Welcome to the Common Component Architecture Tutorial

ACTS Collection Workshop
27 August 2004

CCA Forum Tutorial Working Group
http://www.cca-forum.org/tutorials/
tutorial-wg@cca-forum.org
# Agenda & Table of Contents

<table>
<thead>
<tr>
<th>Time</th>
<th>Title</th>
<th>Slide No.</th>
<th>Presenter</th>
</tr>
</thead>
<tbody>
<tr>
<td>11:30-11:35am</td>
<td>Welcome</td>
<td>1</td>
<td>David Bernholdt, ORNL</td>
</tr>
<tr>
<td>11:35am-12:30pm</td>
<td>A Pictorial Introduction to Components in Scientific Computing</td>
<td>6</td>
<td>David Bernholdt, ORNL</td>
</tr>
<tr>
<td></td>
<td>An Introduction to Components &amp; the CCA</td>
<td>26</td>
<td>David Bernholdt, ORNL</td>
</tr>
<tr>
<td>12:30-1:30pm</td>
<td>Lunch</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1:30pm-1:50pm</td>
<td>Distributed Computing with the CCA</td>
<td>67</td>
<td>David Bernholdt, ORNL</td>
</tr>
<tr>
<td>1:50-2:50pm</td>
<td>CCA Applications</td>
<td>87</td>
<td>Jaideep Ray, SNL</td>
</tr>
<tr>
<td>2:50-3:20pm</td>
<td>Language Interoperable CCA Components with Babel</td>
<td>136</td>
<td>Tom Epperly, LLNL</td>
</tr>
<tr>
<td>3:20-3:30pm</td>
<td>Questions/Discussion</td>
<td></td>
<td>The Team</td>
</tr>
<tr>
<td>3:30-4:00pm</td>
<td>Break/Relocate to Tolman Hall</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4:00-4:45pm</td>
<td>TAU Hands-On</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4:45-6:30pm</td>
<td>CCA Hands-On</td>
<td></td>
<td>Rob Armstrong, SNL &amp; the Team</td>
</tr>
</tbody>
</table>
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 “Standard” 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/
Acknowledgements: Tutorial Working Group

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Acknowledgements: The CCA

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- **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!
A Pictorial Introduction to Components in Scientific Computing

CCA Forum Tutorial Working Group
http://www.cca-forum.org/tutorials/
tutorial-wg@cca-forum.org
Once upon a time...
As Scientific Computing grew...
Tried to ease the bottle neck
SPMD was born.
SPMD worked.

But it isn’t easy!!!
Meanwhile, corporate computing was growing in a different way.

**Diagram:**
- Input
- Output

**Components:**
- email client
- spreadsheet
- browser
- graphics
- editor
- Unicode
- multimedia
- database

**Legend:**
- Red
- Orange
- Yellow
- Light Blue
- Dark Blue
- Light Gray
- Gray
This created a whole new set of problems → complexity

- Interoperability across multiple languages
- Interoperability across multiple platforms
- Incremental evolution of large legacy systems (esp. w/ multiple 3rd party software)
Component Technology addresses these problems
So what’s a component ???

Implementation: No Direct Access

Interface Access: Generated by Tools

Matching Connector: Assigned by Framework Hidden from User
1. Interoperability across multiple languages

Language & Platform independent interfaces

Automatically generated bindings to working code
2. Interoperability Across Multiple Platforms

Imagine a company migrates to a new system, OS, etc.

What if the source to this one part is lost???
Transparent Distributed Computing

These wires are very, very smart!
3. Incremental Evolution With Multiple 3rd party software
Now suppose you find this bug...
Good news: an upgrade available
Bad news: there’s a dependency
Great News:
Solvable with Components
Great News: Solvable with Components
Why Components for Scientific Computing

→ Complexity

- Interoperability across multiple languages
- Interoperability across multiple platforms
- Incremental evolution of large legacy systems (esp. w/ multiple 3rd party software)
The Model for Scientific Component Programming
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
Component-Based Software Engineering

- CBSE methodology is an emerging approach to software development
  - Both in research and in practical application
  - Especially popular in business and internet areas

- Addresses software complexity issues

- Increases software productivity
Motivation: For Library Developers

- People want to use your software, but need wrappers in languages you don’t support
  - Many component models provide language interoperability

- Discussions about standardizing interfaces are often sidetracked into implementation issues
  - Components separate interfaces from implementation

- You want users to stick to your published interface and prevent them from stumbling (prying) into the implementation details
  - Most component models actively enforce the separation
Motivation: For Application Developers and Users

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

• No universally accepted definition in computer science research …yet

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

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

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

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

• These standards **define**…
  – The rights and responsibilities of a **component**
  – How components express their **interfaces**
  – The environment in which are composed to form an application and executed (**framework**) 
  – The rights and responsibilities of the framework
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...
Application 3...

