

**CCA**
Common Component Architecture


Welcome to the Common Component Architecture Tutorial

SC2007
12 November 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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Common Component Architecture

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 - [CCA Forum Tutorial Working Group, Common Component Architecture Tutorial, 2007, http://www.cca-forum.org/tutorials/](http://www.cca-forum.org/tutorials/)





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About the Printed Notes


- The printed version of these presentations includes additional slides marked *“Supplementary material for handouts”*
- Additional material to address questions sometimes raised, or provide more detail on a topic
- We are happy to discuss this material if asked


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Agenda & Table of Contents

Time	Title	Slide No.	Presenter
8:30-8:35am	Welcome	1	David Bernholdt, ORNL
8:35-9:30am	What Can Component Technology do for Scientific Computing	6	David Bernholdt, ORNL
	An Intro to Components & the CCA	17	David Bernholdt, ORNL
9:30-10:00am	CCA Tools	72	Rob Armstrong, SNL
10:00-10:30am	Break		
10:30-11:10am	Language Interoperable CCA Components with Babel	109	Gary Kumfert, LLNL
11:10am-11:55am	Using CCA: Approaches & Experience	136	Boyana Norris, ANL
11:55am-12:00n	Closing	183	Boyana Norris, ANL
12:00-1:30pm	Lunch		
1:30-3:00pm	Hands-On	Hands-On Guide	Rob Armstrong, SNL
3:00-3:30pm	Break		
3:30-5:00pm	Hands-On (continued)		


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Who We Are: The Common Component Architecture (CCA) Forum

- Combination of standards body and user group for the CCA
- Define [specifications](#) for high-performance scientific components & frameworks
- Promote and facilitate development of [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/>

- Center for Technology for Advanced Scientific Component Software (TASCS)
 - 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?

CCA Forum Tutorial Working Group

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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:

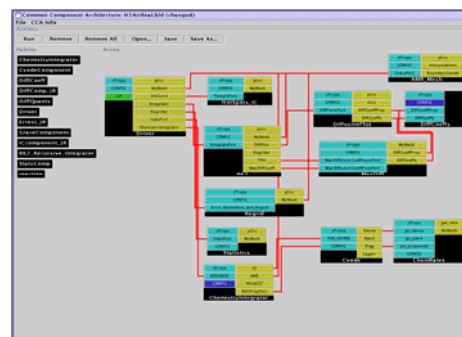
- Components help you think about software in manageable chunks that interact only in well-defined ways
- Components provide a “plug-and-play” environment that allows easy, flexible application assembly

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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*



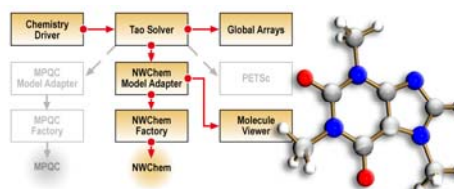
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Example: Quantum Chemistry

- 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-gui

Languages: C, C++, F77, Python



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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

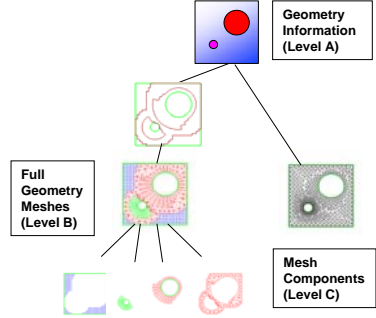



Illustration of geometry domain hierarchy used in TSTT mesh interface.

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?

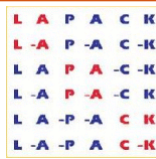
How CCA Can Help:


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

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Examples

hydre

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


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


-- Jeff Painter, LLNL. 2 June 2003

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)

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:

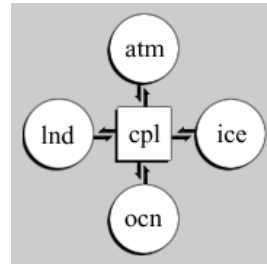
- Components are isolated from one another
 - Interactions via well-defined interfaces
 - An application can include multiple versions of a component
- Components can be composed flexibly, hierarchically
 - Standalone application as one assembly, coupled simulation as another
- CCA can be used in SPMD,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


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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



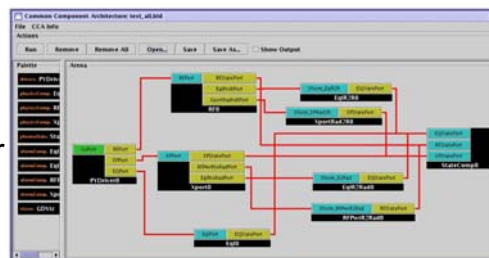
Schematic of CCSM showing coupler managing data exchanges between atmosphere, sea ice, ocean, and land models.
 (From <http://www.cesm.ucar.edu/models/ccsm3.0/cpl6/>)

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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



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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**



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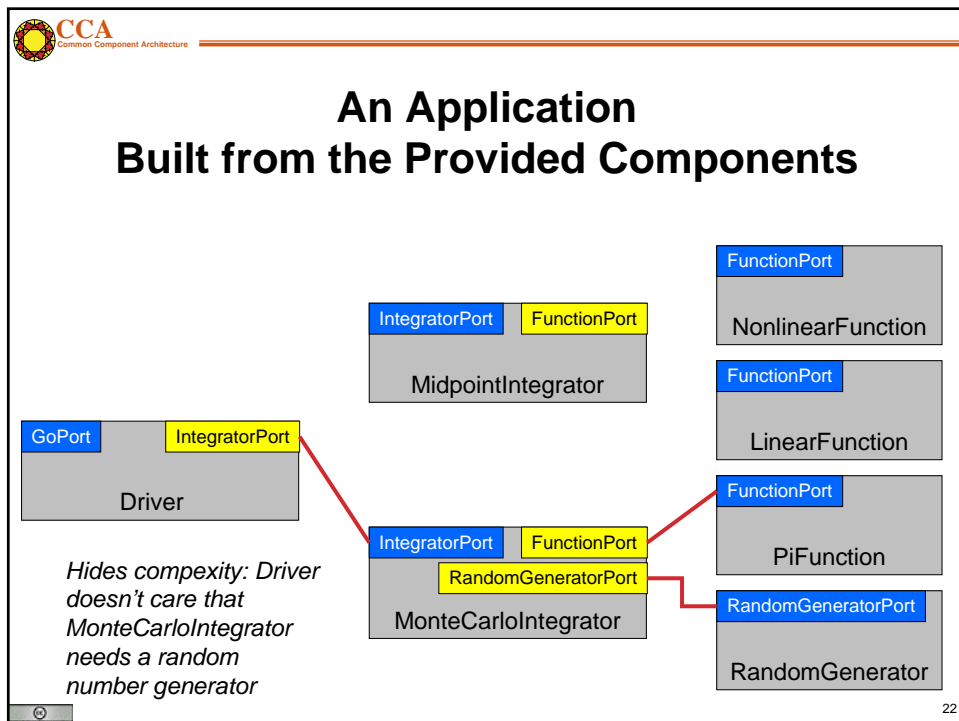
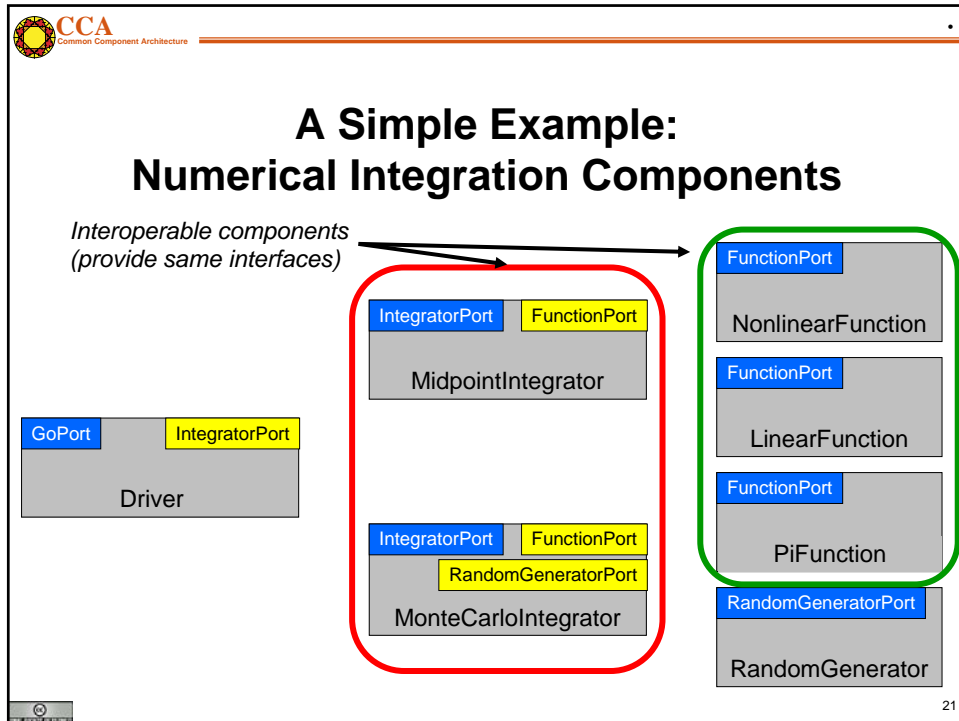


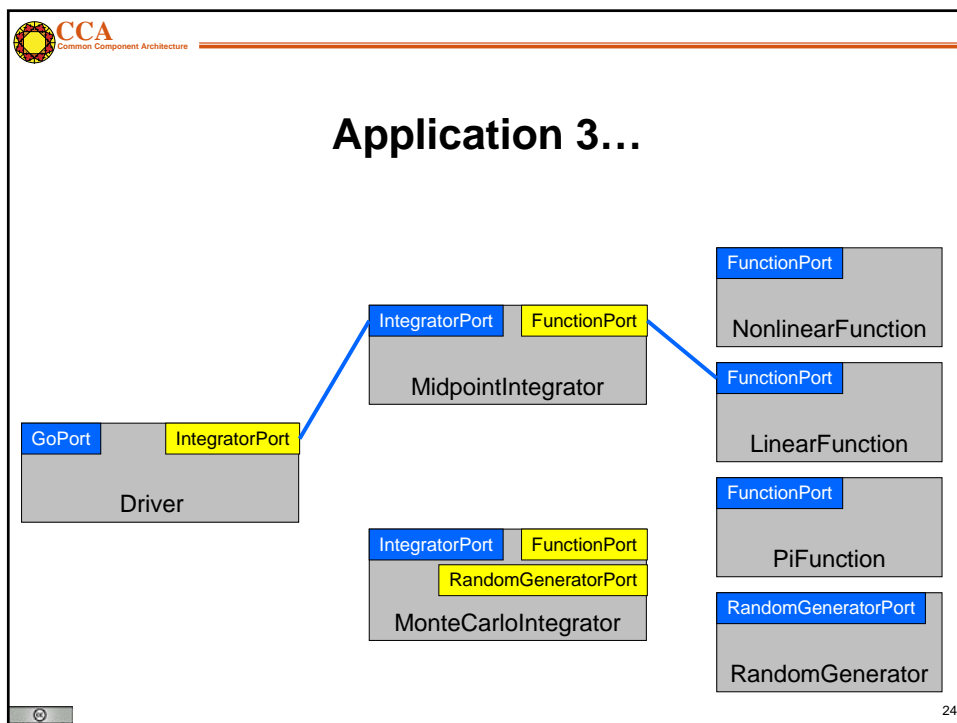
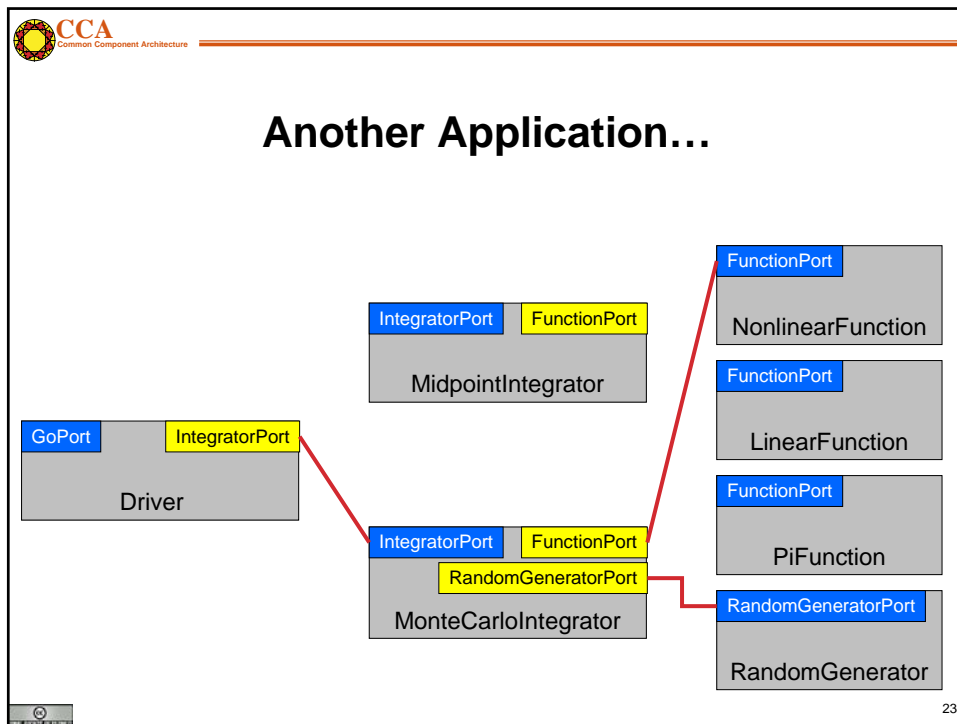
What is a Component Architecture?

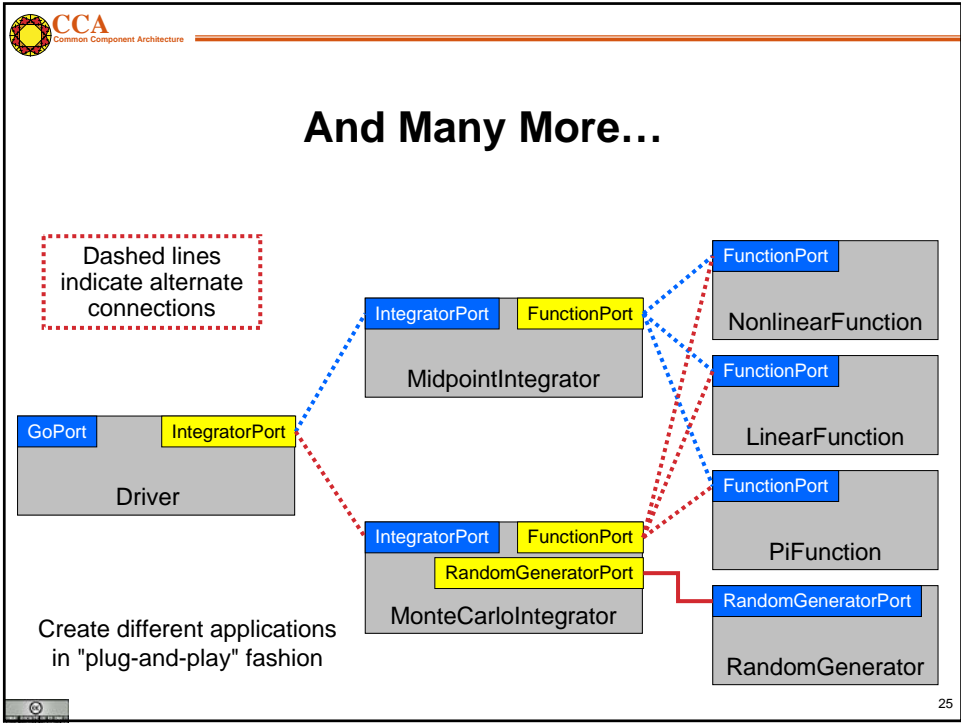
- A set of **standards** that allows:
 - Multiple groups to write units of software (**components**)...
 - And have confidence that their components will **work with other components** written in the same architecture
- These standards **define**...
 - The rights and responsibilities of a **component**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




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Supplementary material for handouts

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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Supplementary material for handouts

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



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?



