Welcome to the
Common Component Architecture Tutorial

ACTS Collection Workshop
25 August 2006

CCA Forum Tutorial Working Group
http://www.cca-forum.org/tutorials/
tutorial-wg@cca-forum.org
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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 Domain-Specific *Common Interfaces*
- Goal: *Interoperability* between components developed by different expert teams across different institutions
- Quarterly Meetings, Open membership…

Mailing List: cca-forum@cca-forum.org
http://www.cca-forum.org/
What Can Component Technology do for Scientific Computing?

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

CCA tools used: Babel (SIDL), Chasm
Library languages: C, C++, F77, F90
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
Examples

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

**LAPACK07**
- Update to LAPACK linear algebra library
  - To be released 2007
  - Library written in F77, F95
- Will use Babel-generated interfaces for: C, C++, F77, F95, Java, Python
- Possibly also ScaLAPACK (distributed version)

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

-- Jeff Painter, LLNL. 2 June 2003

CCA tools used: Babel, Chasm
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
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.ccas.ucar.edu/models/ccsm3.0/cpl6/)
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
An Introduction to Components and the Common Component Architecture

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

- Introduce basic concepts and vocabulary of component-based software engineering and the CCA

- Highlight the special demands of high-performance scientific computing on component environments

- Give you sufficient understanding of the CCA to begin evaluating whether it would be useful to you
What are Components?

• No universally accepted definition in computer science research, but key features include…

• A unit of software development/deployment/reuse
  – i.e. has interesting functionality
  – Ideally, functionality someone else might be able to (re)use
  – Can be developed independently of other components

• Interacts with the outside world only through well-defined interfaces
  – Implementation is opaque to the outside world

• Can be composed with other components
  – “Plug and play” model to build applications
  – Composition based on interfaces
What is a Component Architecture?

• A set of standards that allows:
  – Multiple groups to write units of software (components)…
  – And have confidence that their components will work with other components written in the same architecture

• These standards define…
  – The rights and responsibilities of a component
  – How components express their interfaces
  – The environment in which components are composed to form an application and executed (framework)
  – The rights and responsibilities of the framework
A Simple Example: Numerical Integration Components

Interoperable components (provide same interfaces)
An Application
Built from the Provided Components

Hides complexity: Driver doesn’t care that MonteCarloIntegrator needs a random number generator
Another Application…

Diagram:
- GoPort
- Driver
- MidpointIntegrator
  - IntegratorPort
  - FunctionPort
- MonteCarloIntegrator
  - IntegratorPort
  - FunctionPort
  - RandomGeneratorPort
- NonlinearFunction
  - FunctionPort
- LinearFunction
  - FunctionPort
- PiFunction
  - FunctionPort
  - RandomGeneratorPort
  - RandomGenerator
Application 3...
And Many More…

Dashed lines indicate alternate connections

Create different applications in "plug-and-play" fashion
### Comparison of Application Development Approaches

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

- **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**
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
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
CCA Concepts: Ports

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

- Ports and connections between them are a procedural (caller/callee) relationship, *not dataflow!*
  - e.g., *FunctionPort* could contain a method like `evaluate(in Arg, out Result)` with data flowing both ways
CCA Concepts: *Provides* and *Uses* Ports

- 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
Components and Ports (in UML)

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

A component must implement the CCA spec’s component interface

A port must extend the CCA spec’s port interface

A component must implement the port(s) it provides

Key: ▲ = Inheritance

SIDL keywords

Class for Midpoint Integrator component
Components and Ports (in SIDL)

package gov.cca {
  interface Component {
    void setServices(...);
  }
}

packagegov.cca {
  interface Port {
    }
}

package integrators {
  interface IntegratorPort extends gov.cca.Port {
    double integrate(...);
  }
}

package integrators {
  class Midpoint implements gov.cca.Component, integrator.IntegratorPort {
    double integrate(...);
    void setServices(...);
  }
}
Using Ports