- Driver
  - GoPort
  - IntegratorPort

- MidpointIntegrator
  - IntegratorPort
  - FunctionPort

- MonteCarloIntegrator
  - IntegratorPort
  - FunctionPort
  - RandomGeneratorPort

- NonlinearFunction
  - FunctionPort

- LinearFunction
  - FunctionPort

- PiFunction
  - FunctionPort
  - RandomGeneratorPort

- RandomGenerator
And Many More…

Dashed lines indicate alternate connections

Create different applications in "plug-and-play" fashion
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
Domain-Specific Frameworks vs Generic Component Architectures

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

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

- Interfaces define how components interact…
- Therefore interfaces are key to interoperability and reuse of components

- In many cases, “any old interface” will do, but…
- Achieving reuse across multiple applications requires agreement on the same interface for all of them

- “Standard” or “community” interfaces facilitate reuse and interoperability
  - Typically domain specific
  - Formality of “standards” process varies
  - Significant initial investment for long-term payback

More about community interface development efforts in “Applications” module
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?
Commodity Component Models

- CORBA Component Model (CCM), COM, Enterprise JavaBeans
  - Arise from business/internet software world

- Componentization requirements can be high
- Can impose significant performance overheads
- No recognition of tightly-coupled parallelism
- May be platform specific
- May have language constraints
- May not support common scientific data types
What is the CCA?

- CCA is a *specification* of a component environment designed for *high performance scientific computing*
  - Specification is decided by the CCA Forum
    - CCA Forum membership open to all
  - “CCA-compliant” just means conforming to the specification
    - Doesn’t require using any of our code!

- A *tool* to enhance the productivity of scientific programmers
  - Make the hard things easier, make some intractable things tractable
  - Support & promote reuse & interoperability
  - Not a magic bullet
CCA Philosophy and Objectives

• Local and remote components
  – Support local, HPC parallel, and distributed computing

• High Performance
  – Design should support high-performance mechanisms wherever possible (i.e. minimize copies, extra communications, extra synchronization)
  – Support SPMD and MPMD parallelism
  – Allow user to chose parallel programming models

• Heterogeneity
  – Multiple architectures, languages, run-time systems used simultaneously in an application

• Integration
  – Components should be easy to make and easy to use

• Openness and simplicity
  – CCA spec should be open & usable with open software
CCA Concepts: Components

- Components provide/use one or more **ports**
  - A component with no ports isn’t very interesting

- Components include some **code which interacts with a CCA framework**
CCA Concepts: Ports

- Components interact through well-defined *interfaces*, or *ports*
  - In OO languages, a port is a *class* or *interface*
  - In Fortran, a port is a bunch of subroutines or a *module*

- Components may *provide* ports – *implement* the class or subroutines of the port ("Provides" Port)

- Components may *use* ports – *call* methods or subroutines in the port ("Uses" Port)

- Links between ports denote a procedural (caller/callee) relationship, *not* *dataflow!*
  - e.g., FunctionPort could contain: *evaluate*(in Arg, out Result)
CCA Concepts: Frameworks

• The framework provides the means to “hold” components and compose them into applications

• Frameworks allow connection of ports without exposing component implementation details

• Frameworks provide a small set of standard services to components

• *Currently*: specific frameworks support specific computing models (parallel, distributed, etc.)

• *Future*: full flexibility through integration or interoperation
Writing Components

• Components…
  – Inherit from `gov.cca.Component`
    • Implement `setServices` method to register ports this component will *provide* and *use*
  – Implement the ports they provide
  – Use ports on other components
    • `getPort`/`releasePort` from framework `Services` object

• Interfaces (ports) extend `gov.cca.Port`

*Full details in the hands-on!*
Adapting Existing Code into Components

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

1. Decide **level of componentization**
   - Can evolve with time (start with coarse components, later refine into smaller ones)

2. Define **interfaces** and write wrappers between them and existing code

3. Add **framework interaction code** for each component
   - setServices

4. Modify component internals to use **other components** as appropriate
   - getPort, releasePort and method invocations

Example in the hands-on!
Writing Frameworks

- There is no reason for most people to write frameworks – just use the existing ones!

- Frameworks must provide certain ports…
  - ConnectionEventService
    - Informs the component of connections
  - AbstractFramework
    - Allows the component to behave as a framework
  - BuilderService
    - Instantiate components & connect ports
  - ComponentRepository
    - A default place where components are found

- Frameworks must be able to load components
  - Typically shared object libraries, can be statically linked

- Frameworks must provide a way to compose applications from components
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
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.
    \[
    \text{sum} = \text{sum} + \text{function->evaluate}(x)
    \]
- **Release** port

**Diagram:**
- Framework interaction code
  - CCA.Services
    - uses FunctionPort
      (connected to NonlinearFunction FunctionPort), ...
  - Integrator code
    - MonteCarloIntegrator
CCA Supports Local, Parallel and Distributed Computing

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

- Distributed computing has same uses/provides pattern, but framework intervenes between user and provider
  - Framework provides a proxy provides port local to the uses port
  - Framework conveys invocation from proxy to actual provides port
CCA Concepts: “Direct Connection” Maintains Local Performance

- Calls *between* components equivalent to a C++ virtual function call: lookup function location, invoke it
  - Cost equivalent of ~2.8 F77 or C function calls
  - ~48 ns vs 17 ns on 500 MHz Pentium III Linux box