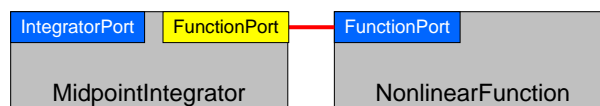


CCA: Concept and Practice


- 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



CCA Concepts: Components

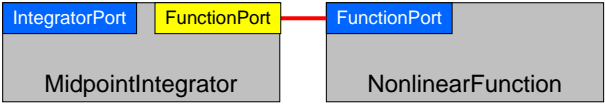


- A component encapsulates some computational functionality
- Components provide/use one or more interfaces
 - A component with no interfaces is formally okay, but isn't very interesting or useful
- In SIDL, a component is a **class** that **implements** (inherits from) **gov.cca.Component**
 - This 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




```

graph LR
    MI[MidpointIntegrator] -- FunctionPort --- NF[NonlinearFunction]
    
```

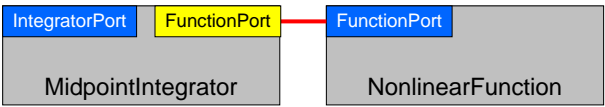
- Components interact through well-defined **interfaces**, or **ports**
 - A port expresses some **computational functionality**
 - In Fortran, a port is a bunch of subroutines or a **module**
 - In OO languages, a port is an **abstract class** or **interface**
- Ports and connections between them are 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

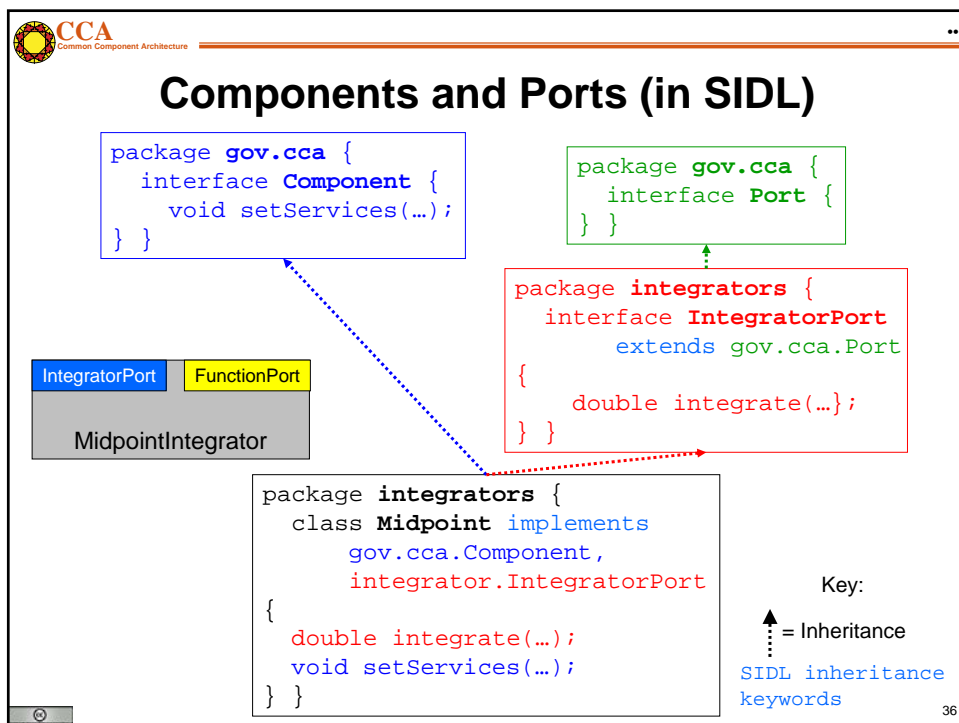
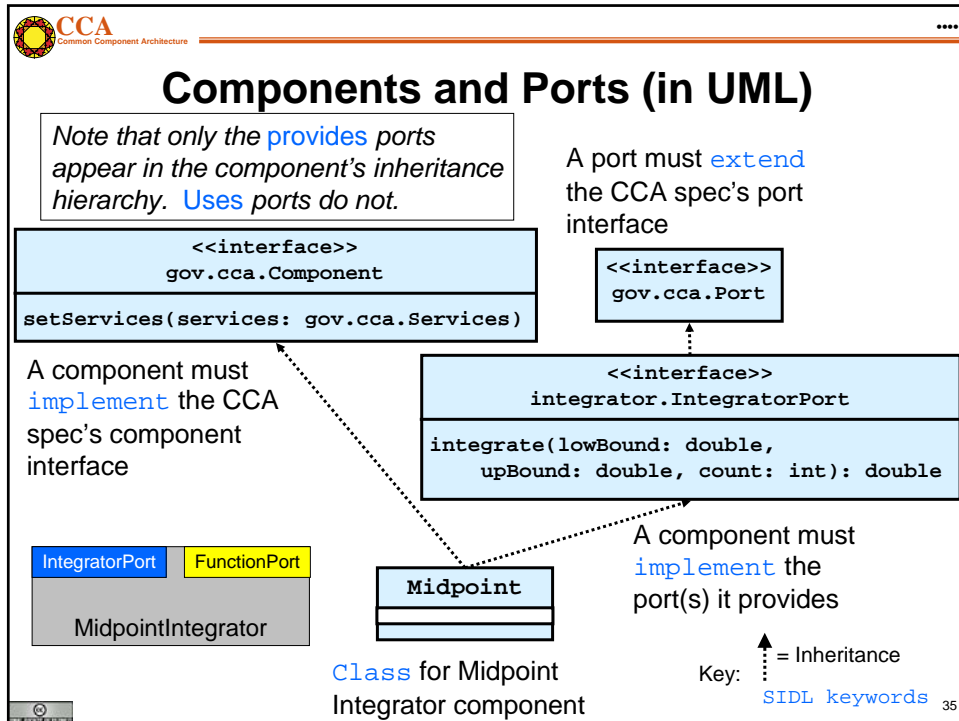



```

graph LR
    MI[MidpointIntegrator] -- FunctionPort --- NF[NonlinearFunction]
    
```

- 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

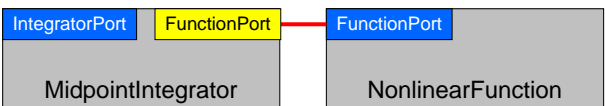

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Using Ports




```

graph LR
    MI[MidpointIntegrator] -- IntegratorPort --> FP1[FunctionPort]
    FP1 -- FunctionPort --> NF[NonlinearFunction]
    
```

- Calling methods on a port you use requires that you first obtain a “handle” for the port
 - Done by invoking `getPort()` on the user’s `gov.cca.Services` object
 - Free up handle by invoking `releasePort()` when done with port
- Best practice is to bracket actual port usage as closely as possible without using `getPort()`, `releasePort()` too frequently
 - Can be expensive operations, especially in distributed computing contexts
 - Performance is in tension with dynamism
 - can’t “re-wire” a ports that is “in use”



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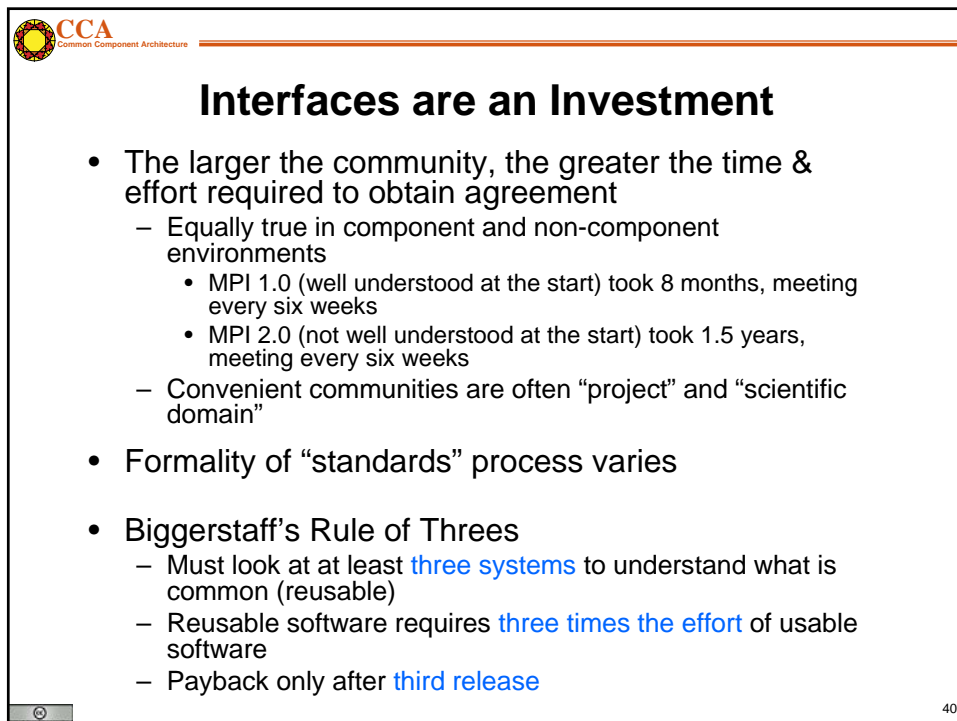
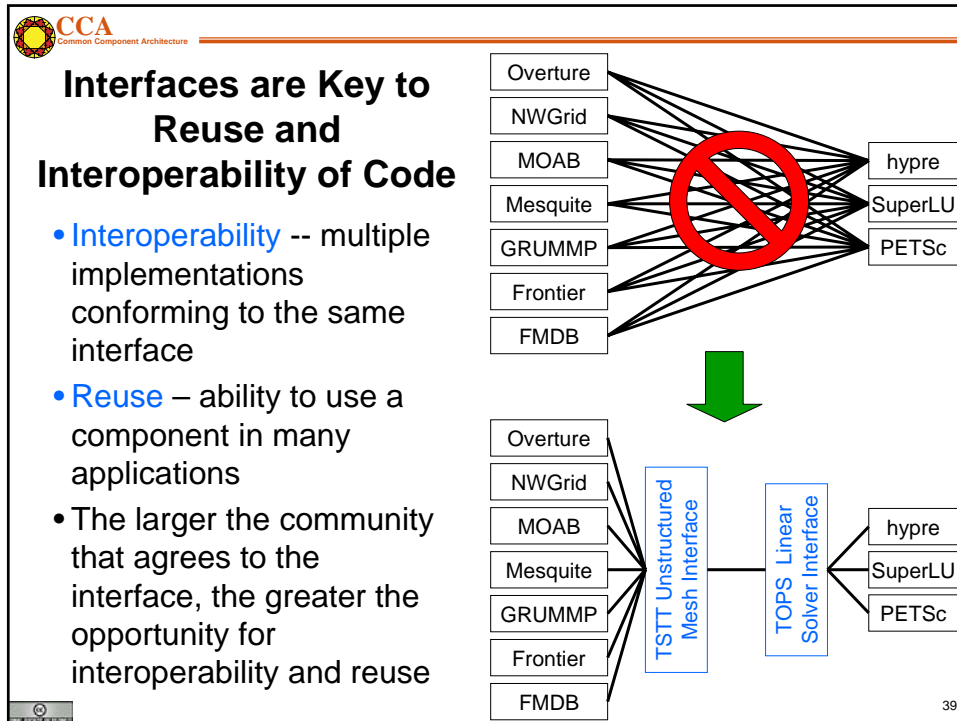



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Where Do Ports Come From?

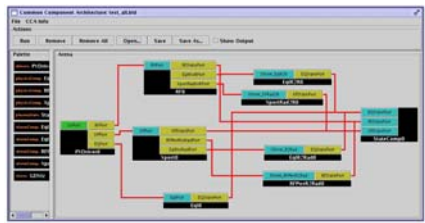
- Most ports are designed and implemented by **users** of CCA
 - May be specific to an application or used more broadly (i.e. community-wide)
- The **CCA specification** defines a *small* number of ports
 - Most are services CCA frameworks must provide for use by components
 - Some are intended for users 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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CCA Concepts: Frameworks

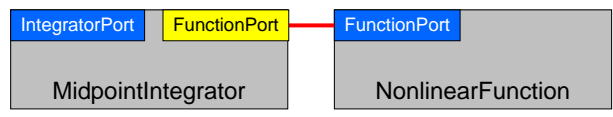


- The framework provides the means to “hold” components and **compose** them into applications
- Frameworks allow **connection of ports** without exposing component implementation details
- Frameworks provide a small set of **standard services** to components
 - Framework services are CCA ports, just 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



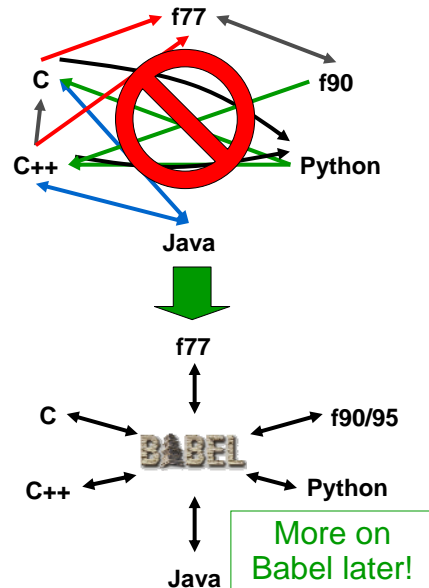
- Components must tell the framework about the ports they are providing and using
 - Framework will not allow connections to ports it isn't aware of
- Register them using methods on the component's **gov.cca.Services** object
 - **addProvidesPort()** and **removeProvidesPort()**
 - **registerUsesPort()** 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

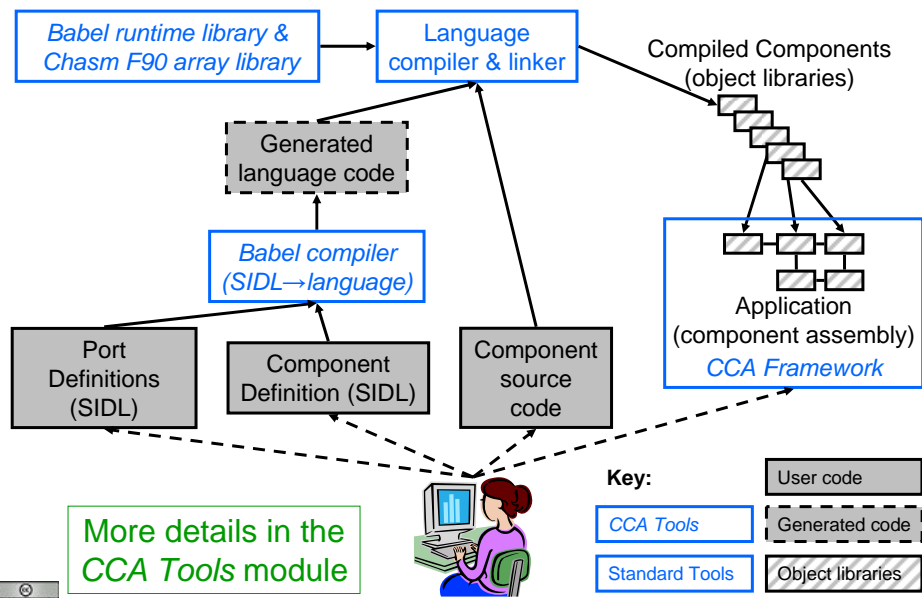
- Scientific software is increasingly diverse in use of programming languages
- In a component environment, users should not care what language a component is implemented in
- “Point-to-point” solutions to language interoperability are not suitable for a component environment
- The **Babel** language 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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Coding in a CCA Environment



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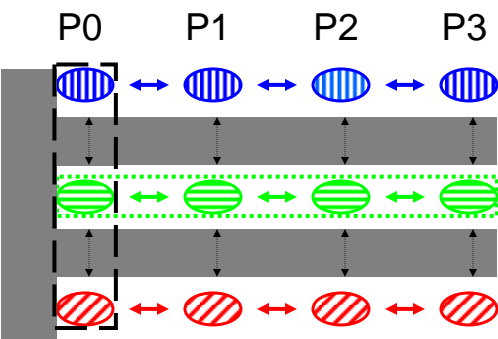


Common Component Architecture

CCA Supports Parallelism -- by “Staying Out of the Way” of it

- Single component multiple data (SCMD) model is component analog of widely used SPMD model
- Each process loaded with the same set of components wired the same way
- Different components in same process “talk to each” other via ports and the framework