- 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”
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
Interfaces are Key to Reuse and Interoperability of Code

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

- The larger the community, the greater the time & effort required to obtain agreement
  - Equally true in component and non-component environments
    - MPI 1.0 (well understood at the start) took 8 months, meeting every six weeks
    - MPI 2.0 (not well understood at the start) took 1.5 years, meeting every six weeks
  - Convenient communities are often “project” and “scientific domain”
- Formality of “standards” process varies
- Biggerstaff’s Rule of Threes
  - Must look at at least three systems to understand what is common (reusable)
  - Reusable software requires three times the effort of usable software
  - Payback only after third release
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
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
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

More on Babel later!
Coding in a CCA Environment

- **Port Definitions (SIDL)**
- **Component Definition (SIDL)**
- **Component source code**
- **Compiled Components (object libraries)**
- **Application (component assembly)**
- **CCA Framework**

- **Babel runtime library & Chasm F90 array library**
- **Language compiler & linker**
- **Generated language code**
- **Babel compiler (SIDL → language)**

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

More details in the **CCA Tools** module
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
“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)
MCMD Within A Single Framework

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

- Framework
- Application driver & MCMD support component
- Components on all processes
- Components only on process group A
- Components only on process group B
CCA Supports High-Performance Local and Distributed Computing

- “Direct connection” preserves high performance of local (“in-process”) and parallel components
  - Framework makes connection
  - But is not involved in invocation

- Distributed computing has same uses/provides pattern, but framework intervenes between user and provider
  - Framework provides a proxy
    - provides port local to the uses port
  - Framework conveys invocation from proxy to actual provides port
“Direct Connection” 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 a 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
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 (CCAneiness)
  - 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
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
Some Performance Results and References


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

<table>
<thead>
<tr>
<th>Function arg type</th>
<th>f77</th>
<th>Component</th>
</tr>
</thead>
<tbody>
<tr>
<td>Array</td>
<td>80 ns</td>
<td>224 ns</td>
</tr>
<tr>
<td>Complex</td>
<td>75 ns</td>
<td>209 ns</td>
</tr>
<tr>
<td>Double complex</td>
<td>86 ns</td>
<td>241 ns</td>
</tr>
</tbody>
</table>
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
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

Advanced CCA Concepts

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

- The Proxy Component pattern *(Hands-On Ch. 6, papers)*
- Component lifecycle *(tutorial notes, Hands-On)*
- Components can be dynamic *(papers)*
- Frameworks can provide a specialized programming environment *(papers)*
The Proxy Component Pattern

- Component interfaces offer an obvious place to collect information about method invocations for performance, debugging, or other purposes
  - No intrusion on component internals
- A “proxy” component can be inserted between the user and provider of a port without either being aware of it
- Proxies can often 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
Component Lifecycle

- **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.
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
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
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

MonteCarloIntegrator

CCA.Services
  provides IntegratorPort
  uses FunctionPort, RandomGeneratorPort

Integrator code

MonteCarloIntegrator

Supplementary material for handouts
CCA.

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
Component’s View of Using a Port

- User calls `getPort` to obtain (handle for) port from `Services`
  - Finally user code can “see” provider
- **Cast** port to expected type
  - OO programming concept
  - Insures type safety
  - Helps enforce declared interface
- **Call** methods on port
  - e.g.
    `sum = sum + function->evaluate(x)`
- Call `releasePort`
Components can be Dynamic

- *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.
- **Encapsulation** of reusable complex component assemblies
  - Create a “container component” which exposes selected ports from the enclosed components
Frameworks can Provide Specialized Parallel Programming Environments

- By definition, all execution of components takes place within a framework
- CCA does not dictate a particular approach to parallelism
- Therefore, a specialized parallel programming environment can be made part of a CCA framework
  - May simplify design
  - Components depending on it won’t be useable in other frameworks, even if they are also CCA-compliant