- Language interoperability can impose additional overheads
  - Some arguments require conversion
  - Costs vary, but small for typical scientific computing needs

- Calls *within* components have no CCA-imposed overhead

- Implications
  - Be aware of costs
  - Design so inter-component calls do enough work that overhead is negligible

More about performance in the “Applications” module
CCA Concepts: Framework Stays “Out of the Way” of Component Parallelism

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

Components: Blue, Green, Red
Framework: Gray

MCMD/MPMD also supported
Other component models ignore parallelism entirely
“Multiple-Component Multiple-Data” Applications in CCA

• Simulation composed of multiple SCMD sub-tasks

• Usage Scenarios:
  – Model coupling (e.g. Atmosphere/Ocean)
  – General multi-physics applications
  – Software licensing issues

• Approaches
  – Run single parallel framework
    • Driver component that partitions processes and builds rest of application as appropriate (through BuilderService)
  – Run multiple parallel frameworks
    • Link through specialized communications components (e.g. MxN)
    • Link as components (through AbstractFramework service; highly experimental at present)
MCMD Within A Single Framework

Working examples available using Ccaffeine framework, with driver coded in Python.

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

Group A
Group B
CCA Concepts: Language Interoperability

- Existing language interoperability approaches are "point-to-point" solutions
- **Babel** provides a unified approach in which all languages are considered peers
- Babel used primarily at interfaces

*Babel presentation coming up!*

Few other component models support all languages and data types important for scientific computing
Advanced CCA Concepts

- Components are peers
  - Application architecture determines relationships, not CCA specification

- Frameworks provide a **BuilderService** which allows programmatic composition of components

- Frameworks may present themselves as components to other frameworks

- A “traditional” application can treat a CCA framework as a library

- **Meta-component models** enable bridging between CCA components and other component(-like) environments
  - e.g. SCIRun Dataflow, Visualization Toolkit (VTK), …

No time to go into detail on these, but ask us for more info after the tutorial
What the CCA isn’t…

• CCA doesn’t specify who owns “main”
  – CCA components are peers
  – Up to application to define component relationships
    • “Driver component” is a common design pattern

• CCA doesn’t specify a parallel programming environment
  – Choose your favorite
  – Mix multiple tools in a single application

• CCA doesn’t specify I/O
  – But it gives you the infrastructure to create I/O components
  – Use of stdio may be problematic in mixed language env.

• CCA doesn’t specify interfaces
  – But it gives you the infrastructure to define and enforce them
  – CCA Forum supports & promotes “standard” interface efforts

• CCA doesn’t require (but does support) separation of algorithms/physics from data
  – Generic programming
What the CCA is…

- CCA is a specification for a component environment
  - Fundamentally, a design pattern
  - Multiple “reference” implementations exist
  - Being used by applications

- CCA is designed for interoperability
  - Components within a CCA environment
  - CCA environment with other tools, libraries, and frameworks

- CCA provides an environment in which domain-specific application frameworks can be built
  - While retaining opportunities for software reuse at multiple levels
Concept Review

• **Ports**
  – Interfaces between components
  – Uses/provides model

• **Framework**
  – Allows assembly of components into applications

• **Direct Connection**
  – Maintain performance of local inter-component calls

• **Parallelism**
  – Framework stays out of the way of parallel components

• **Language Interoperability**
  – Babel, Scientific Interface Definition Language (SIDL)
Distributed Computing with the CCA

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http://www.cca-forum.org/tutorials/
tutorial-wg@cca-forum.org
Component Composition

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

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

Remote Invocation
• Need global pointers and not local pointers
• Invoke methods across machine boundaries
• Need global namespace for names of components and services
• Mechanism for implementing remote method invocation (RMI)
• Introspection mechanisms to allow ports and services to be discovered and accessed
CCA Concepts that Influence Design of Distributed Frameworks (1)

- **Ports**
  - References to *provides* ports can move across address spaces
  - *Uses* ports are local to each component

- **Services Object** is present in each component
  - Manages all the ports
  - Hides details of framework-specific bindings for ports

- **ComponentID**: opaque handle to the component
  - Should be *serializable* and *deserializable*
  - Usually points to the *services* object
CCA Concepts that Influence Design of Distributed Frameworks (2)

• Builder Service: charged with following operations
  – Create Components in remote address spaces
    • Return a ComponentID of instantiated components
    • Hide details of heterogeneous remote environments
  – Connect ports of components
    • Facilitate connection between uses and provides ports
      – Only if they are of the same SIDL type
    • Place provides port reference in the uses port table

• Introspection
  – Allow remote querying of a component
    • How many and what type of ports does the component have?
Key Design Choices for Distributed CCA Frameworks (1)

• How is the CCA ComponentID represented in a distributed environment?
  – Handle that can be passed to remote components
  – Serialize and deserialize ComponentID
  – Belong to a namespace understood in the entire framework
  – Should enable optimized communication for co-located components

• How is the PortType represented?
  – Provides port should be designed as a remote service
  – Uses port should be a local object
Key Design Choices for Distributed CCA Frameworks (2)