- **Same component in different processes talk to each other through their favorite communications layer (i.e. MPI, PVM, GA)**



Components: Blue, Green, Red
Framework: Gray

Any parallel programming environments that can be mixed outside of CCA can be mixed inside

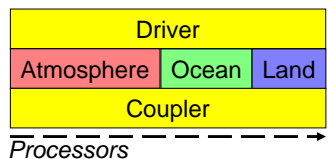
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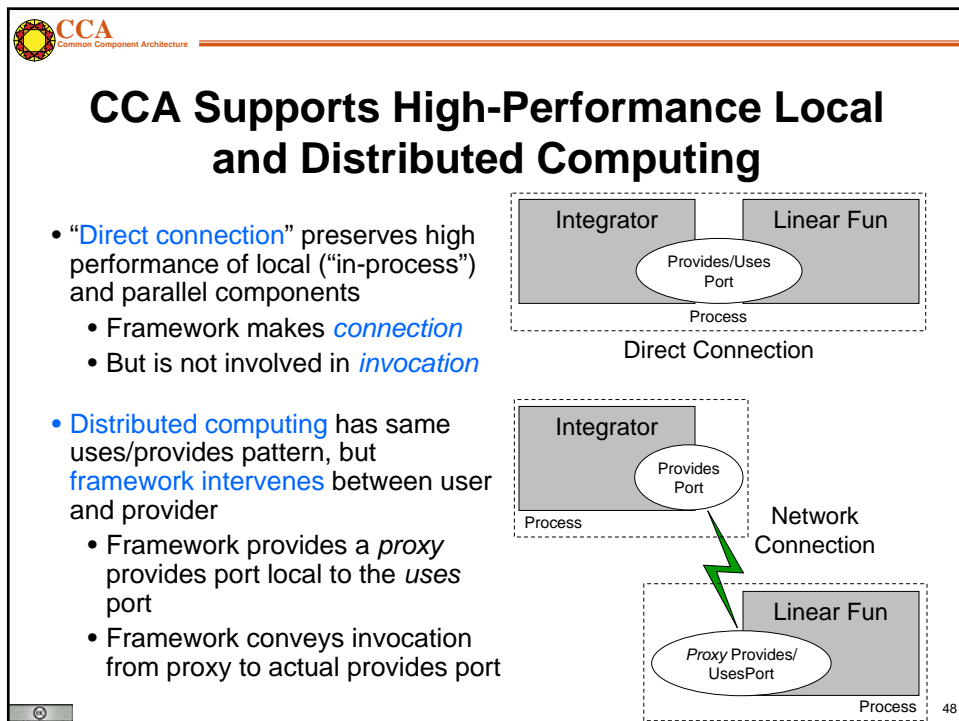
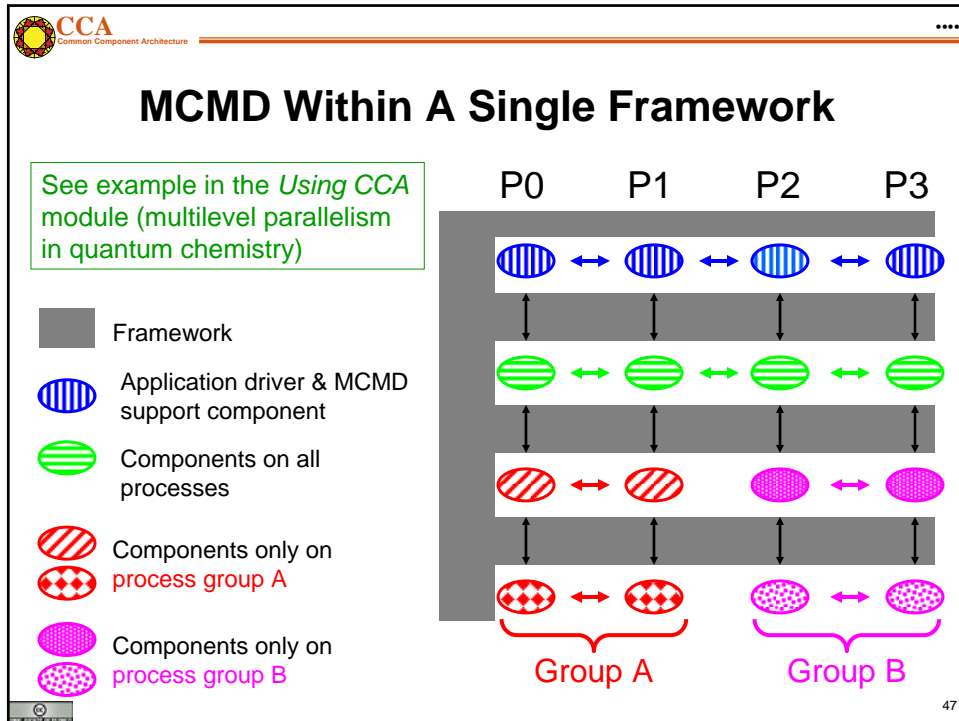
Common Component Architecture

“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)



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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



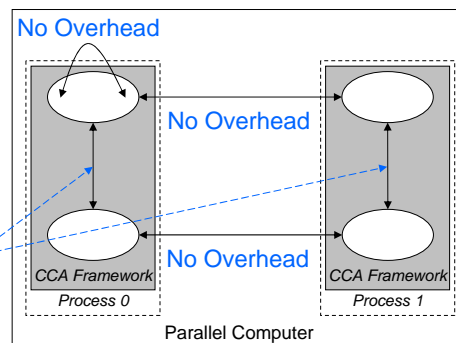
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Performance, the Big Picture

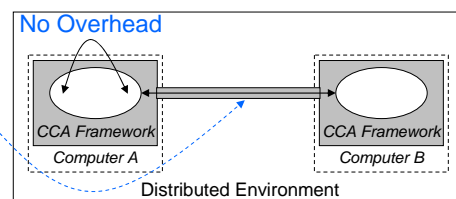
Direct-Connect, Parallel

- 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



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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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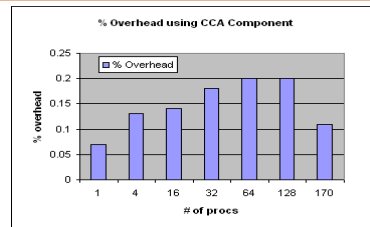


Common Component Architecture

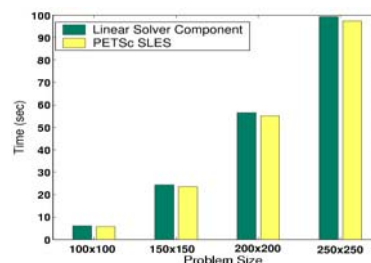
Supplementary material for handouts

Some Performance Results and References

- Lois Curfman McInnes, et al. **Parallel PDE-Based Simulations Using the Common Component Architecture**. In Are Magnus Bruaset, Petter Bjørstad, 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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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

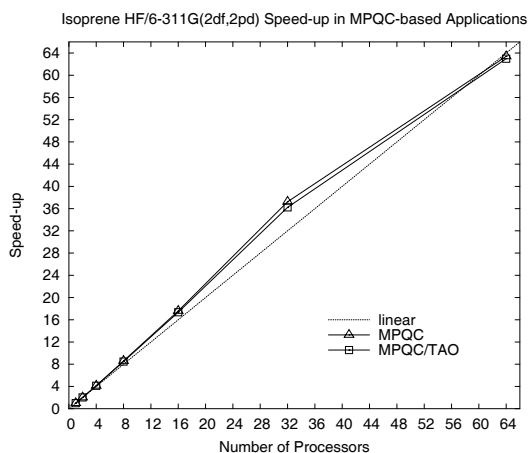
Function arg type	f77	Component
Array	80 ns	224ns
Complex	75ns	209ns
Double complex	86ns	241ns

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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)



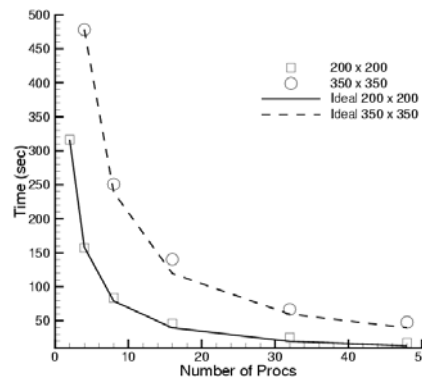
Parallel Scaling of MPQC w/ native and TAO optimizers

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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.



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, 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)



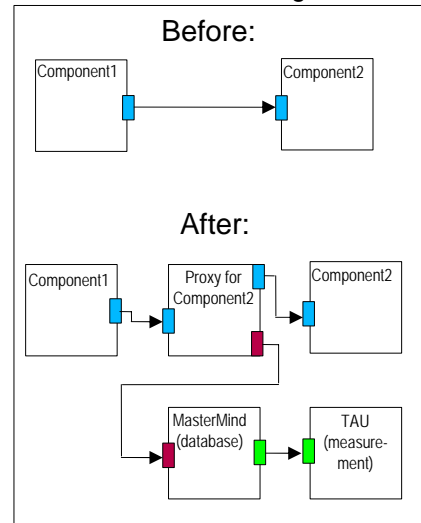
The Proxy Component Pattern

- 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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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

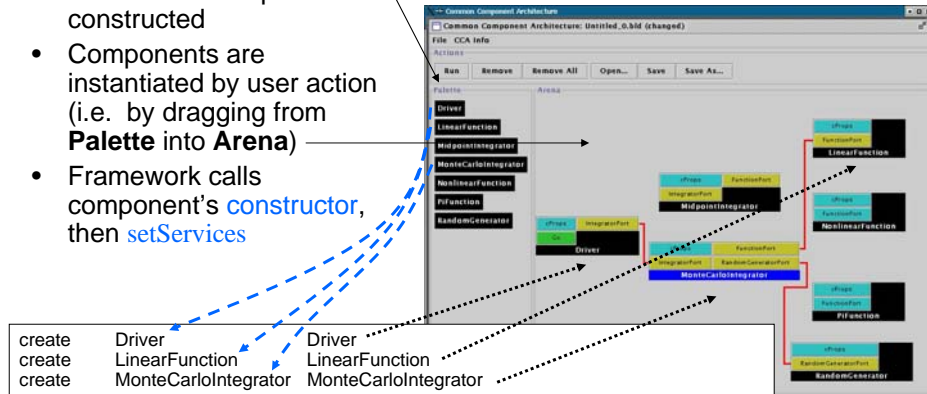
Steps may be under human or software control

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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

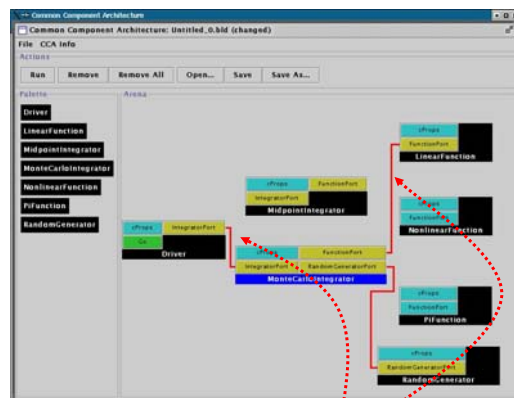


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User Connects Ports

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

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CCA Common Component Architecture Supplementary material for handouts

Component's View of Instantiation

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

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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.

$$\text{sum} = \text{sum} + \text{function} \rightarrow \text{evaluate}(x)$$
- Call `releasePort`

The diagram illustrates the interaction between user code and the MonteCarloIntegrator. The user code calls `getPort` to obtain a port handle from the Services. This handle is then cast to the expected type. The user code then calls methods on the port, such as `evaluate(x)`, to perform calculations. Finally, the user code calls `releasePort` to release the port handle. The MonteCarloIntegrator component contains the Framework interaction code, the CCA.Services interface (which uses FunctionPort and is connected to NonlinearFunction FunctionPort), and the Integrator code.

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CCA
Common Component Architecture

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



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 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



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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Common Component Architecture

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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CCA
Common Component Architecture

Goal of This Module

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

IDE = Interactive Development Environment

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CCA
Common Component Architecture


CCA adds value to component development

Babel runtime library & Chasm F90 array library → Language compiler & linker
 Language compiler & linker → Compiled Components (object libraries)
 Compiled Components (object libraries) → Application (component assembly) CCA Framework
 Application (component assembly) CCA Framework → CCA IDE
 Port Definitions (SIDL) → Babel compiler (SIDL → language) → Generated language code → Language compiler & linker
 Component Definition (SIDL) → Babel compiler (SIDL → language)
 Component source code → Language compiler & linker
 CCA IDE

Key:

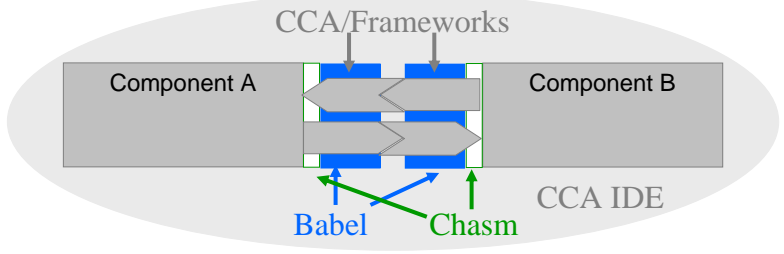
- User code
- CCA Tools
- Standard Tools
- Generated code
- Object libraries


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CCA
Common Component Architecture

Tools Module Overview






- Language interoperability tools
- Frameworks
- CCA Interactive Development Environment



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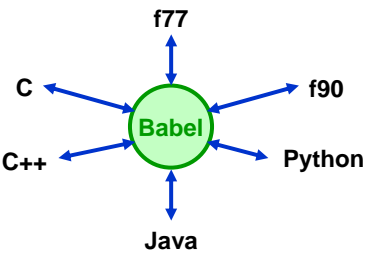


CCA
Common Component Architecture

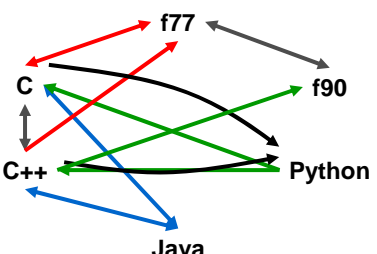
Babel

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



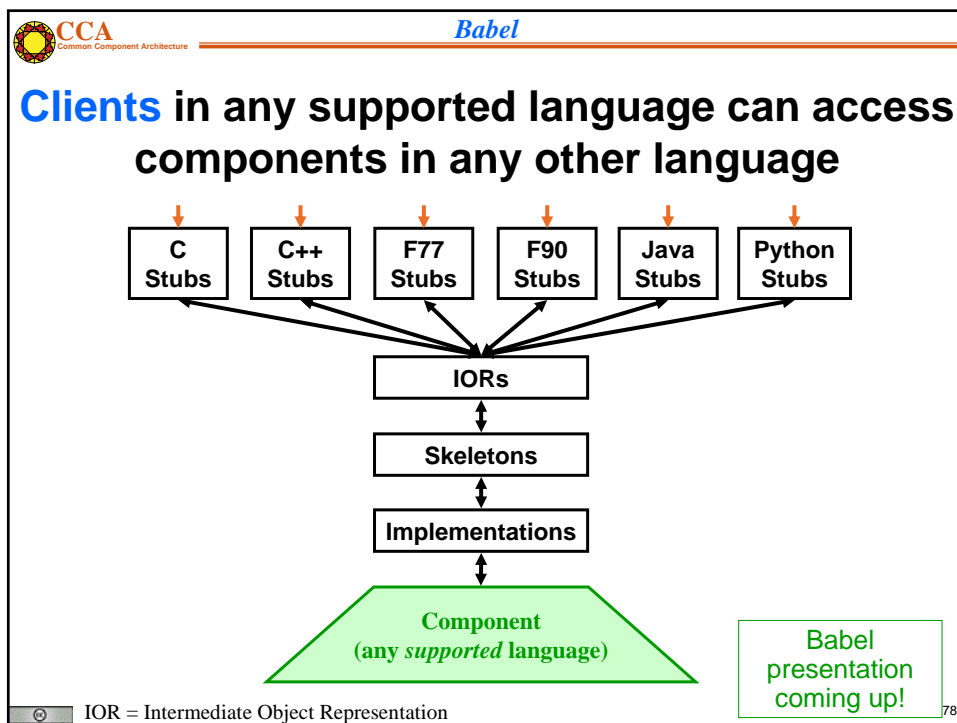
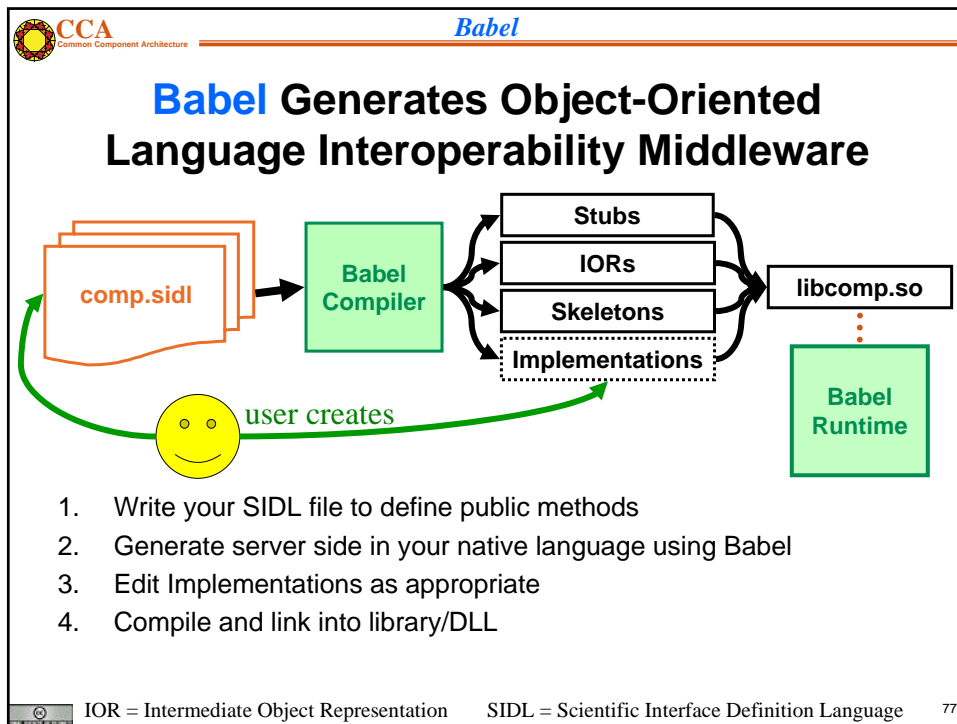
vs.