Example:
- Uintah Computational Framework, based on SCIRun2 (Utah) provides a multi-threaded parallel execution environment based on task graphs
  - Graphs express interdependencies of each task’s inputs and outputs
  - Specialized to a class of problems using structured adaptive mesh refinement
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
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
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 it’s not perfect
  – We’re not “done” by any stretch

• Talk to us…
  – If you’re evaluating CCA and need help or have questions
  – If you don’t think CCA meets your needs
  – If you’ve got suggestions for things we might do better
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
  – Ports in progress for Cray X1 and XT3
  – Porting is driven by user needs
CCA Tools – Language Interoperability and Frameworks

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

- Describe tools for multi-lingual, scientific component ‘plug-and-play’
CCA adds value to component development

**Babel runtime library & Chasm F90 array library**

**Language compiler & linker**

**Compiled Components (object libraries)**

**Application (component assembly)**

**CCA Framework**

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

Port Definitions (SIDL)

Component Definition (SIDL)

Component source code

Generated language code

Babel compiler (SIDL→language)

CCA IDE
Tools Module Overview

- Language interoperability tools
- Frameworks
- CCA Interactive Development Environment
**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

**Supported on Linux, AIX, and Solaris 2.7, works on OSX; C (ANSI C), C++ (GCC), F77 (g77, Sun f77), F90 (Intel, Lahey, GNU, Absoft), Java (1.4)**
Babel Generates Object-Oriented Language Interoperability Middleware

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

IOR = Intermediate Object Representation
SIDL = Scientific Interface Definition Language
**Clients** in any supported language can access components in any other language

IOR = Intermediate Object Representation
Recent and Upcoming Features

- Remote Method Invocation (BabelRMI)  ALPHA
- Design-by-Contract  ALPHA
- Pre- and post-method invocation hooks  ALPHA
Chasm Provides Language Interoperability for Fortran, C, and C++

- Extracts interfaces from C/C++ and Fortran90 codes
- Uses library of XSLT stylesheets for language transformations → easily extended
  - Generates XML and SIDL representations
  - Generates Fortran90 Babel implementation glue
- Provides Fortran array descriptor library used by Babel

Supported on Linux, AIX, and Solaris 2.7, works on OSX;
C (ANSI C), C++ (GCC), F90 (Intel, Lahey, GNU, Absoft)
The Entire **Chasm** Process Involves Three Basic Steps

1. Start with a Fortran (or C/C++) source file
2. Create an XML description of the component (or port)
3. Generate the SIDL specification and glue code files

**XML** = Extensible Markup Language  
**PTD** = Parse Tree Dump
Chasm-Assisted Glue Code Generation

1. Create functions_LinearFunction.impl.xml
2. Create xml description of source procedures
   % gfortran -fdump-parse-tree LinearFunction.f90 > LinearFunction.ptd
   % gfortran2xml < LinearFunction.ptd > LinearFunction.xml
3. Create .sidl, _Impl.F90, and _Mod.F90
   % xalan -o functions_LinearFunction.sidl functions_LinearFunction.impl.xml cca-f90-comp.sidl.xsl
   % xalan -o functions_LinearFunction_Impl.F90 functions_LinearFunction.impl.xml cca-f90.impl.xsl
   % xalan -o functions_LinearFunction_Mod.F90 functions_LinearFunction.impl.xml cca-f90.mod.xsl
4. Run Babel...
User-Created XML Component Description File

```xml
<componentImplementation name="LinearFunction" package="functions">
  <language name="F90">
    <property name="impl-scope" value="LinearFunction"/>
    <property name="impl-xml" value="/home/cca/LinearFunction.xml"/>

    <ports>
      <provides name="FunctionPort" package="function">
        <MethodsBlock>
          <Method name="evaluate" impl="evaluate_lf"/>
        </MethodsBlock>
      </provides>
    </ports>
  </language>
</componentImplementation>
```
Recent and Upcoming Features