• Where can the key CCA functions be called from? Are they remote or local?
  – `getPort()` call on the services object
    • Should return a remote reference for provides ports
    • Note that the same call in the Ccaffeine framework returns a local object
  – Details of remote and local calls should be hidden
    • Framework should internally distinguish local and remote calls

• How can components be connected?
  – Need internal mechanism for uses port to obtain remote reference of the provides port
    • Information can be stored in a central table, facilitate development of GUIs to show component assembly
    • Distributed across components so they are aware of who they are connected to
Key Design Choices for Distributed CCA Frameworks (3)

• Should Builder Service be centralized or distributed?
  – A component can have its own builder service if
    • The builder service is lightweight
    • The components has special create/connect requirements
Current CCA Distributed Frameworks

- SCIRun2
  - University of Utah

- LegionCCA
  - Binghamton University - State University of New York (SUNY)

- XCAT (Java and C++)
  - Indiana University and Binghamton University

- DCA
  - Indiana University
  - A research framework for MXN

- Frameworks address the design questions in different ways
  - Each has a different set of capabilities
  - Specialized for different kinds of applications
SCIRun2

**Remote Method Invocation (RMI)**
- Allows distributed components to interact through normal mechanisms
- Components in the same address space incur no additional overhead
- Based on a C++ in-house SIDL compiler
  - Currently not based on Babel

**Remote creation of distributed components**
- A distributed CCA framework uses RMI to coordinate components
- A *slave framework* resides on each remote address space
- Uses *ssh* to start the slave framework
- CCA BuilderService communicates with *master framework* which coordinates *slave frameworks*
SCIRun2

- Support for distributed and parallel components
  - Able to launch MPI–parallel components
    - Parallel components interact with other parallel components (on different machines) through **Parallel Remote Method Invocation (PRMI)**
    - Each MPI process may contain multiple threads
      - Increases concurrency and efficiency in the face of a large parallel invocation load
Architecture of Distributed SCIRun2

SCIRun2 Framework (Master Framework)

Component Loader (Slave Framework)

Component

Provides Ports

Component Code (User)

Component Code (PIDL-Generated)

Uses Ports

Service Object

Component Loader (Slave Framework)

Component

Provides Ports

Component Code (User)

Component Code (PIDL-Generated)

Uses Ports

Service Object

Builder Service

PRMI

Connection Table
(Referencing remote Components)

Component ID Table
(Referencing remote provides ports)
SCIRun2 Meta-Component Model

- In the same way that components plug into a CCA framework, component models (such as CCA) plug into SCIRun2
- Allows components of several different families to be used together
- Currently supports: CCA (Babel), SCIRun Dataflow, Visualization Toolkit (Vtk); others coming…
- Bridging between components of different models is semi-automatic; current research is defining a more automatic form of bridging
LegionCCA

- Legion is a collection of software services for the Grid
  - Provides illusion of a virtual machine for geographically-distributed resources

- LegionCCA: models CCA components as Legion objects

- Component Communication
  - Uses Legion’s built-in RPC mechanisms, based on Unix sockets

- ComponentID: based on Legion LOID
  - LOID: globally unique object id

- Component Connections:
  - Information distributed across components
  - Tables can be dynamically updated as connections are made and broken
Anatomy of a Legion CCA Component

CCA
Common Component Architecture

Legion Library

CCALegion Library

Connection Table
Component-Specific Code
ComponentID

Services Object
ProvidesPortsTable
UsesPortsTable
Registration and Discovery Service
Builder Service

Legion Context Space
Connection Table
getProvidesPorts()
contextLookup()
addContextName()
createObject()
destroyObject()

Legion Object Space
ComponentID
Object Proxy, LOID’s, binding, messaging, etc.

Remote Invocations, Calls to remote ports

Interface defined in the CCA Specification
XCAT-Java

• Uses XSOAP for remote invocations
  – XSOAP: implementation of the SOAP protocol from Indiana University
  – ComponentID: uses the XSOAP remote reference
    • An XML document that has a subset of WSDL features

• Remote and Local Access to CCA functions
  – Services object implements different interfaces for local and remote calls

• Component Connections
  – Uses an event mechanism to propagate connection information

• Builder Service
  – Each component has a builder service
  – Creation can currently be done via GRAM or ssh
    • GRAM: Grid Resource Allocation and Management
XCAT-C++

- **Remote Method Invocation**
  - Uses the *Proteus* multi-protocol library for remote communication
    - Proteus supports both messaging and RMI models
    - Currently supports two protocols: binary and SOAP
  - Stub-Skeleton generation is based on WSDLPull
    - A toolkit for parsing WSDL (Web Service Description Language)
  - Support for SIDL will be provided via BabelRMI
    - BabelRMI: Currently in the research phase

- **Remote creation of distributed components**
  - Each component has a BuilderService
  - Creation can be based on GRAM or ssh
Architecture of an XCAT-C++ Component
Proteus: Multi-Protocol Library

- One protocol does not suit all applications
- Proteus provides single-protocol abstraction to components
  - Allows users to dynamically switch between protocols
    - Example: RMI A and RMI B, in the picture
  - Facilitates use of specialized implementations of serialization and deserialization
Babel RMI