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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 **CCA**
Common Component Architecture

Babel

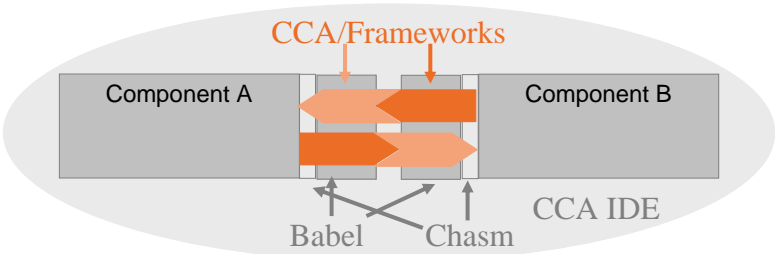
Recent and Upcoming Features

- 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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 **CCA**
Common Component Architecture

Tools Module Overview



The diagram illustrates the Tools Module Overview. It shows two components, Component A and Component B, represented as gray rectangles. Between them are two orange arrows pointing from Component A to Component B, labeled 'CCA/Frameworks'. Below the components, there are two gray rectangles labeled 'Babel' and 'Chasm'. Arrows point from 'Babel' and 'Chasm' up to the space between Component A and Component B. To the right of these rectangles is the label 'CCA IDE'.

- 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


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CCA
Common Component Architecture

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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 **CCA**
Common Component Architecture


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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 **CCA**
Common Component Architecture


Ccaffeine Framework

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.

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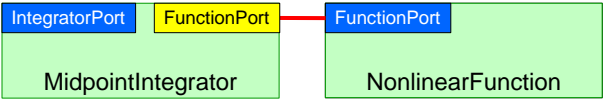



CCA
Common Component Architecture

Ccaffeine Framework (ccafe-gui)


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





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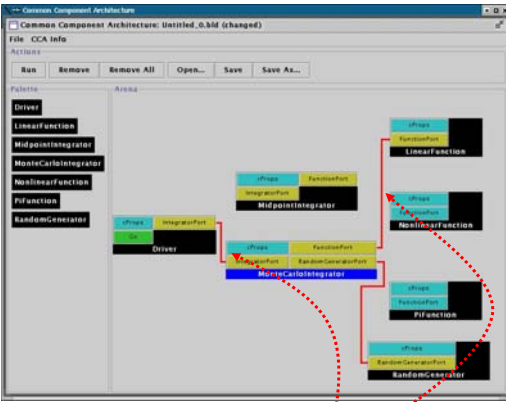


CCA
Common Component Architecture


Ccaffeine 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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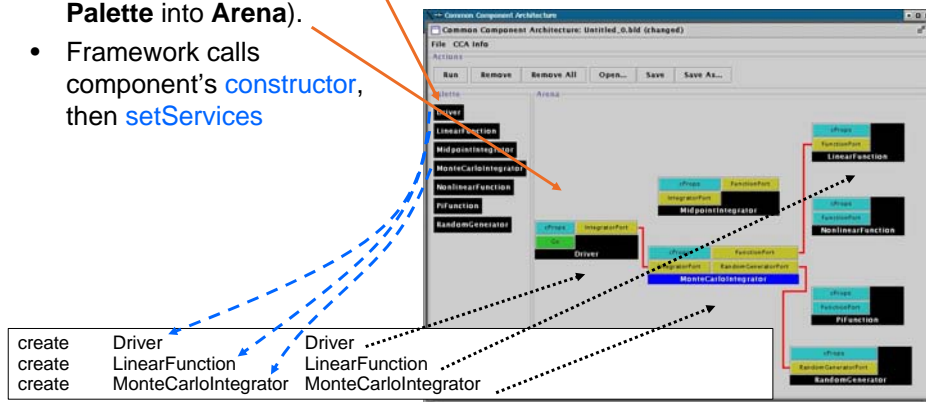


Common Component Architecture

Ccaffeine 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**



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Common Component Architecture

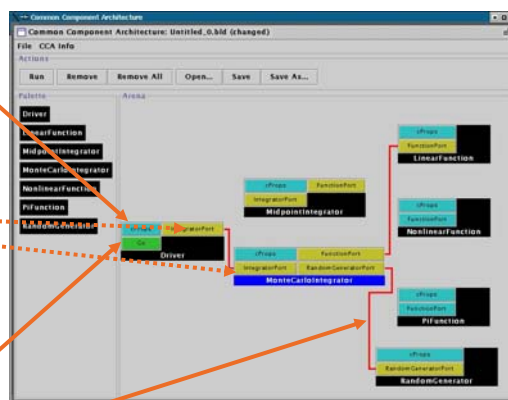
Ccaffeine Framework (ccafe-gui)

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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**CCA**
Common Component Architecture


XCAT-C++ Framework



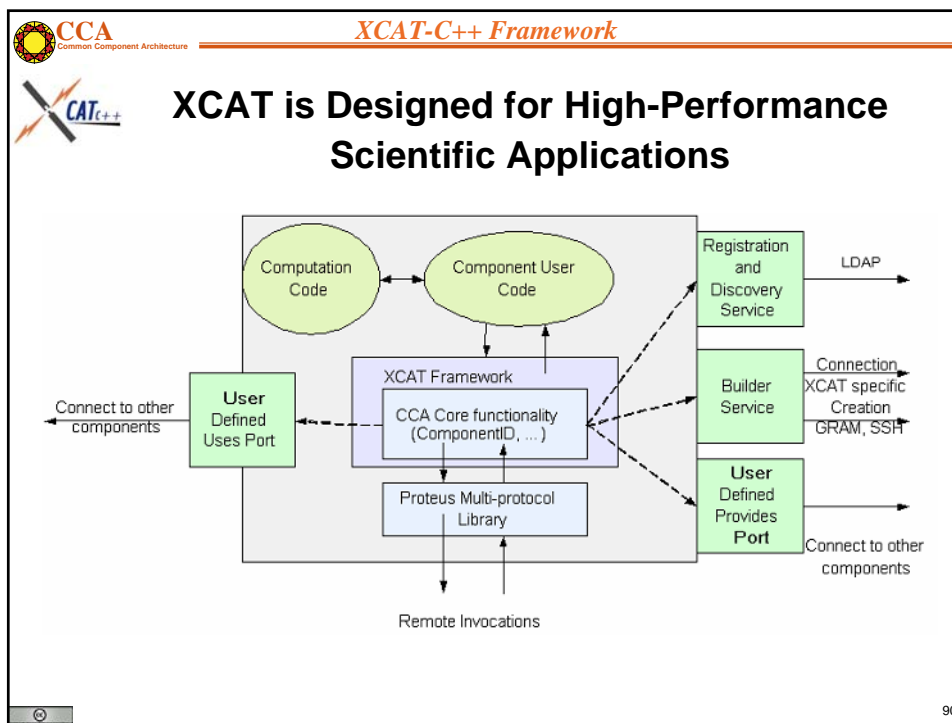
XCAT is a Web-services based Distributed Component Framework

- 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

Basic How-To

1. Define port interfaces as C++ header files or WSDL docs
2. Indicate ports used by each component in a config file
3. Run scripts to generate code for stub-skeletons (for ports)
 - Can also generate component-templates for new components
 - Use component-templates to convert a scientific library into a CCA component
4. Build components using XCAT-C++ make scripts
5. Deploy component executables on the target remote hosts
 - Also set up SSH access to remote hosts
6. Write python scripts (edit examples) to use CCA API to connect components and invoke a Go port
 - Alternatively, can use a C++ front-end
7. Execute the python script (or C++ front-end)



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Common Component Architecture




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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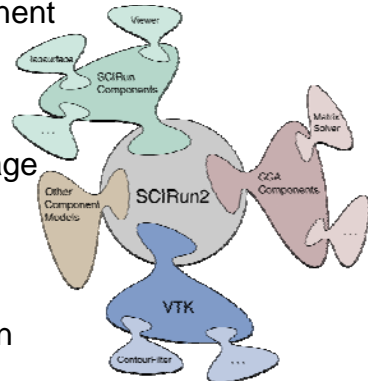


CCA
Common Component Architecture

SCIRun2 Framework

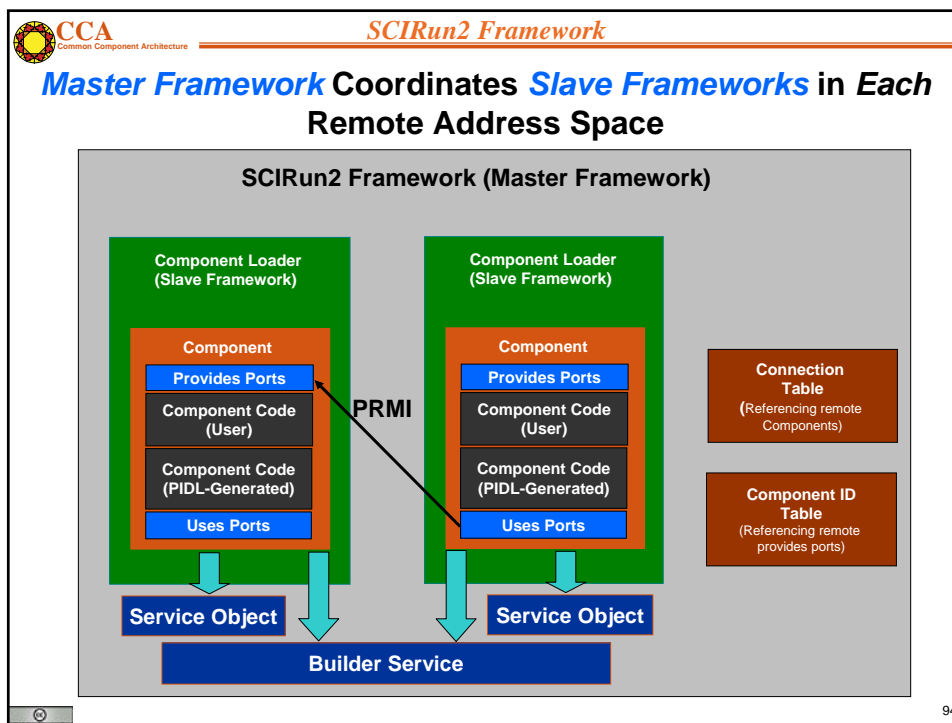
SCIRun2 is a Cross-Component Model, Distributed Component Framework

- 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)



Supported on Linux.

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Basic How-To

1. Add component source files and makefile to SCIRun2 sources
 - May need to define ports in SIDL
2. Add component information to the component model xml file
3. Build component using SCIRun2 make scripts
 - Alternatively, build component using Babel
4. Start the framework and graphical (default) or text builder
5. Graphically connect component to other CCA-based or non CCA-based components
 - May need to create bridge components to go between models
6. Press the “Go” button on the driver component

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Experimental Frameworks

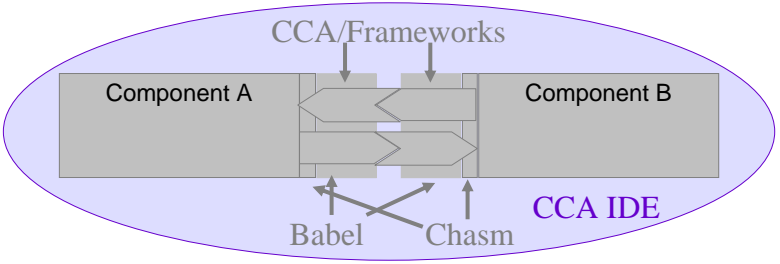
Framework	Purpose	Summary
Distributed CCA Framework (DCA)	MxN research	<ul style="list-style-type: none"> • Goal: explore MxN Parallel-Remote Method Invocation (PRMI) using MPI • Parallel data transfer and redistribution integrated into port invocation mechanism
LegionCCA	Grid-based research	<ul style="list-style-type: 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.



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**CCA**
Common Component Architecture


Tools Module Overview



The diagram illustrates the Tools Module Overview. It features a central light blue oval containing two grey rectangular blocks labeled 'Component A' and 'Component B'. Between these components are four interlocking puzzle-piece shapes. Above the oval, the text 'CCA/Frameworks' has two arrows pointing down to the puzzle pieces. Below the oval, the text 'CCA IDE' is in purple. Two arrows, labeled 'Babel' and 'Chasm', point upwards from below the oval towards the puzzle pieces. 'Babel' points to the left puzzle piece, and 'Chasm' points to the right puzzle piece.

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

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**CCA**
Common Component Architecture

CCA IDE

Supplementary material for notes

Component Development Environment

- Bocca
 - Provides a light-weight, portable environment

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Eclipse Environment Provided via Eclipse Plug-ins

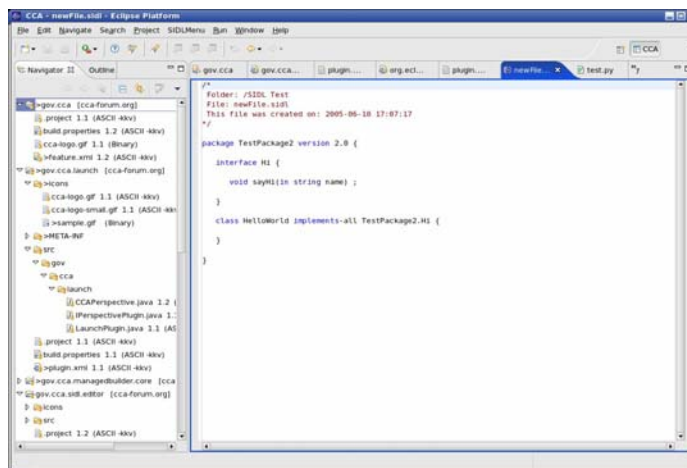
- Provides a high-level graphical environment
 - Creating new SIDL-based components
 - Componentizing legacy codes
 - C, C++, Java and Fortran
- Automatic code generation

Supported on Linux, Windows, MacOS.