• Generate Fortran 2003 MPI Bindings 1Q 2006

• Update XML processor and generator to new PDToolkit releases 1Q 2006
Tools Module Overview

- Language interoperability tools
- Frameworks
- CCA Interactive Development Environment
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
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

None of these (yet) plug into your favorite Integrated Development Environment (e.g., Eclipse, MS Dev. Studio, Java Studio, …).
Ccaffeine is a Direct-Connect, Parallel-Friendly Framework

- Supports SIDL/Babel components
  - Conforms to latest CCA specification (0.7)
  - 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.
Caffeine 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 Caffeine input file to load the component at runtime.

• Proceed to plug & play...

There are many details and automated tools that help manage components.
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
  - *use* ports call methods or subroutines in the port.
  - Links denote caller/callee relationship *not* data flow

---

Java is required.
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 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
...
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**
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.
Application Configurations can be Re-used

1. Click Save or Save As… to save actions.

2. Click Open to replay actions.

- Script optimization
  
  % simplify-bld saved_file.bld > faster_file.bld

- Batch conversion
  
  % bld2rc faster_file.bld > faster_file.batch

- C++ stand-alone execution
  
  % bld2babel-cpp faster_file.bld faster_file_babel outdir

  or
  
  % bld2neo faster_file.bld faster_file.batch outdir
Recent and Upcoming Features

• Interoperate with other CCA frameworks
  – Via Babel RMI 2H 2006
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
XCAT is Designed for High-Performance Scientific Applications

XCAT-C++ Framework
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)
Recent and Upcoming Features

- Support GRAM for component creation *1H 2006*
  - Allow use of grid resources

- Automated component registration and discovery *2H 2006*

- Support new protocols such as UDT (in Proteus) *1H 2006*

- Support Babel’s Remote Method Invocation *2H 2006*
  - Allows access to Babel objects through remote Babel stubs
  - Provides direct support for SIDL in distributed applications
  - Leverages Proteus

GRAM = Grid Resource Allocation Management  
UDT = UDP-based Data Transfer protocol
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.
**Master Framework** Coordinates **Slave Frameworks** in Each Remote Address Space
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
Simple SCIRun2 CCA (PIDL) and Babel Bridge
Recent and Upcoming Features

- Merge PIDL with SIDL/Babel \textit{1H 2005}

- Support additional component models
  - Kepler workflows \textit{1H 2006}

- Support Babel’s Remote Method Invocation PRMI \textit{2H 2006}

- Automate bridging \textit{On-going}
## Experimental Frameworks

<table>
<thead>
<tr>
<th>Framework</th>
<th>Purpose</th>
<th>Summary</th>
</tr>
</thead>
</table>
| **Distributed CCA Framework (DCA)** | MxN research                     | • **Goal**: explore MxN Parallel-Remote Method Invocation (PRMI) using MPI  
• Parallel data transfer and redistribution integrated into port invocation mechanism   |
| **LegionCCA**              | Grid-based research              | • **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       | • **Goal**: explore web interface for launching distributed applications  
• This (alpha) version compatible with latest CCA specification and provides built-in seamless compatibility with OGSI. |

OGSI = Open Grid Services Infrastructure
Tools Module Overview

- Language interoperability tools
- Frameworks
- CCA Interactive Development Environment
Component Development 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
A Wizard is also Available for Adding Methods
Recent and Upcoming Features

• Provide automated build support  1H 2005

• Launch application via GUI  1H 2006
### CCA Tools Contacts (1 of 2)