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

Research!
CCA Applications

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
Overview

- Examples (scientific) of increasing complexity
  - Laplace equation
  - Time-dependent heat equation
  - Nonlinear reaction-diffusion system
  - Quantum chemistry
  - Climate simulation

- Tools
  - MxN parallel data redistribution
  - Performance measurement, modeling and scalability studies

- Community efforts & interface development
  - TSTT Mesh Interface effort
  - CCTTSS’s Data Object Interface effort
Laplace Equation

\[ \nabla^2 \varphi(x,y) = 0 \in [0,1] \times [0,1] \]
\[ \varphi(0,y) = 0 \quad \varphi(1,y) = \sin(2\pi y) \]
\[ \frac{\delta \varphi}{\delta y}(x,0) = \frac{\delta \varphi}{\delta y}(x,1) = 0 \]
Laplace Equation with Components

- **The Driver Component**
  - Responsible for the overall application flow
  - Initializes the mesh, discretization, solver and visualization components
  - Sets the physics parameters and boundary condition information
Laplace Equation with Components

- The Driver
  - Responsible for the overall application flow
  - Initializes the mesh, discretization, solver and visualization components
  - Sets the physics parameters and boundary condition information

- The Mesh Component
  - Provides geometry, topology, and boundary information
  - Provides the ability to attach user-defined data as tags to mesh entities
  - Is used by the driver, discretization and visualization components
Laplace Equation with Components

- The Driver
  - Responsible for the overall application flow
  - Initializes the mesh, discretization, solver and visualization components
  - Sets the physics parameters and boundary condition information

- The Mesh
  - Provides geometry and topology information
  - Provides the ability to attach user defined data to mesh entities
  - Is used by the driver, discretization and visualization components

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

- **The Driver**
  - Responsible for the overall application flow
  - Initializes the mesh, discretization, solver and visualization components
  - Sets the physics parameters and boundary condition information

- **The Mesh**
  - Provides geometry and topology information
  - Provides the ability to attach user defined data to mesh entities
  - Is used by the driver, discretization and visualization components

- **The Discretization**
  - Provides a finite element discretization of basic operators (gradient, laplacian, scalar terms)
  - Provides mechanisms for general Dirichlet and Neumann boundary condition manipulations

- **The Solver Component**
  - Provides access to vector and matrix operations (e.g., create, destroy, get, set)
  - Provides a “solve” functionality for a linear operator
Laplace Equation with Components

- The Driver
  - Responsible for the overall application flow
  - Initializes the mesh, discretization, solver and visualization components
  - Sets the physics parameters and boundary condition information

- The Mesh
  - Provides geometry and topology information
  - Provides the ability to attach user defined data to mesh entities
  - Is used by the driver, discretization and visualization components

- The Discretization Component
  - Provides a finite element discretization of basic operators (gradient, laplacian, scalar terms)
  - Provides mechanisms for general Dirichlet and Neumann boundary condition manipulations
  - Computes

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

- The Visualization Component
  - Uses the mesh component to print a vtk file of \( \phi \) on the unstructured triangular mesh
  - Assumes user data is attached to mesh vertex entities
**Time-Dependent Heat Equation**

\[
\frac{\partial \phi}{\partial t} = \nabla^2 \phi \ (x,y,t) \in [0,1] \times [0,1]
\]

\[
\phi(0,y,t)=0 \quad \phi(1,y,t)=.5\sin(2\pi y)\cos(t/2)
\]

\[
\frac{\partial \phi}{\partial y}(x,0) = \frac{\partial \phi}{\partial y}(x,1) = 0
\]

\[
\phi(x,y,0)=\sin(.5\pi x) \sin (2\pi y)
\]
Some things change…

- Requires a time integration component
  - Based on the LSODE library
- Uses a new visualization component
  - Based on AVS
  - Requires an MxN data redistribution component
- The MxN redistribution component requires a Distributed Array Descriptor component
  - Similar to HPF arrays
- The driver component changes to accommodate the new physics
... and some things stay the same

- The mesh component doesn’t change
- The discretization component doesn’t change
- The solver component doesn’t change
  - What we use from the solver component changes
  - Only vectors are needed
Heat Equation Wiring Diagram

CCA
Common Component Architecture

Reused
Integration
Visualization
Driver/Physics
What did this exercise teach us?

• Easy to incorporate the functionalities of components developed at other labs and institutions given a well-defined interface.
  – In fact, some components (one uses and one provides) were developed simultaneously across the country from each other after the definition of a header file.
  – Amazingly enough, they usually “just worked” when linked together (and debugged individually).