Component Development Environment Starts at the Eclipse Platform Level

- Plug-ins for:
- SIDL Editor
 - Wizards
 - Preliminary automated build support

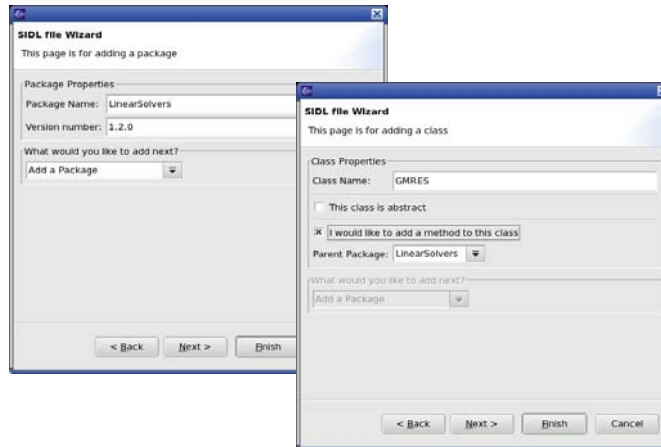


Imperative that you start by creating a new project!



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 system maintenance.
 - Easy to adopt or abandon while preserving code, build.
- No GUI required.
- Still in the early beta stage of development
 - Being tested by managing the tutorial source and a regression test suite.
 - Basis for common CCA toolkit installation.
 - Manages components in all Babel-supported languages (C, C++, Fortran 77, Fortran 90, Java, Python).

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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 also meant to support very rapid prototyping.
- Complementary to a normal IDE
 - Does not provide an integrated editor for creating code.
 - Invoke your own editor with bocca assistance (no need to remember paths to files, build system optionally automatically updated).



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Bocca Creates Skeletons for CCA

- Including **ports** and **interfaces**
 - Give the SIDL name and an empty port or interface is created.
- Including **components** and **classes**
 - Give the name and an empty component or class is created.
 - Some extra options: the component uses/provides ports, implemented interfaces or extended classes
- 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
./configure

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

# compile application
make
```


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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 Tools Contacts (2 of 2)

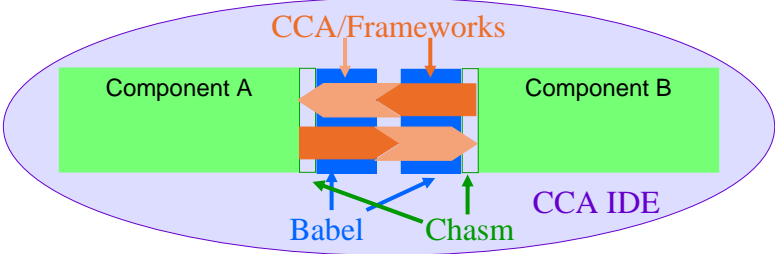
Tool	Purpose	More information
SCIRun2	Cross-component model framework	URL: www.sci.utah.edu/ Email: Steve Parker, sparker@cs.utah.edu
XCAT-C++	Globus-based GRID framework	URL: grid.cs.binghamton.edu/projects/xcats/ Email: Madhu Govindaraju, mgovinda@cs.binghamton.edu


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
Module Summary




The diagram illustrates the CCA architecture. At the top, 'CCA/Frameworks' is shown with arrows pointing to 'Component A' and 'Component B', which are represented as green rectangles. Between the components are orange arrows indicating interaction. Below the components, 'Babel' (blue) and 'Chasm' (green) are shown with arrows pointing up towards the components. A purple oval labeled 'CCA IDE' encompasses the Babel, Chasm, and the interaction area between the components.

- 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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BABEL

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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Goal of This Module

Expose Attendees to How Existing Code is

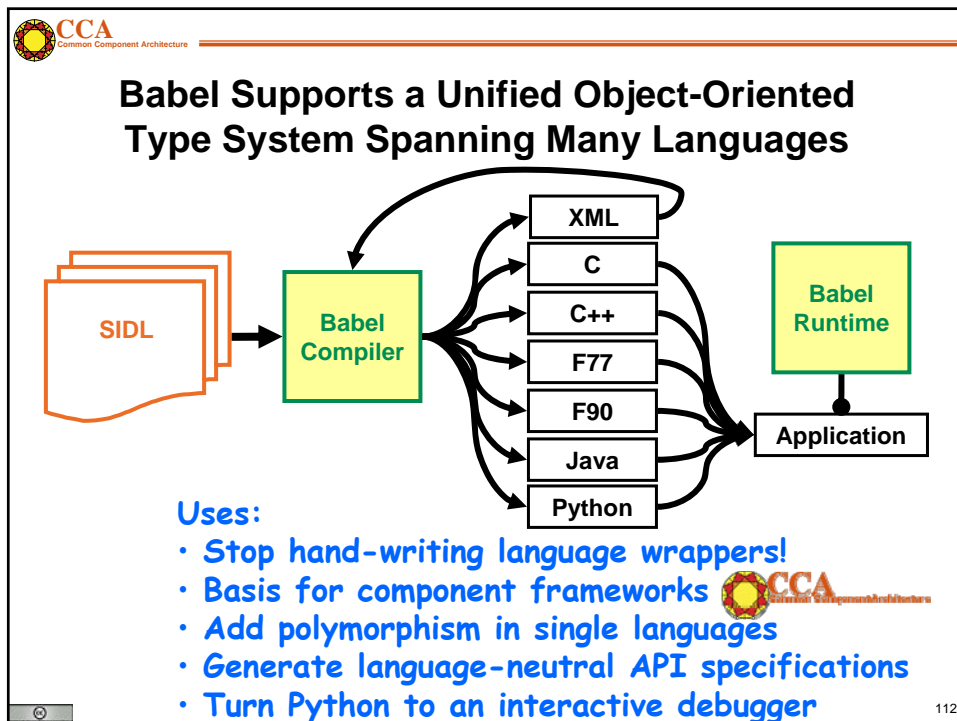
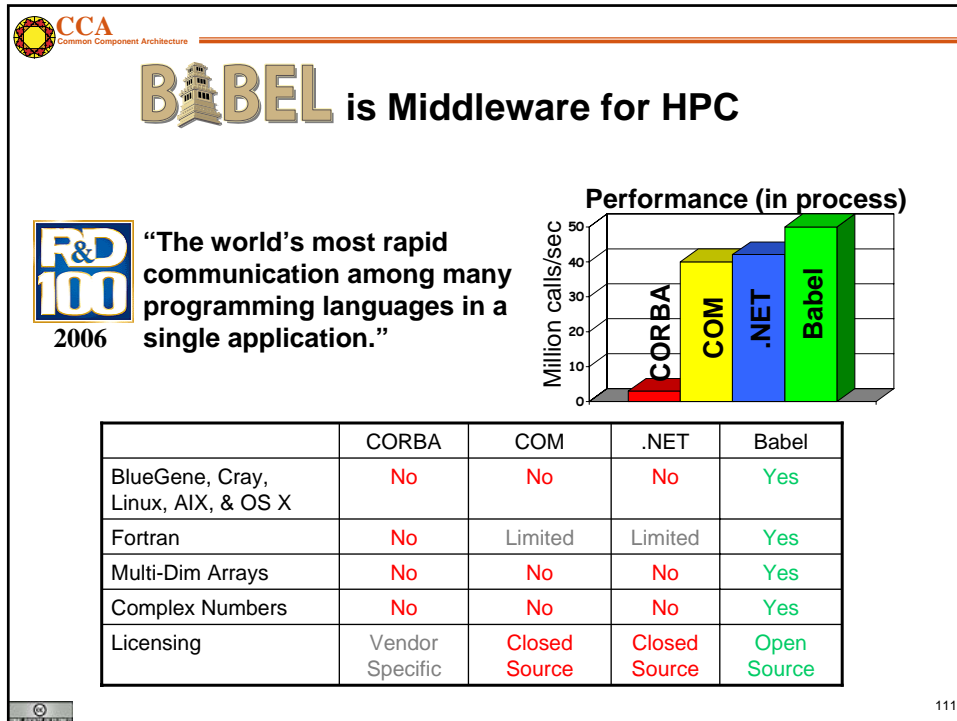
- **Wrapped into Babel objects, and then**
- **Promoted to CCA components**

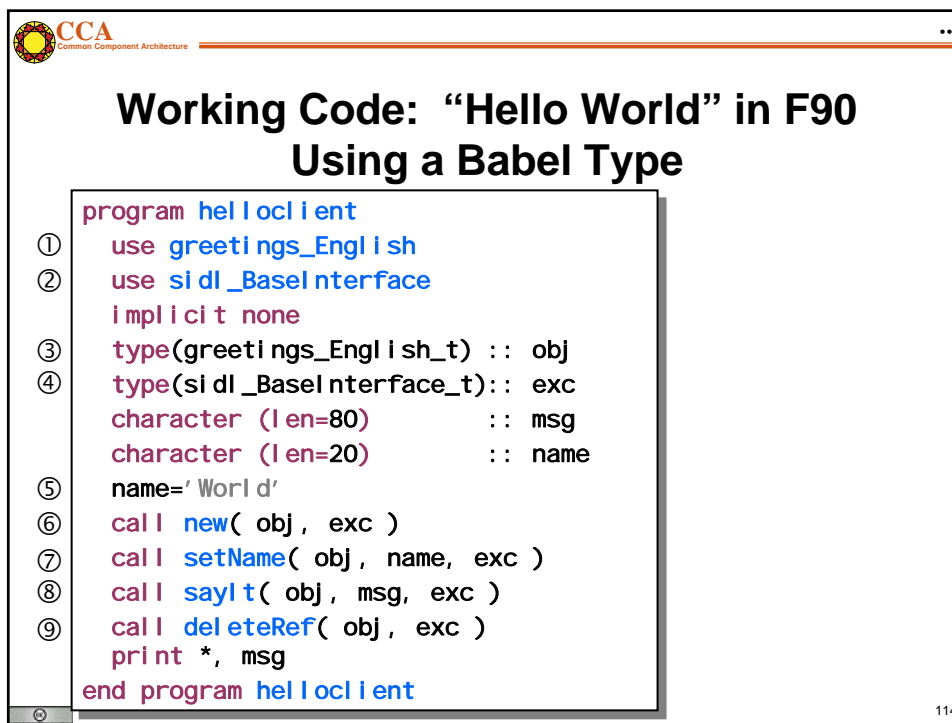
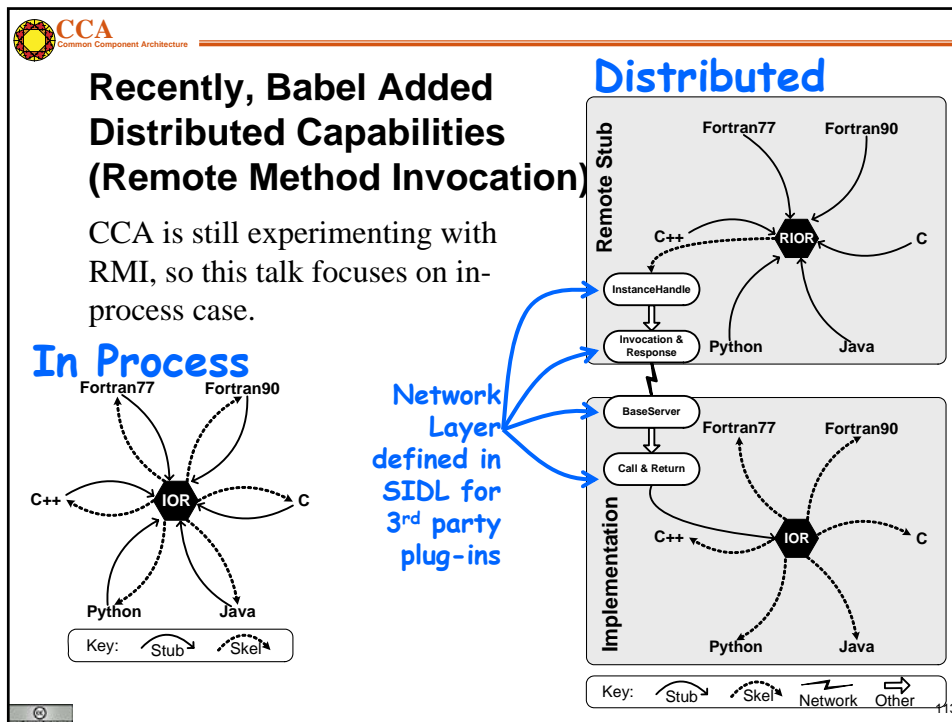
In the process, will also cover

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



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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 hellocient
  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 hellocient

```

Answer: Can't Know!

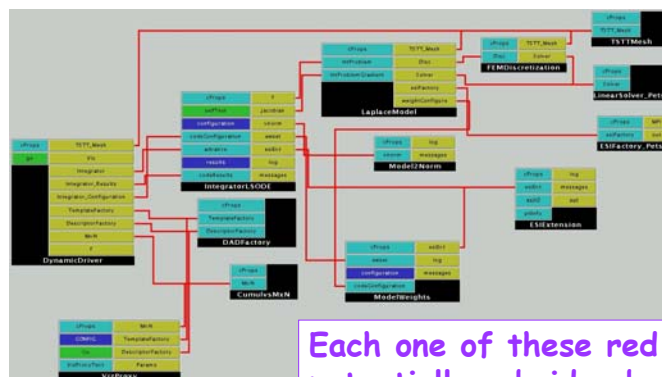
With Babel, it could be C, C++, Python, Java, Fortran77, or Fortran90/95

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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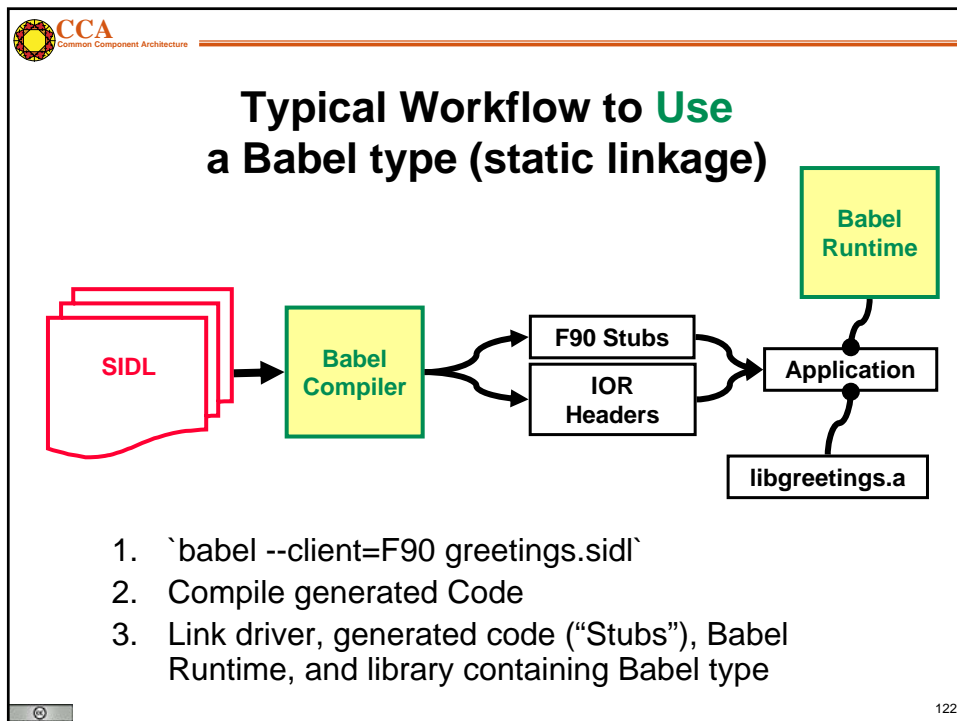
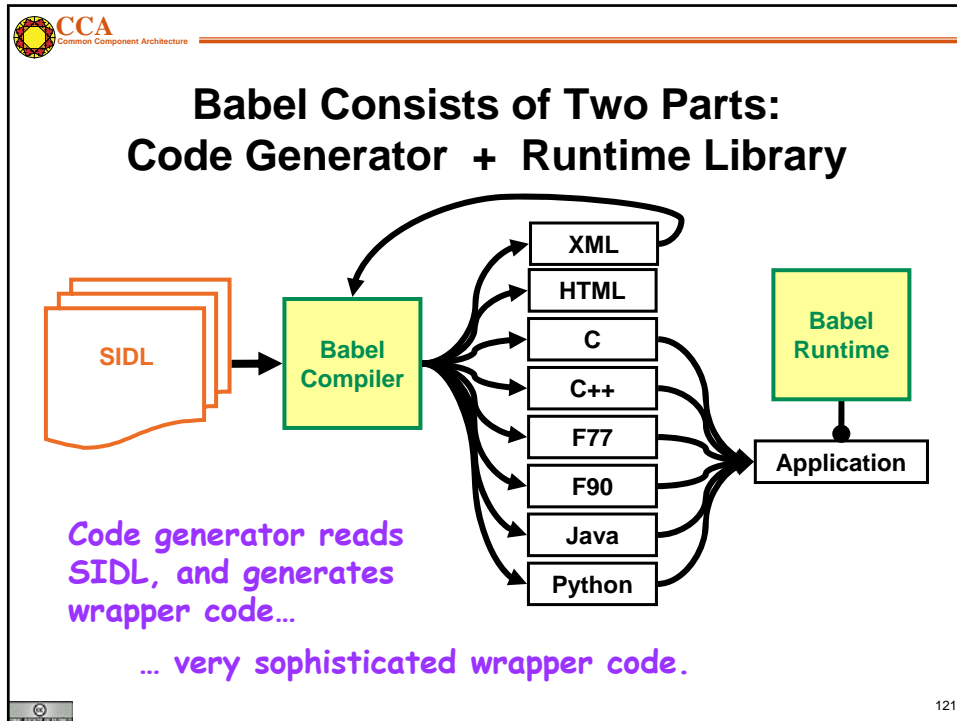