<table>
<thead>
<tr>
<th>Tool</th>
<th>Purpose</th>
<th>More information</th>
</tr>
</thead>
</table>
| **Babel** | **Scientific** language interoperability tool kit | URL: [www.llnl.gov/CASC/components](http://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/](http://www.cca-forum.org/software/)  
Email: Ben Allan, ccafe-help@z.ca.sandia.gov  
Wiki: [https://www.cca-forum.org/wiki](https://www.cca-forum.org/wiki) |
| **Chasm** | Fortran90 interoperability wrapper            | URL: [chasm-interop.sourceforge.net](http://chasm-interop.sourceforge.net)  
Examples: [chasm/example/cca-tutorial](http://chasm/example/cca-tutorial) |
| **DCA**   | MxN research framework                       | URL: [www.cs.indiana.edu/~febertra/mxn](http://www.cs.indiana.edu/~febertra/mxn)  
Email: Felipe Bertrand, febertra@cs.indiana.edu |
| **CCA IDE** | CCA development environment               | Email: usability@cca-forum.org |
# CCA Tools Contacts (2 of 2)

<table>
<thead>
<tr>
<th>Tool</th>
<th>Purpose</th>
<th>More information</th>
</tr>
</thead>
</table>
| LegionCCA     | Grid-based research framework | URL: grid.cs.binghamton.edu/projects/legioncca.html  
Email: Michael J. Lewis, mlewis@binghamton.edu |
| 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/xcat/  
Email: Madhu Govindaraju, mgovinda@cs.binghamton.edu |
| XCAT-Java     | Grid research framework   | URL: www.extreme.indiana.edu/xcat/  
Email: Dennis Gannon, gannon@cs.indiana.edu        |
Module Summary

- 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 Environment via Eclipse plug-in
CCA Forum Tutorial Working Group

http://www.cca-forum.org/tutorials/

tutorial-wg@cca-forum.org
Goal of This Module

Learn how existing code is
- Wrapped into Babel objects, and
- Promoted to CCA components

In the process, also need to learn about
- Scientific Interface Definition Language (SIDL)
- Using the Babel tool
- Characteristics of Babelized software
Working Code: “Hello World” in F90 Using a Babel Type

```fortran
program helloclient
  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 helloclient
```
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 helloclient
  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 helloclient
```

Looks like a native F90 derived type

These subroutines were specified in the SIDL.

Other basic subroutines are “built in” to all Babel types.
The SIDL File that defines the “greetings.English” type

```
package greetings version 1.0 {
    interface Hello {
        void setName( in string name );
        string sayIt();
    }
    class English implements-all Hello {
    }
}
```
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.
Question: What language is “obj” really implemented in?

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!
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.
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.
Babel Consists of Two Parts: Code Generator + Runtime Library

Code generator reads SIDL, and generates wrapper code...

... very sophisticated wrapper code.
Typical Workflow to **Use** a Babel type (static linkage)

1. `babel --client=F90 greetings.sidl`
2. Compile generated Code
3. Link driver, generated code ("Stubs"), Babel Runtime, and library containing Babel type
Typical Workflow to Use a Babel type (dynamic linkage)

1. `babel --client=F90 greetings.sidl`
2. Compile same generated code with different flags
3. Link driver, and stubs only (both generated code and F90 stubs to Babel Runtime library)
4. Set SIDL_DLL_PATH environment variable to include relevant *.scl (or *.cca) files.
5. Actual implementations are linked in at runtime
Static vs. Dynamic Linkage

• Static
  – Least runtime overhead
  – Easiest to get right, debug, etc.

• Dynamic
  – Allows new types to “plug-in” without relinking driver
  – Necessary for Java or Python calling to other languages (unless you relink their virtual machine)
  – Induces very nondeterministic behavior if done incorrectly
Workflow for a Developer Wrapping Their Code into Babel Objects

1. `babel --server=C++ greetings.sidl`
2. Fill in the implementation details (see next slide)
3. Compile and link into a library/DLL
Implementation Details Must be Filled in Between Splicer Blocks

namespace greetings {
    class English_impl {
        private:
            // DO NOT DELETE splicer.begin(greetings.English._impl)
            string d_name;
            // DO NOT DELETE splicer.end(greetings.English._impl)

    string
    greetings::English_impl::sayIt() throw () {
        // DO NOT DELETE splicer.begin(greetings.English.sayIt)
        string msg("Hello ");
        return msg + d_name + "!";
        // DO NOT DELETE splicer.end(greetings.English.sayIt)
    }
}
Quick Review of Babel in general before proceeding to CCA specifics

- Babel can be used as a standalone tool
- Each language binding strikes a balance
  - support the SIDL type system (OO, exceptions, etc.)
  - provide it in a manner “natural” to experienced programmers in the target language
- For more details about Babel and SIDL
  - SC|04 tutorial slides for Babel
    http://www.llnl.gov/CASC/components/docs/sc04.html
  - Babel User’s Guide (aka. the BUG)
    http://www.llnl.gov/CASC/components/docs/users_guide/
How to write a Babelized CCA Component (1/3)

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

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