• In this case, the complexity of the component-based approach was higher than the original code complexity.
  – Partially due to the simplicity of this example
  – Partially due to the limitations of the some of the current implementations of components
Nonlinear Reaction-Diffusion Equation

- Flame Approximation
  - $\text{H}_2$-Air mixture; ignition via 3 hot-spots
  - 9-species, 19 reactions, stiff chemistry
- Governing equation
  $\frac{\partial Y_i}{\partial t} = \nabla \cdot \alpha \nabla Y_i + \dot{w}_i$
- Domain
  - 1cm X 1cm domain
  - 100x100 coarse mesh
  - finest mesh = 12.5 micron.
- Timescales
  - $O(10\text{ns})$ to $O(10\text{ microseconds})$
Numerical Solution

- Adaptive Mesh Refinement: GrACE
- Stiff integrator: CVODE
- Diffusive integrator: $2^{nd}$ Order Runge Kutta
- Chemical Rates: legacy f77 code
- Diffusion Coefficients: legacy f77 code
- New code less than 10%
Reaction-Diffusion Wiring Diagram
Evolution of the Solution

Temperature

0 ms.

0.4 ms

1 ms

OH Profile

Temperature (K)
The need for AMR

- $\text{H}_2\text{O}_2$ chemical subspecies profile
  - Only 100 microns thick (about 10 fine level cells)
  - Not resolvable on coarsest mesh
Unconstrained Minimization Problem

- Given a rectangular 2-dimensional domain and boundary values along the edges of the domain
- Find the surface with minimal area that satisfies the boundary conditions, i.e., compute
  \[ \min f(x), \text{ where } f: \mathbb{R} \to \mathbb{R} \]
- Solve using optimization components based on TAO (ANL)
Unconstrained Minimization Using a Structured Mesh
Computational Chemistry: Molecular Optimization

- **Investigators:** Yuri Alexeev (PNNL), Steve Benson (ANL), Curtis Janssen (SNL), Joe Kenny (SNL), Manoj Krishnan (PNNL), Lois McInnes (ANL), Jarek Nieplocha (PNNL), Jason Sarich (ANL), Theresa Windus (PNNL)

- **Goals:** Demonstrate interoperability among software packages, develop experience with large existing code bases, seed interest in chemistry domain

- **Problem Domain:** Optimization of molecular structures using quantum chemical methods
Molecular Optimization Overview

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

Components in gray can be swapped in to create new applications with different capabilities.
Wiring Diagram for Molecular Optimization

- Electronic structures components:
  - MPQC (SNL)  
    http://aros.ca.sandia.gov/~cljanss/mpqc
  - NWChem (PNNL)  
    http://www.emsl.pnl.gov/pub/docs/nwchem

- Optimization components: TAO (ANL)  
  http://www.mcs.anl.gov/tao

- Linear algebra components:
  - Global Arrays (PNNL)  
  - PETSc (ANL)  
    http://www.mcs.anl.gov/petsc
## Actual Improvements

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<th>Molecule</th>
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<th>MPQC</th>
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<td>Cholesterol</td>
<td>33</td>
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<td>27</td>
<td>30</td>
</tr>
</tbody>
</table>

**Function and gradient evaluations**
Componentized Climate Simulations

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

- **Climate Component:**
  - Schedule component coupling
  - Data flow is via pointer NOT data copy.
  - All components in C++; run in CCAFFEINE.
- **Multiple ocean models with the same interface**
  - Can be selected by a user at runtime
Simulation Results

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

...changes a field variable (e.g., wind) in the atmosphere!
Concurrency At Multiple Granularities

- Certain simulations need multi-granular concurrency
  - Multiple Component Multiple Data, multi-model runs

- Usage Scenarios:
  - Model coupling (e.g. Atmosphere/Ocean)
  - General multi-physics applications
  - Software licensing issues

- Approaches
  - Run single parallel framework
    - Driver component that partitions processes and builds rest of application as appropriate (through BuilderService)
  - Run multiple parallel frameworks
    - Link through specialized communications components (e.g. MxN)
    - Link as components (through AbstractFramework service; highly experimental at present)
Componentizing your own application

• The key step: think about the decomposition strategy
  – By physics module?
  – Along numerical solver functionality?
  – Are there tools that already exist for certain pieces? (solvers, integrators, meshes?)
  – Are there common interfaces that already exist for certain pieces?
  – Be mindful of the level of granularity

• Decouple the application into pieces
  – Can be a painful, time-consuming process

• Incorporate CCA-compliance

• Compose your new component application

• Enjoy!
Overview

- Examples (scientific) of increasing complexity
  - Laplace equation
  - Time-dependent heat equation
  - Nonlinear reaction-diffusion system
  - Quantum chemistry
  - Climate simulation

- Tools
  - MxN parallel data redistribution
  - Performance measurement, modeling and scalability studies

- Community efforts & interface development
  - TSTT Mesh Interface effort
  - CCTTSS’s Data Object Interface effort
CCA Concepts: MxN Parallel Data Redistribution

- Share Data Among Coupled Parallel Models
  - Disparate Parallel Topologies (M processes vs. N)
  - e.g. Ocean & Atmosphere, Solver & Optimizer…
  - e.g. Visualization (Mx1, increasingly, MxN)

Research area -- tools under development
“MxN” Parallel Data Redistribution: The Problem…