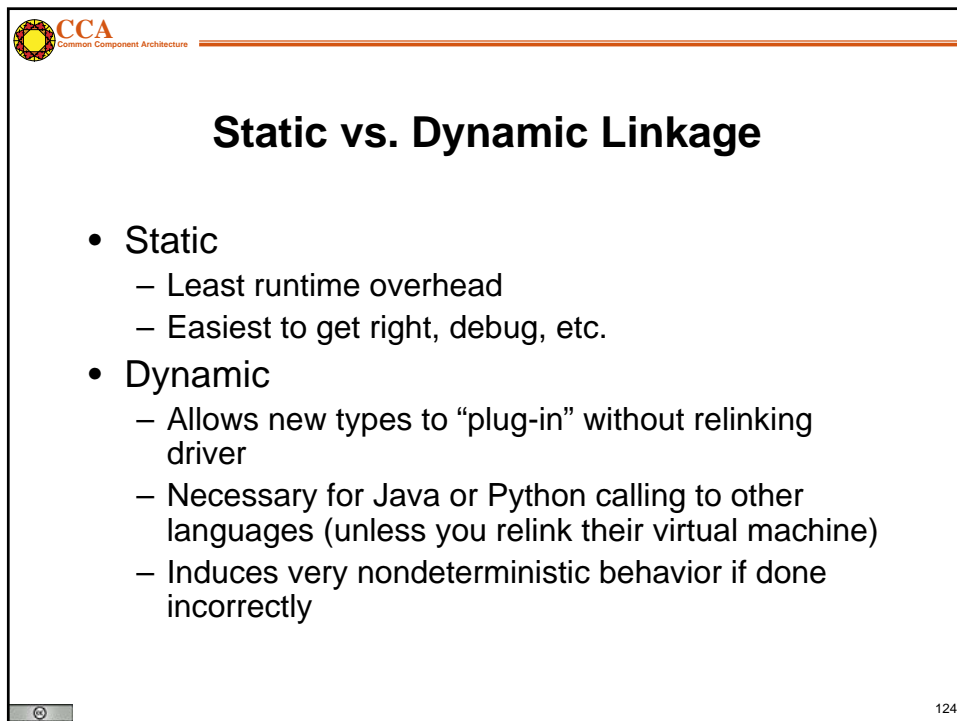
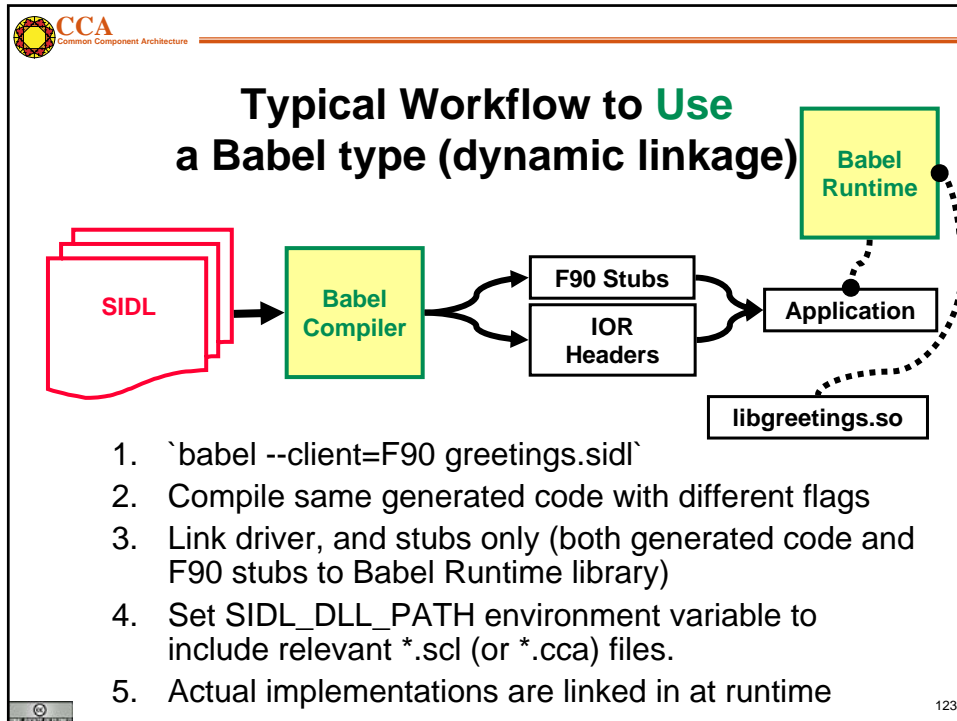
Supplementary material for handouts

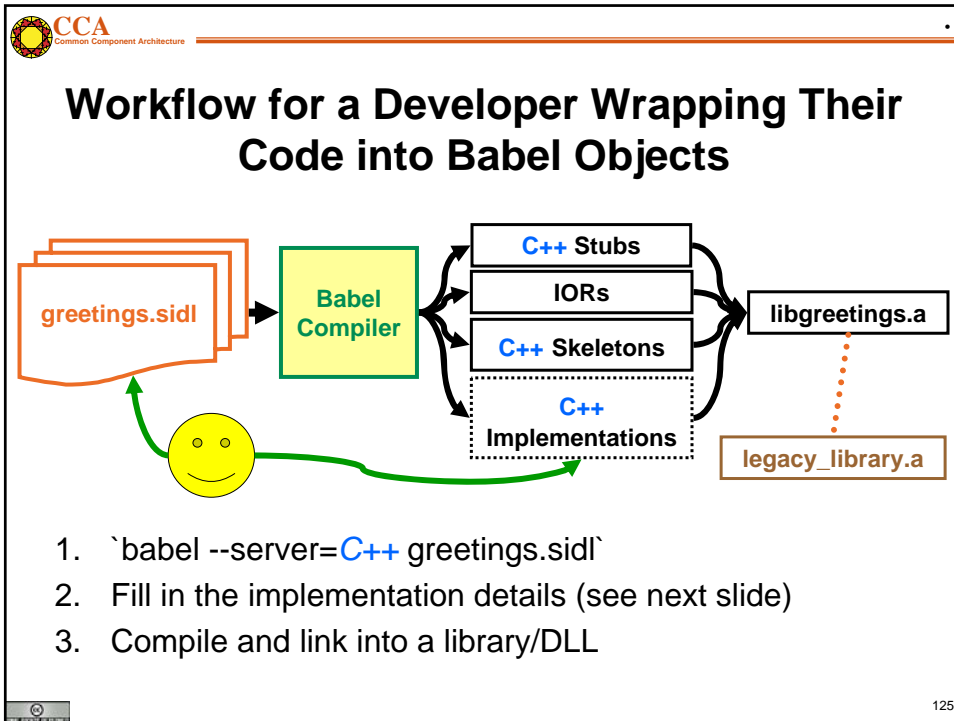
Handout Material: Code Notes

- 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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Implementation Details Must be Filled in Between Splicer Blocks

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

string
greeti ngs:: Engli sh_ i mpl :: sayl t()
throw ()
{
    // DO-NOT-DELETE spl i cer. begi n(greeti ngs. Engli sh. sayl t)
    string msg("Hello ");
    return msg + d_name + "!";
    // DO-NOT-DELETE spl i cer. end(greeti ngs. Engli sh. sayl 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|07 tutorial slides for Babel
<http://www.llnl.gov/CASC/components/docs/sc07.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