```java
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 {
}
```
Tip: Use Babel’s XML output like precompiled headers in C++

1. Precompile SIDL into XML using ‘--text=xml’
2. Store XML in a directory
3. Use Babel’s –R option to specify search directories
How to write a Babelized CCA Component (3/3)

3. Use Babel to generate the interoperability glue
   - Execute `babel --server=\texttt{C} --repo \texttt{functions.sidl}`

4. Fill in Implementations as needed
Review: Goal of This Module

Learn how existing code is
  • Wrapped into Babel objects, and
  • Promoted to CCA components

In the process, also need to learn about
  • Scientific Interface Definition Language (SIDL)
  • Using the Babel tool
  • Characteristics of Babelized software
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
Using CCA: Approaches & Experience

CCA Forum Tutorial Working Group
http://www.cca-forum.org/tutorials/
tutorial-wg@cca-forum.org
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
Using CCA to Help Manage Complexity

• Application areas participating in the CCA: astronomy, astrophysics, biological and medical simulations, chemically reacting flow, climate and weather modelling, combustion, computational chemistry, data management, fusion and plasma physics modelling, linear algebra, materials science, molecular electronics, nanoscience, nuclear power plant simulations, structured adaptive meshes, unstructured meshes, and visualization

• Research agencies sponsoring software development using the CCA: DOE (SciDAC, Office of Science, NNSA/ASC), NASA, NIH, NSF, DoD, European Union
Outline

• Developing Components
  – Strategies for both developing new codes and wrapping existing codes

• Case Studies
  – Chemistry project
    • Moderate-sized multi-disciplinary, multi-institutional team
    • Using Ccaffeine framework, SIDL components
  – Combustion toolkit
    • Small team, both new and wrapped codes
    • Using Ccaffeine framework, C++ components
Developing Components
(Both New Codes and Wrappers to Existing Codes)

• Productivity Benefits

• Application Decomposition Strategies

• Interface Design Issues
  – Social factors
  – Technical factors

• Implementation Issues and Patterns
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
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 management
  as 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
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 (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
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)
CCA-Chemistry Project Participants

Pacific Northwest National Laboratory
Theresa L. Windus
Yuri Alexeev
Manojkumar Krishnan
Jarek Nieplocha
Carl Fahlstrom
Elizabeth Jurrus

Sandia National Laboratory
Curtis L. Janssen
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Argonne National Laboratory
Steve Benson
Lois Curfman McInnes
Jason Sarich
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
CCA quantum chemistry application using components based on:
- MPQC, NWChem (chemistry – energy evaluation)
- GA, PETSc (parallel data management and linear algebra)
- TAO (numerical optimization)
Molecular Geometry Optimization

Compute the molecular geometry with minimum energy, i.e. solve \( \min f(u) \), where \( f: \mathbb{R}^n \rightarrow \mathbb{R} \).

\[ u_{i+1} = u_i + \alpha s \ldots \]

**Builder**
Construct application using framework builder services

**User Input**

- **f(u)** energy
- **u** Cartesian coordinates
- **u** internal coordinates
- **g** gradient (in Cartesians)
- **g** gradient (in internals)
- **H** Hessian (in Cartesians)
- **H** Hessian (in internals)
- **s** update (in internals)

**Model Factory** (instantiate model)

**Coordinate Model** (perform transformations)

**Linear Algebra**

PETSc
GA

**Optimization**

**GUI**

**Model Factory** (instantiate model)

MPQC
NWChem

Relatively high-level interfaces
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

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

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