- Create complex scientific simulations by coupling together multiple parallel component models
  - Share data on “M” processors with data on “N”
    - M ≠ N ~ Distinct Resources (Pronounced “M by N”)
  - Model coupling, e.g., climate, solver / optimizer
  - Collecting data for visualization
    - Mx1; increasingly MxN (parallel rendering clusters)

- Define “standard” interface
  - Fundamental operations for any parallel data coupler
    - Full range of synchronization and communication options
Hierarchical MxN Approach

• Basic MxN Parallel Data Exchange
  – Component implementation
  – Initial prototypes based on CUMULVS & PAWS
    • Interface generalizes features of both

• Higher-Level Coupling Functions
  – Time & grid (spatial) interpolation, flux conservation
  – Units conversions…

• “Automatic” MxN Service via Framework
  – Implicit in method invocations, “parallel RMI”

http://www.csm.ornl.gov/cca/mxn/
CCA Delivers Performance

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

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

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

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

Aggregate time for linear solver component in unconstrained minimization problem w/ PETSc
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>
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<tr>
<th>Function arg type</th>
<th>f77</th>
<th>Component</th>
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<td>80 ns</td>
<td>224ns</td>
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<tr>
<td>Complex</td>
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<td>209ns</td>
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<tr>
<td>Double complex</td>
<td>86ns</td>
<td>241ns</td>
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</table>
Parallel Scaling of the QC Simulation

Isoprene HF/6-311G(2df,2pd) Speed-up in MPQC-based Applications

Parallel Scaling of MPQC w/ native and TAO optimizers
Scalability of Scientific Data Components in CFRFS Combustion Applications

- Investigators: S. Lefantzi, J. Ray, and H. Najm (SNL)
- 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

CCA provides a novel means of profiling & modeling component performance

Need to collect incoming inputs and match them up with the corresponding performance but how?
  - Need to “instrument” the code
    • But has to be non-intrusive, since we may not “own” component code

What kind of performance infrastructure can achieve this?
  - Previous research suggests proxies
    • Proxies serve to intercept and forward method calls
“Integrated” Performance Measurement Capability

Measurement infrastructure:

- **Proxy**
  - Notifies MasterMind of all method invocations of a given component, along with performance dependent inputs
  - Generated automatically using PDT

- **MasterMind**
  - Collects and stores all measurement data

- **TAU**
  - Makes all performance measurements
Component Application With Proxies
Overview

- **Examples (scientific) of increasing complexity**
  - Laplace equation
  - Time-dependent heat equation
  - Nonlinear reaction-diffusion system
  - Quantum chemistry
  - Climate simulation

- **Tools**
  - MxN parallel data redistribution
  - Performance measurement, modeling and scalability studies

- **Community efforts & interface development**
  - TSTT Mesh Interface effort
  - CCTTSS’s Data Object Interface effort
Scientific Data Objects & Interfaces

- Define “Standard” Interfaces for HPC Scientific Data
  - Descriptive, Not (Necessarily) Generative…

- Basic Scientific Data Object
  - David Bernholdt, ORNL

- Structured & Unstructured Mesh
  - Lori Freitag, LLNL
  - Collaboration with SciDAC TSTT Center

- Block Structured AMR
  - Phil Colella, LBNL
  - Collaboration with APDEC & TSTT
The Next Level

• Common Interface Specification
  – Provides plug-and-play interchangeability
  – Requires domain specific experts
  – Typically a difficult, time-consuming task
  – A success story: MPI

• A case study… the TSTT/CCA mesh interface
  – TSTT = Terascale Simulation Tools and Technologies (www.tstt-scidac.org)
  – A DOE SciDAC ISIC focusing on meshes and discretization
  – Goal is to enable
    • hybrid solution strategies
    • high order discretization
    • Adaptive techniques
Proliferations of interfaces – the $N^2$ problem

Current Situation

- Public interfaces for numerical libraries are unique
- Many-to-Many couplings require $Many^2$ interfaces
  - Often a heroic effort to understand the inner workings of both codes
  - Not a scalable solution
Common Interface Specification

Reduces the *Many-to-Many* problem to a *Many-to-One* problem

– Allows interchangeability and experimentation

– Challenges

  • Interface agreement
  • Functionality limitations
  • Maintaining performance
TSTT Philosophy

• Create a small set of interfaces that existing packages can support
  – AOMD, CUBIT, Overture, GrACE, …
  – Enable both interchangeability and interoperability
• Balance performance and flexibility
• Work with a large tool provider and application community to ensure applicability
  – Tool providers: TSTT and CCA SciDAC centers
  – Application community: SciDAC and other DOE applications
CCTTSS Research Thrust Areas and Main Working Groups

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

- Complex applications that use components are possible
  - Combustion
  - Chemistry applications
  - Optimization problems
  - Climate simulations
- Component reuse is significant
  - Adaptive Meshes
  - Linear Solvers (PETSc, Trilinos)
  - Distributed Arrays and MxN Redistribution
  - Time Integrators
  - Visualization
- Examples shown here leverage and extend parallel software and interfaces developed at different institutions
  - Including CUMULVS, ESI, GrACE, LSODE, MPICH, PAWS, PETSc, PVM, TAO, Trilinos, TSTT.
- Performance is not significantly affected by component use
- Definition of domain-specific common interfaces is key
Language Interoperable CCA Components via BABEL