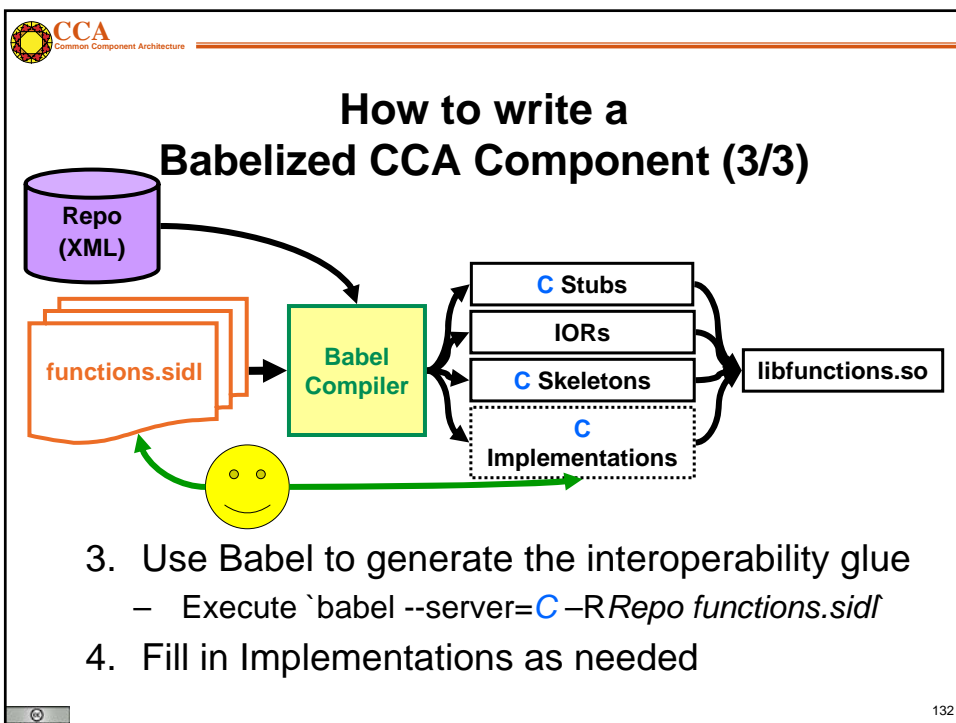
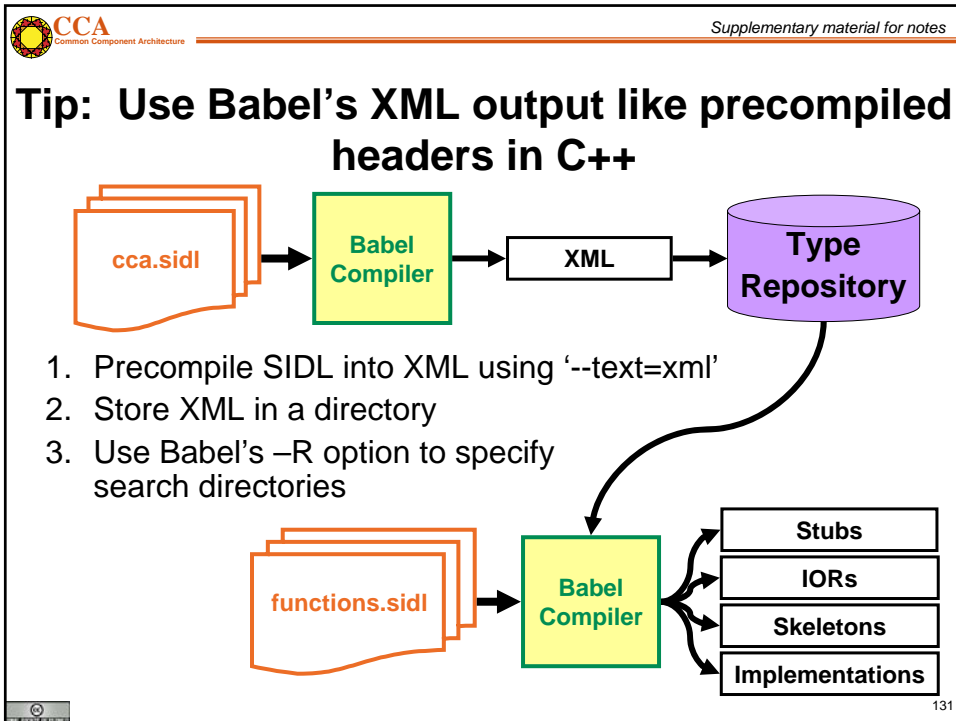
- CCA Component =
 - SIDL Class
 - implements gov.cca.Component (and any provided ports)

```
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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Review: Goal of This Module

Learn how existing code is

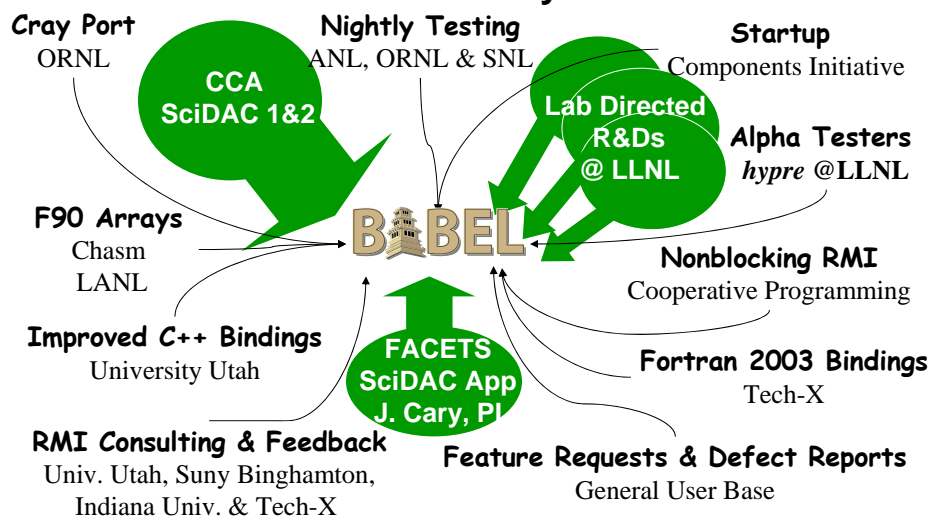
- Wrapped into Babel objects, and
- Promoted to CCA components

In the process, will also covered

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



Babel Thrives on Research Collaborations & Community






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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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Using CCA: Approaches & Experience

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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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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Common Component Architecture

Supplementary material for handouts

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

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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



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





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**



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



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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?



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





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



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)





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.***



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`





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

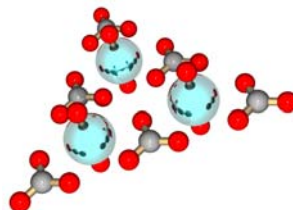


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Case Study 1: Chemistry Project

- 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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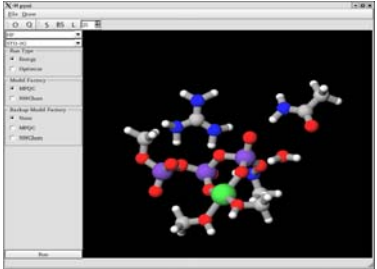
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CCA-Chemistry Project Participants

<u>Pacific Northwest National Laboratory</u>	<u>Argonne National Laboratory</u>
Theresa L. Windus	Steve Benson
Yuri Alexeev	Lois Curfman McInnes
Manojkumar Krishnan	Jason Sarich
Jarek Nieplocha	
Carl Fahlstrom	
Elizabeth Jurrus	


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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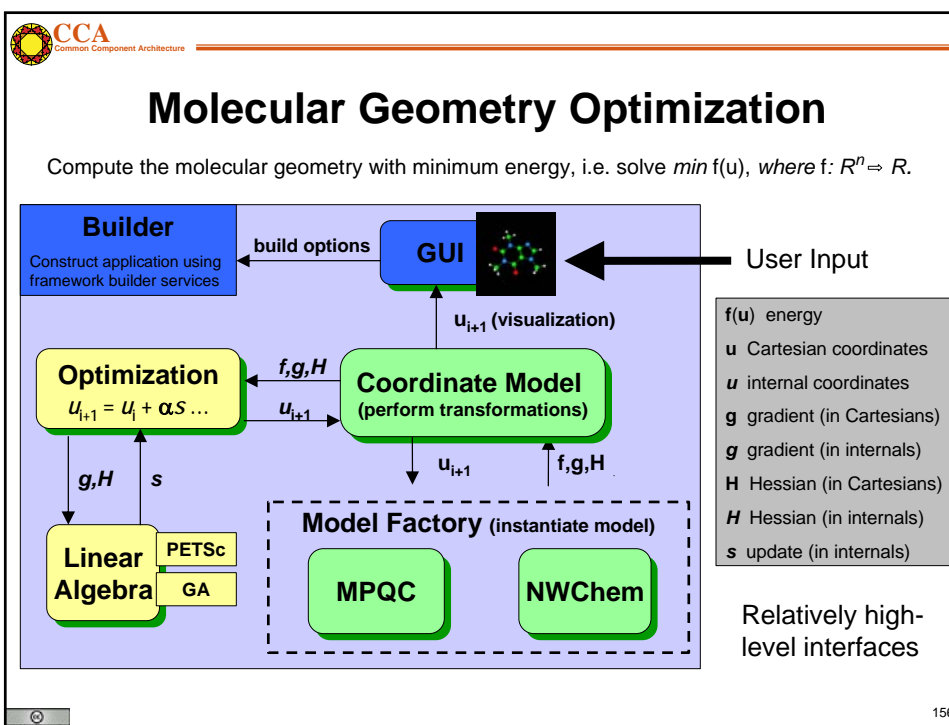
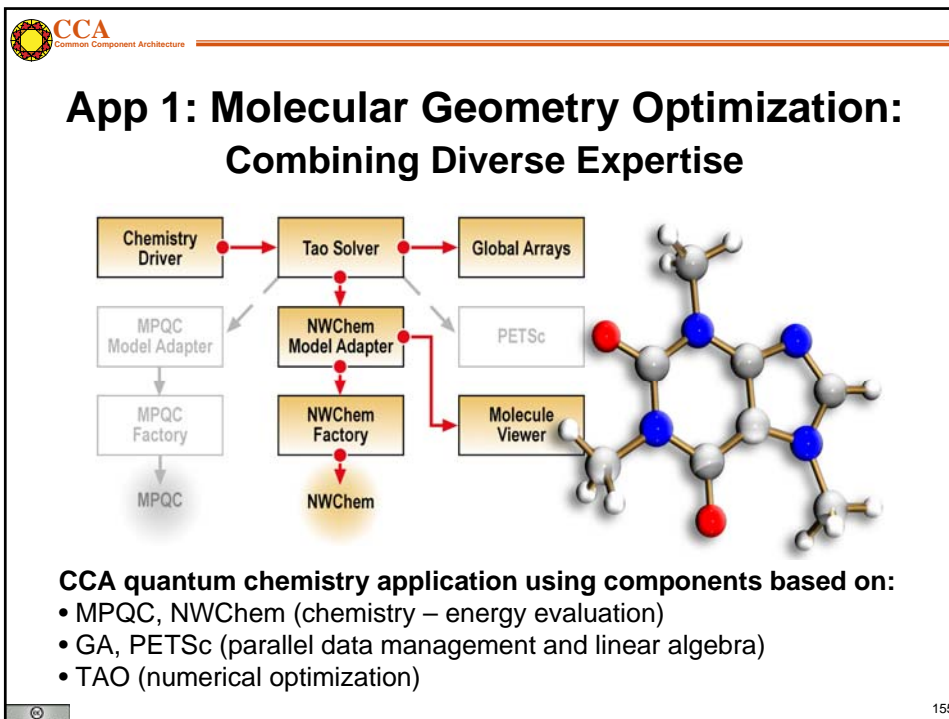
CCA Impacts in Computational Chemistry

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



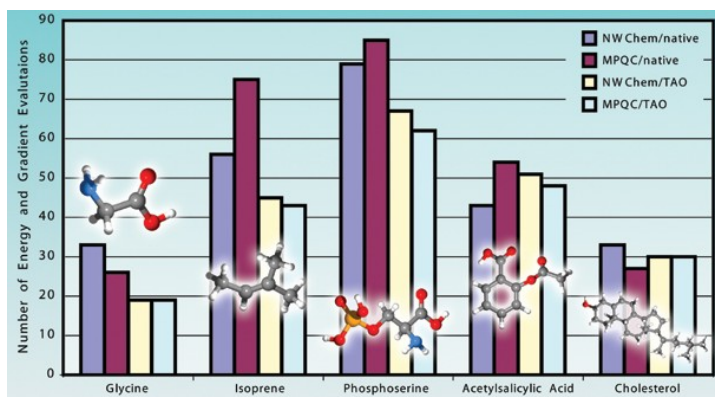
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Common Component Architecture

Performance Gains with Better Optimization Algorithms



CCA-based integration of state of the art optimization algorithms from the TAO toolkit provides up to 40% improvement in the time required to optimize molecular structures with MPQC and NWChem.¹

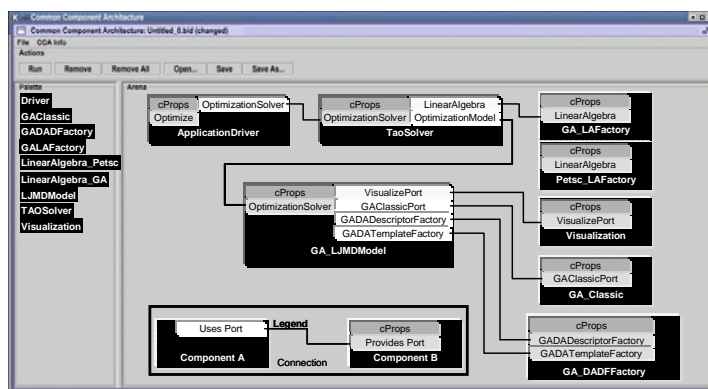
¹Journal of Computational Chemistry 25: 1717-1725, 2004.

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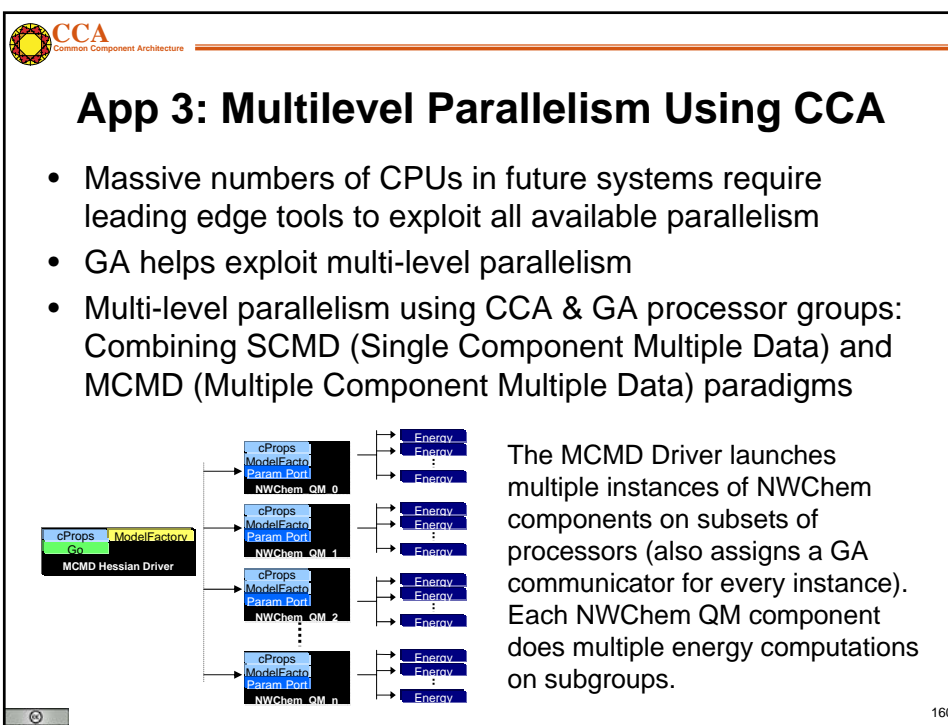
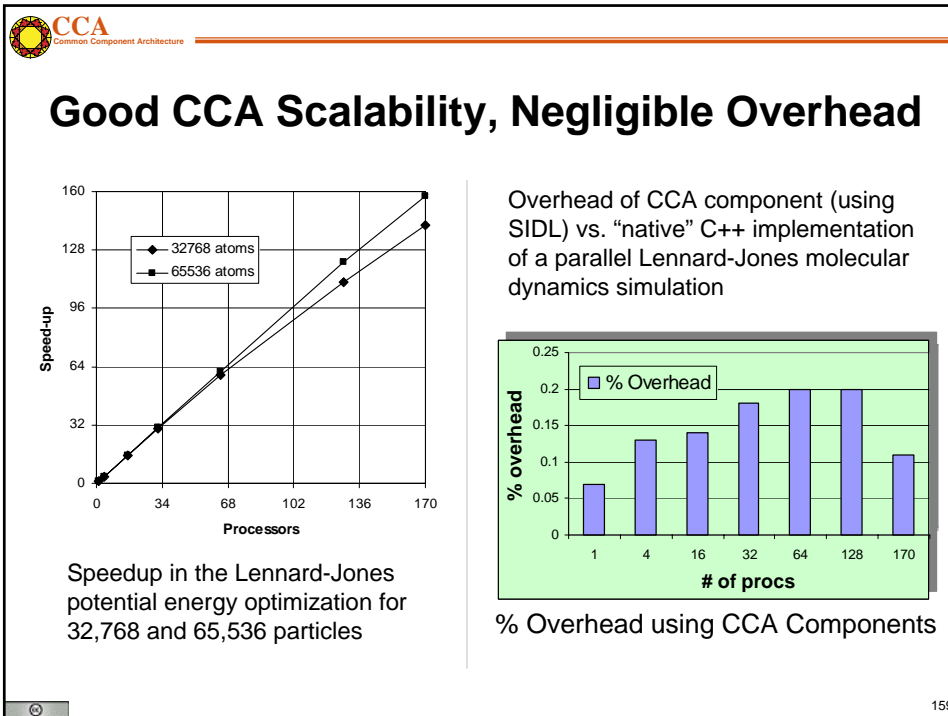
Common Component Architecture

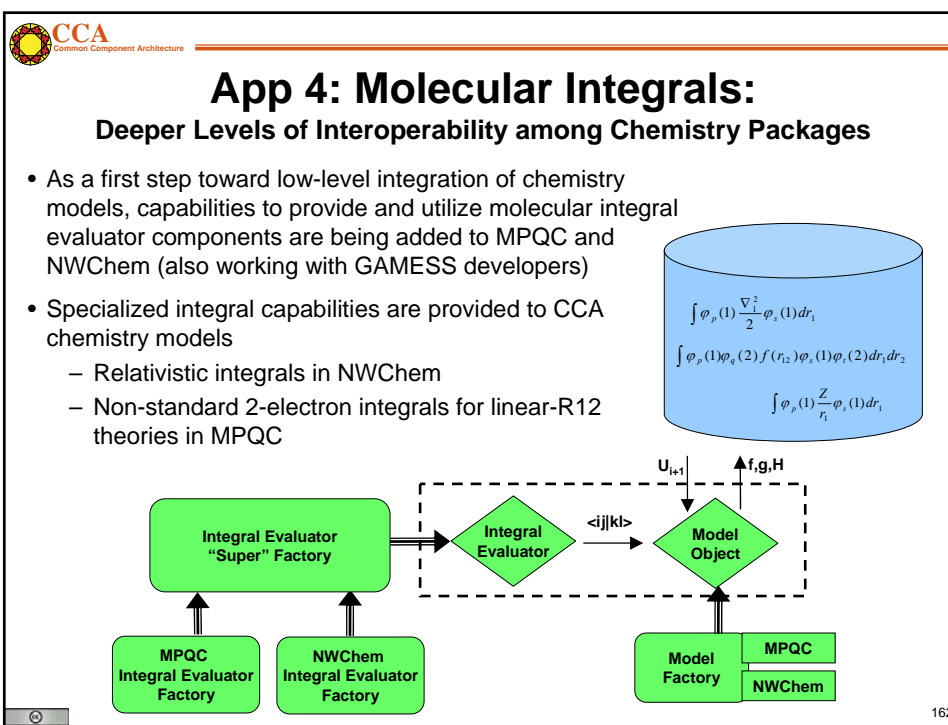
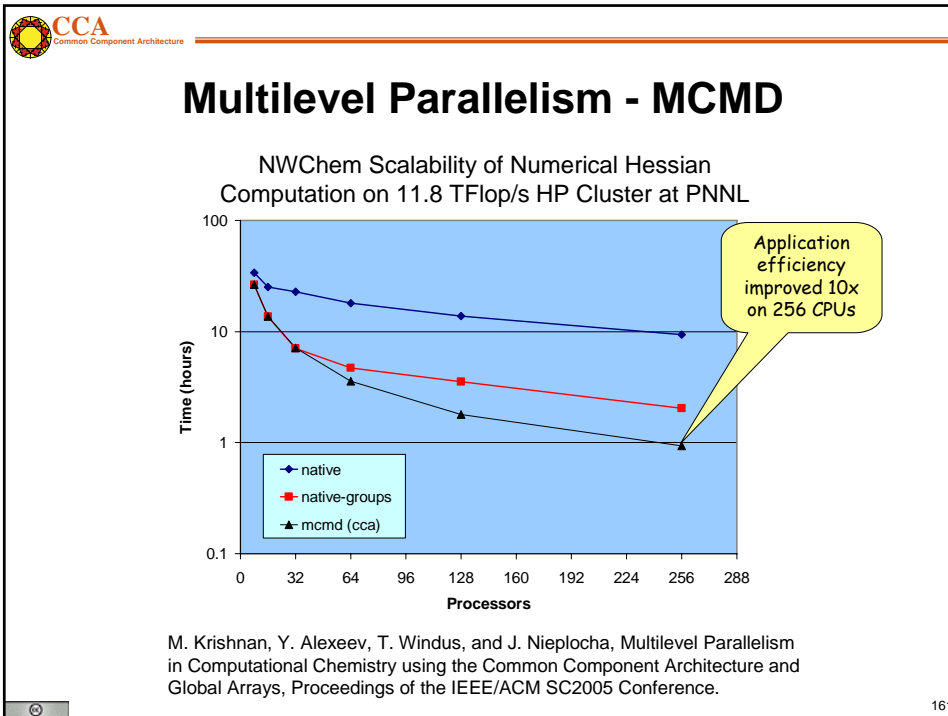
App 2: Molecular Dynamics



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