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

% Overhead using CCA Components
App 3: Multilevel Parallelism Using CCA

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

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

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

Application efficiency improved 10x times on 256 CPUs

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

- As a first step toward low-level integration of chemistry models, capabilities to provide and utilize molecular integral evaluator components are being added to MPQC and NWChem (also working with GAMESS developers).

- Specialized integral capabilities are provided to CCA chemistry models:
  - Relativistic integrals in NWChem.
  - Non-standard 2-electron integrals for linear-R12 theories in MPQC.

\[
\int \varphi_{p}(1) \nabla \varphi_{s}(1) dr_{1} \\
\int \varphi_{p}(1)\varphi_{q}(2) f(r_{12}) \varphi_{s}(1)\varphi_{s}(2) dr_{1}dr_{2} \\
\int \varphi_{p}(1) \frac{Z}{r_{1}} \varphi_{s}(1) dr_{1}
\]
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
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
Case Study 2: Combustion Project

- Computational Facility for Reacting Flow Science (CFRFS)
  - Funded via SciDAC initiative (PI: H. Najm)

- Focus: A toolkit to perform simulations of lab-sized unsteady flames
  - Solve the Navier-Stokes with 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

- Contributions to research and codebase:
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)
Design Principles of the Toolkit - 1

- **Principal Aim: Reduce software complexity**
  - We can deal with the rest

- Functional decomposition into components
  - “Data Object” and Mesh components
  - (Large) set of numerical algorithmic components (integrators, linear/nonlinear solvers, etc.)
  - (Large) set of physical models components (gas-phase combustion chemistry, thermodynamics, fluid dynamic quantities, e.g. viscous stress tensor)
  - Handful of adaptors
Design Principles of the Toolkit - 2

- Decomposition reflected in the port design and implementation
  - Most re-implemented port is the one that exchanges a rectangular sub-domain’s data for processing by components

- Sparse connectivity between components
  - i.e., components communicate with a few others
  - Large apps (component assemblies) are composed by assembling smaller, largely independent sub-assemblies
    - Sub-assemblies usually deal with a certain physics
  - Intuitive way to assemble a multiphysics code
Separate component subsystems for transport (dark blue) 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?

Questions to consider:

• 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).
Scalability: Capability Growth without Rewrites

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

- Most components are < 1000 lines, i.e., they are easily maintainable
- Components based on GrACE (M. Parashar, Rutgers) and Chombo (P. Colella, LBNL) are the largest in size: parallel mesh libraries with load-balancers
Taming Complexity: Code Size

- Most components are < 250 kB
- The larger the binary, the more complexity is being hidden in underlying (externally contributed) libraries
Taming Complexity: Interface Size

- A CCA port is a unit of task exchange and generally also a unit of thought.
- In CFRFS code, this is typically in the range of 5-10 functions.
- Exception: SAMR mesh data port.

![Bar chart showing the distribution of functions per port with frequencies ranging from 0 to 18.](chart.png)
Taming Complexity: Implementations

- CFRFS ports may have just one or many implementations, as needed, but ...
- Most ports have 1 or 2 implementations
- High-utility ports exist, e.g., for exchanging a patch’s worth of data
Taming Complexity: Callers

- Most CFRFS ports are used by only a few clients, but ...
- Key ports are used by many components
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?
Adaptive Codes

• A CCA code is an assembly of components
  – Components are shared libraries