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

Legacy codes → Babelized CCA Components

• Introduction To:
  – Babel
  – SIDL

• See Babel in use
  – “Hello World” example

• Babel aspects of writing a CCA component
What I mean by “Language Interoperability”

- **Scripting Driver (Python)**
- **Simulation Framework (C)**
- **Numerical Routines (f77)**
- **Solver Library (C++)**
- **Visualization System (Java)**
- **Callback Handlers (Python)**
One reason why mixing languages is hard

<table>
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<tr>
<td>Chasm</td>
<td></td>
</tr>
<tr>
<td>Platform Dependent</td>
<td>Platform Dependent</td>
</tr>
</tbody>
</table>

Diagram showing interconnections between different programming languages and tools:

- C
- C++
- Java
- Python
- f77
- f90

Arrows indicate conversion or interoperation methods such as SWIG, JNI, Siloon, and Chasm.
Babel makes all supported languages peers

---

This is not a Lowest Common Denominator Solution!

---

Once a library has been “Babelized” it is equally accessible from all supported languages
Babel Module’s Outline

• Introduction

Babel Basics
  – How to use Babel in a “Hello World” Example
  – SIDL Grammar
  – Wrapping legacy code

• Babel aspects of writing a CCA component
Babel’s Two Parts: Code Generator + Runtime Library
greetings.sidl: A Sample SIDL File

package greetings version 1.0 {
  interface Hello {
    void setName( in string name );
    string sayIt ( );
  }
  class English implements=all Hello {
  }
}
Library Developer Does This...

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

```cpp
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)
        }
    }
```
Library User Does This...

1. `babel --client=F90 greetings.sidl`
2. Compile & Link generated Code & Runtime
3. Place DLL in suitable location
program helloclient
    use greetings_English
    implicit none
    type(greetings_English_t) :: obj
    character (len=80) :: msg
    character (len=20) :: name

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

end program helloclient
SIDL Grammar (1/3): Packages and Versions

- Packages can be nested
  ```
  package foo version 0.1 {
    package bar {
      ... 
    }
  }
  ```
- Versioned Packages
  - defined as packages with explicit version number
  - OR packages enclosed by a versioned package
  - Reentrant by default, but can be declared final
  - May contain interfaces, classes, or enums
- Unversioned Packages
  - Can only enclose more packages, not types
  - Must be re-entrant. Cannot be declared final

You’ll use SIDL in the hands-on
SIDL Grammar (2/3): Classes & Interfaces

- SIDL has 3 user-defined objects
  - Interfaces – APIs only, no implementation
  - Abstract Classes – 1 or more methods unimplemented
  - Concrete Classes – All methods are implemented

- Inheritance (like Java/Objective C)
  - Interfaces may extend Interfaces
  - Classes extend no more than one Class
  - Classes can implement multiple Interfaces

- Only concrete classes can be instantiated
SIDL Grammar (3/3): Methods and Arguments

- Methods are **public virtual** by default
  - **static** methods are not associated with an object instance
  - **final** methods can not be overridden

- Arguments have 3 parts
  - Mode: can be **in**, **out**, or **inout** (like CORBA, but semantically different than F90)
  - Type: one of (bool, char, int, long, float, double, fcomplex, dcomplex, array<Type,Dimension>, enum, interface, class)
  - Name
Babelizing Legacy Code

1. Write your SIDL interface
2. Generate server side in your native language
3. Edit Implementation (Impls) to dispatch to your code (Do NOT modify the legacy library itself!)
4. Compile & Link into Library/DLL
Known Projects Using Babel
(see www.llnl.gov/CASC/components/gallery.html for more)

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

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

-- Charlie Crabb, LLNL (conversation)
Babel Module’s Outline

- Introduction
- Babel Basics
  - How to use Babel in a “Hello World” Example
  - SIDL Grammar

Babel aspects of writing a CCA component
How to Write and Use Babelized CCA Components

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

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

```java
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
   --text=xml
2. store XML in a directory
3. Use Babel’s –R option to specify search directories
3. Use Babel to generate the glue code
   - `babel --server=C -Rrepo function.sidl`

4. Add implementation details
Limitations of Babel’s Approach to Language Interoperability

- Babel is a code generator
  - Do obscure tricks no one would do by hand
  - Don’t go beyond published language standards
- Customized compilers / linkers / loaders beyond our scope
  - E.g. icc and gcc currently don’t mix on Linux
  - E.g. No C++-style templates in SIDL. (Would require special linkers/loaders to generate code for template instantiation, like C++ does.)
- Babel makes language interoperability feasible, but not trivial
  - Build tools severely underpowered for portable multi-language codes
Contact Info

• Project:  http://www.llnl.gov/CASC/components
  – Babel: language interoperability tool
  – Alexandria: component repository
  – Quorum: web-based parliamentary system
  – Gauntlet (coming soon): testing framework

• Bug Tracking:  http://www-casc.llnl.gov/bugs

• Project Team Email:  components@llnl.gov

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