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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

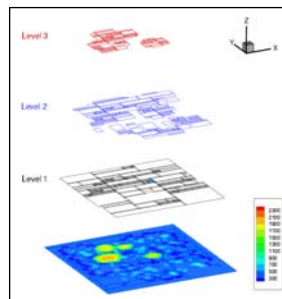


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Case Study 2: Combustion Project

- 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



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CCA
Common Component Architecture

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.



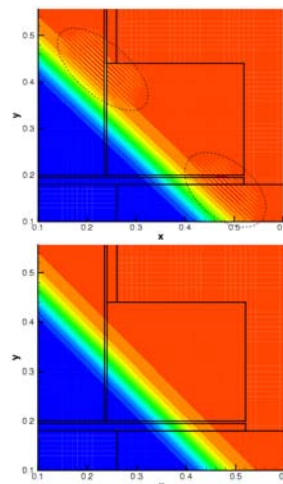
Has the Toolkit Approach Helped Tame Software Complexity?

- 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?



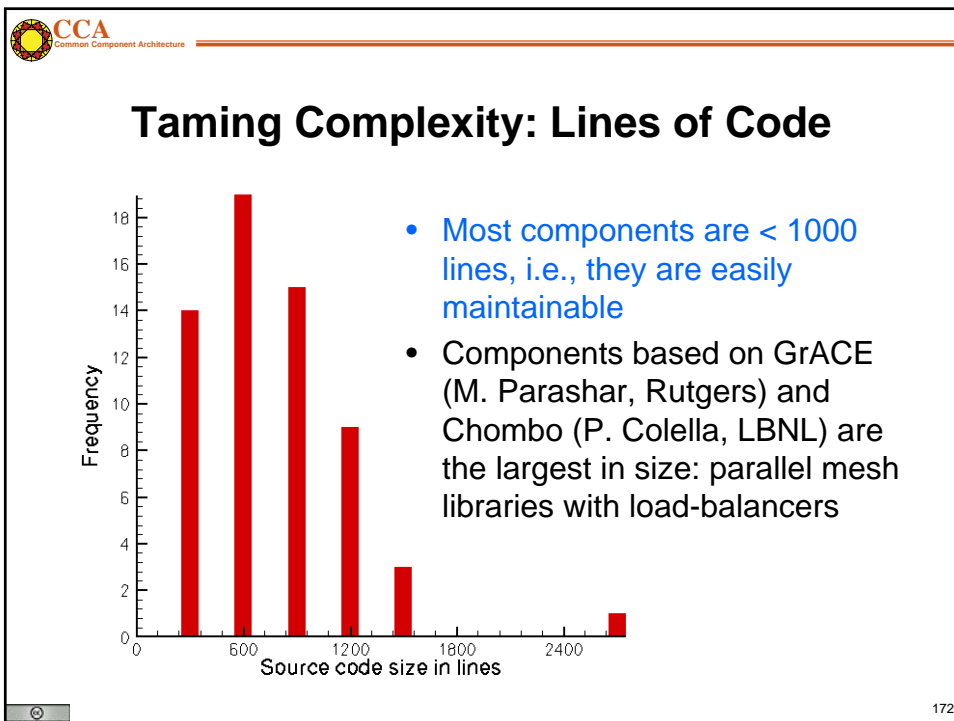
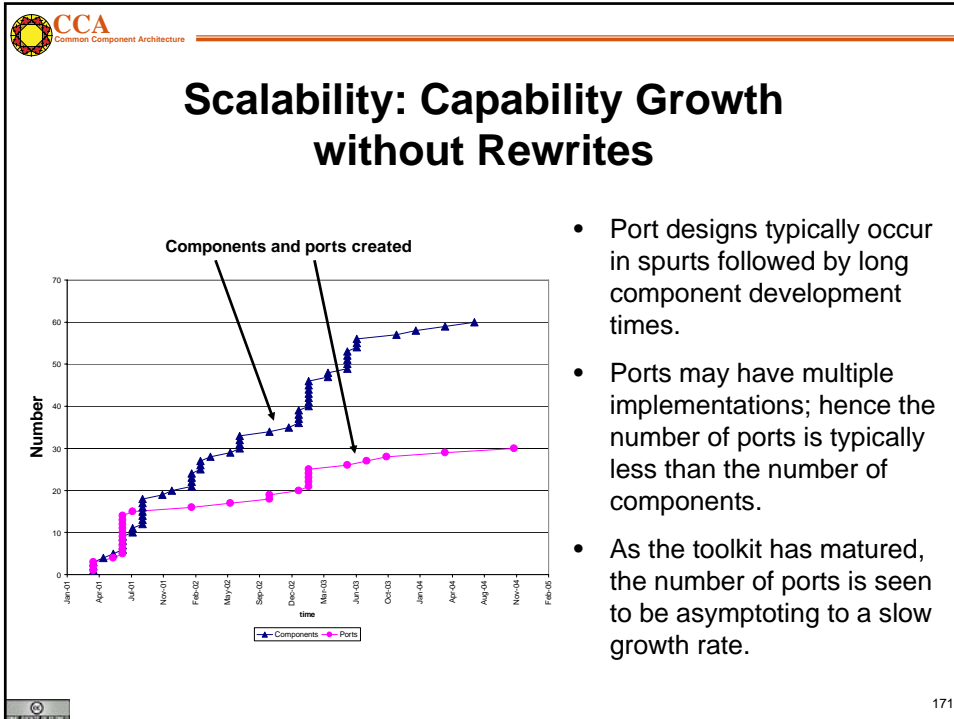
CFRFS Toolkit Status

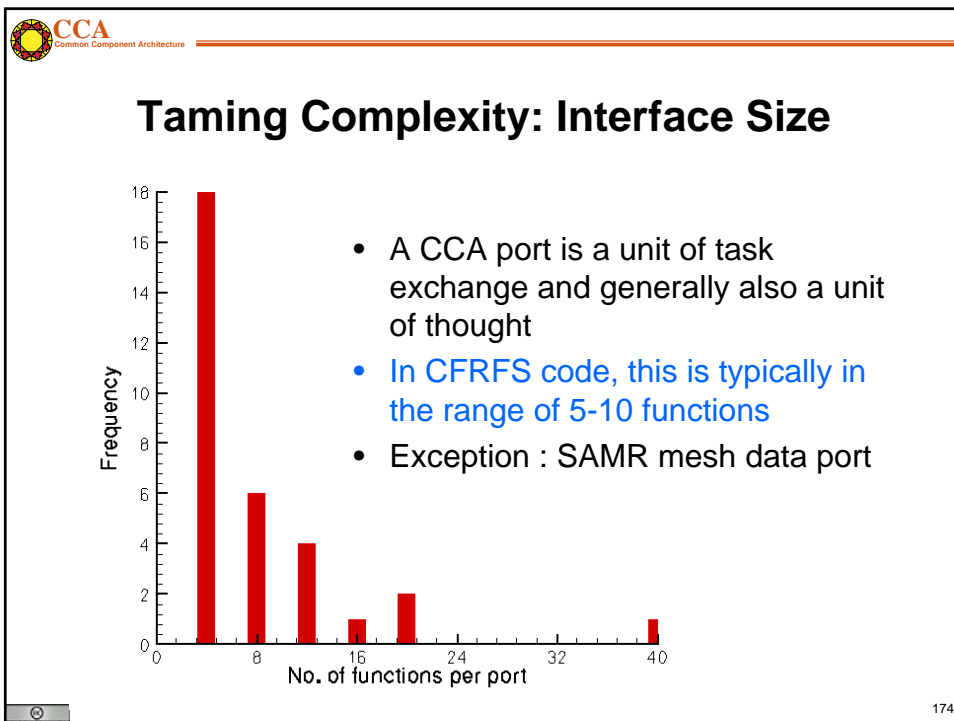
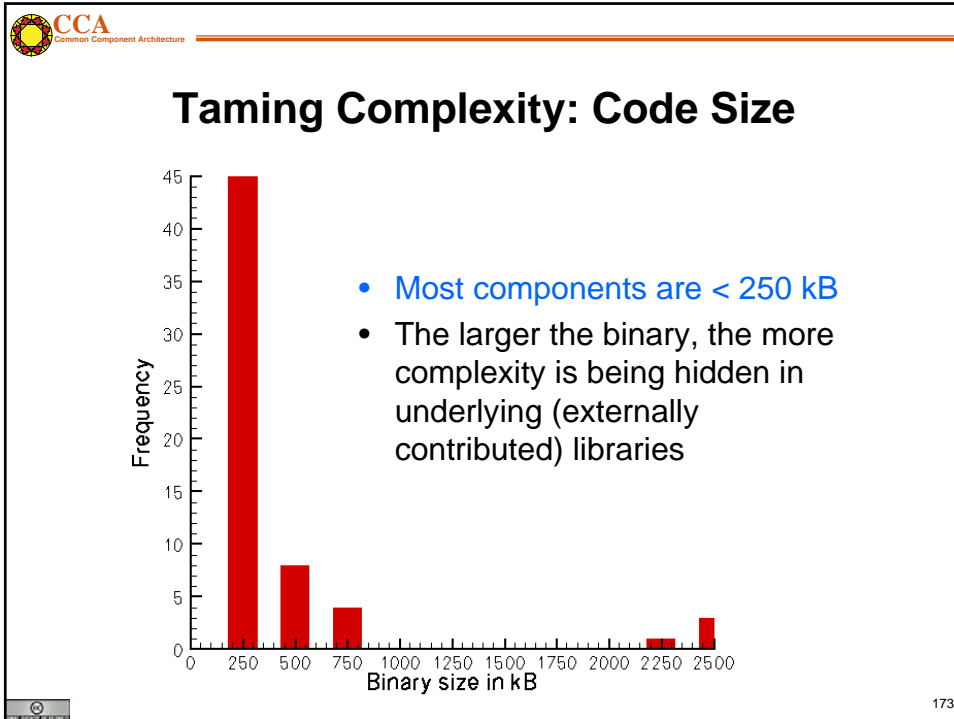
- Started in 2001
- 61 components today, all peers, independent, mixed and matched for combustion and shock hydrodynamics
- 7 external libraries
- Contributors: 9 in all, including 3 summer students
- Only 2 of the 9 contributors are at SNL today

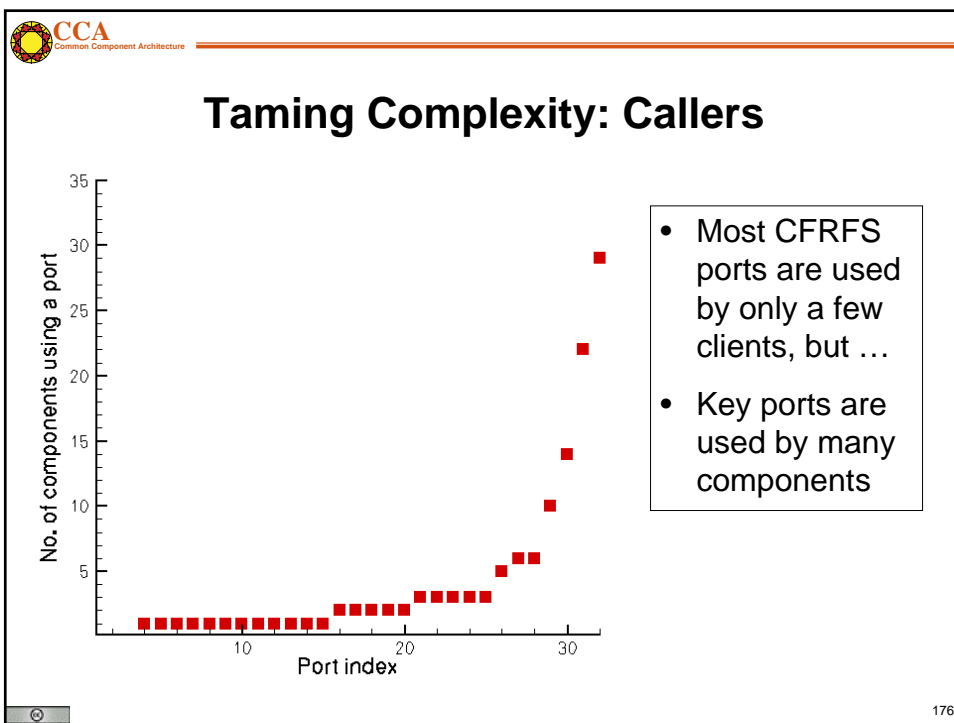
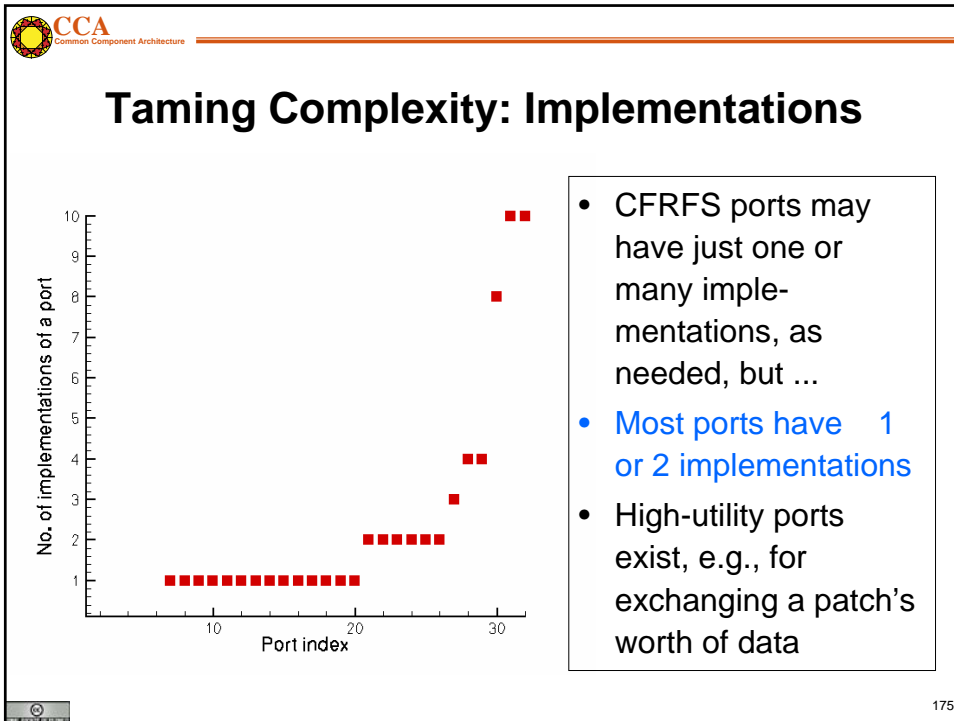


A Fitzhugh-Nagumo equation being solved on a block-structured adaptively refined mesh. The top image illustrates Runge phenomena at coarse-fine interfaces (dashed ovals) when using high-order schemes (6th order interpolations with 4th order discretizations). Filtering them with an 8th order filter removes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





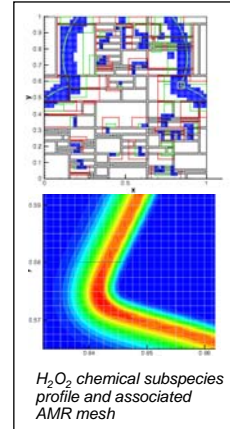






Scientific Productivity

- Conventional Measures
 - 4 journal papers in CFD/Numerics
 - 4 software-oriented journal papers, 1 book chapter
 - ~11 conference papers, including best paper award
 - Over 60 presentations
 - 1 MS and 1 PhD theses
 - 6 test applications
 - See papers at: <http://cfrfs.ca.sandia.gov>
- Unconventional Measures
 - Did the toolkit spawn new research in app-focused CS (e.g., performance evaluation/enhancement/modeling?)
 - Can the design accommodate software which were themselves designed to be *frameworks* and *not components*?



H₂O₂ chemical subspecies profile and associated AMR mesh

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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.



Who's working on CQoS ?

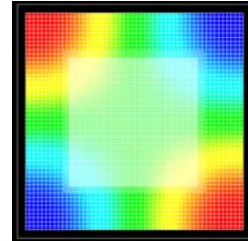
- Control law work:
 - Computational chemistry: evaluation of integrals
 - Partitioning of block-structured adaptive meshes
 - Iterative sparse linear algebra: mix-and-match accelerators and preconditioners
- Infrastructure work
 - Performance measurement: Automatic performance data (statistical) analysis
 - 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





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



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 or cca-tutorial@cca-forum.org





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 or cca-tutorial@cca-forum.org
- Problems with specific tools
 - *check documentation for updated contact info*
 - cca-tools bundle (includes Chasm, Babel, Ccaffeine): [Rob Armstrong](mailto:Rob.Armstrong@cca-forum.org), cca-tools@cca-forum.org
 - Bocca: [Rob Armstrong](mailto:Rob.Armstrong@cca-forum.org), bocca@cca-forum.org
 - Chasm: [Craig Rasmussen](mailto:Craig.Rasmussen@lanl.gov), crasmussen@lanl.gov
 - Babel: babel-users@llnl.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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Thank You!

Thanks for attending this tutorial

We welcome feedback and questions



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