  – 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 a performance model of each component, use the best one
  – Create an expert system that analyzes a problem and picks a good solution strategy
Performance Measurement in a Component World

• Different from traditional software
  – The researcher may not be the author of the component
  – Will need performance info on a component granularity
  – Will need a non-intrusive way of getting it.

• Proxies: Simple component to be inserted between a caller and a callee component
  – Intercepts and forward method calls
  – Can be used to log size of arrays etc
  – Can be use to turn on a “clock” on be called; can turn it off when returning to called.

• A proxy’s ports are the same as the callee’s

• Its functionality is pretty mundane
  – Can it be automatically generated?
Integrated Performance Measurement

Measurement infrastructure:

- **Proxy**
  - Generated automatically using PDT
  - Logs parameters to MasterMind
- **MasterMind**
  - Collects and stores all measurement data
- **TAU**
  - Makes all performance measurements
- Work done at University of Oregon by A. Malony and team
Component Application with Proxies
Extending Ccaffeine to Enable Autonomic Adaptation

- **User component**
- **Component manager**
  - Knows how to replace and tune components
- **Composition manager**
  - Coordinates application processes and triggers component manager when safe

CCA framework + TAU

Node x

CCA framework + TAU

Node y

CCA framework + TAU

Node z

Work done at Rutgers by M. Parashar
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
    - A 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 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, which are shrink-wrapped for easy re-use
  – Apart from the science research, has 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 in these case studies, see:

• Different facets of CCA components may be useful within different projects … What are your needs and priorities?
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…

  tutorial-wg@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
  – tutorial-wg@cca-forum.org

• Problems with specific tools
  – check documentation for updated contact info
  – cca-tools bundle (includes Chasm, Babel, Ccaffeine): Rob Armstrong, rob@sandia.gov
  – Chasm: Craig Rasmussen, crasmussen@lanl.gov
  – Babel: babel-users@llnl.gov
  – Ccaffeine: ccafe-users@cca-forum.org

• General questions, or not sure who to ask?
  – cca-forum@cca-forum.org
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

• “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.
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 Kumfert, Lois Curfman McInnes, Alan Morris, Boyana Norris, Craig Rasmussen, Jaideep Ray, Sameer Shende, Torsten Wilde, Shujia Zhou

- **Institutions:** ANL, Binghamton U, Indiana U, JPL, LANL, LLNL, NASA/Goddard, ORNL, SNL, U Illinois, U Oregon

- **Computer facilities** provided by the Computer Science Department and University Information Technology Services of Indiana University, supported in part by NSF grants CDA-9601632 and EIA-0202048.
Acknowledgements: The CCA

- ANL – Steve Benson, Jay Larson, Ray Loy, Lois Curfman McInnes, Boyana Norris, Everest Ong, Jason Sarich…
- Binghamton University - Madhu Govindaraju, Michael Lewis, …
- Indiana University - Randall Bramley, Dennis Gannon, …
- JPL – Dan Katz, …
- LANL - Craig Rasmussen, Matt Sotille, …
- LLNL – Tammy Dahlgren, Lori Freitag Diachin, Tom Epperly, Scott Kohn, Gary Kumfert, …
- NASA/Goddard – Shujia Zhou
- ORNL - David Bernholdt, Wael Elwasif, Jim Kohl, Torsten Wilde, …
- PNNL - Jarek Nieplocha, Theresa Windus, …
- SNL - Rob Armstrong, Ben Allan, Lori Freitag Diachin, Curt Janssen, Jaideep Ray, …
- Tech-X Corp. – Johan Carlsson, Svetlana Shasharina, Ovsei Volberg, Nanbor Wang
- University of Oregon – Allen Malony, Sameer Shende, …
- University of Utah - Steve Parker, …

and many more… without whom we wouldn’t have much to talk about!
Thank You!

Thanks for attending this tutorial

We welcome feedback and questions