

Welcome to the Common Component Architecture Tutorial

SC2005 Tutorial M02 14 November 2005

CCA Forum Tutorial Working Group

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



This work is licensed under a Creative Commons Attribution 2.5 License



Licensing Information

- This tutorial is distributed under the Creative Commons Attribution 2.5 License
 - http://creativecommons.org/licenses/by/2.5/
- In summary, you are free:
 - to copy, distribute, display, and perform the work
 - to make derivative works
 - to make commercial use of the work
- Under the following conditions:
 - Attribution. You must attribute the work in the manner specified by the author or licensor.
- For any reuse or distribution, you must make clear to others the license terms of this work.
- Any of these conditions can be waived if you get permission from the copyright holder.
- Your fair use and other rights are in no way affected by the above.
- Requested reference:
 - CCA Forum Tutorial Working Group, Common Component Architecture Tutorial, 2005, http://www.cca-forum.org/tutorials/

CCA Common Component Architecture						
	Agenda & Table of Contents					
Time	Title	Slide No.	Presenter			
8:30-8:35am	Welcome	1	David Bernholdt, ORNL			
8:35-9:30am	What can Component Technology do for Scientific Computing	5	Boyana Norris, ANL			
	An Intro. to Components & the CCA	16	Boyana Norris, ANL			
9:30-10:00am	CCA Tools	70	Ben Allan, SNL			
10:00-10:30am	Lunch					
10:30-11:10am	Language Interoperable CCA Components with Babel	113	Gary Kumfert, LLNL			
11:10-11:55am	Using CCA: Approaches & Experience	136	David Bernholdt, ORNL			
11:55am-12:00n	Closing	186	David Bernholdt, ORNL			
12:00-1:30pm	Break					
1:30-3:00pm	Hands-On	Hands-On Guide	All			
3:00-3:30pm	Break					
3:30-5:00pm	Hands-On (continued)					
⊗			3			



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



This work is licensed under a Creative Commons Attribution 2.5 License

5



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:

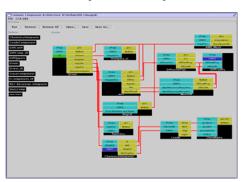
- Components help you think about software in manageable chunks that interact only in well-defined ways
- Components provide a "plug-and-play" environment that allows easy, flexible application assembly

6



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

0



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
- expertise:
 - California chemistry
 - Illinois optimization
 - Washington chemistry, parallel data management
- Effective collaboration with minimal face-to-face interaction



Schematic of CCA-based molecular Geographically distributed 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 N² pairwise interfaces to just N

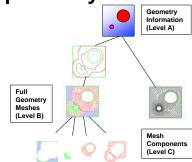


Illustration of geometry domain hierarchy used in TSTT mesh interface.

CCA tools used: Babel (SIDL),

Chasm

Library languages: C, C++, F77, F90 ₁₀



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



solvers

High performance

Library written in C

oriented interfaces

preconditioners and linear

Babel-generated object-

provided in C, C++, Fortran

Examples

LAPACK07

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

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

-- Jeff Painter, LLNL. 2 June 2003

CCA tools used: Babel, Chasm



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

0

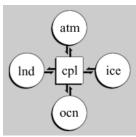
13



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, Babelgenerated bindings for C++, Python
- CCA tools used: Babel, Chasm





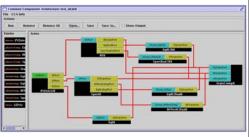
Schematic of CCSM showing coupler managing data exchanges between atmosphere, sea ice, ocean, and land models. (From http://www.ccsm.ucar.edu/models/ccsm3.0/cpl6/)

(6)



Example: Integrated Fusion Simulation

- Proof-of-principle of using CCA for integrated wholedevice modeling needed for the ITER fusion reactor
- Couples radio frequency (RF) heating of plasma with transport modeling
- Coarse-grain encapsulation of preexisting programs
- Follow-on plans for RF, transport, and magnetohydrodynamics



"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

15





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

@

This work is licensed under a Creative Commons Attribution 2.5 License



Goals of This Module

- Introduce basic concepts and vocabulary of component-based software engineering and the CCA
- Highlight the special demands of highperformance scientific computing on component environments
- Give you sufficient understanding of the CCA to begin evaluating whether it would be useful to you

0

17



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 welldefined 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

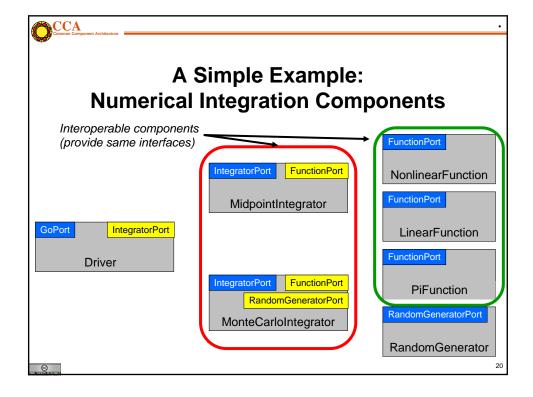
18

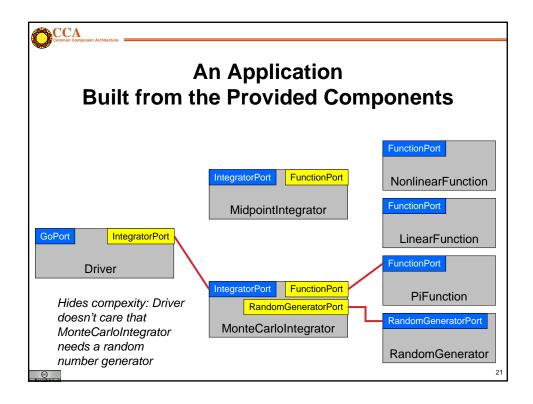


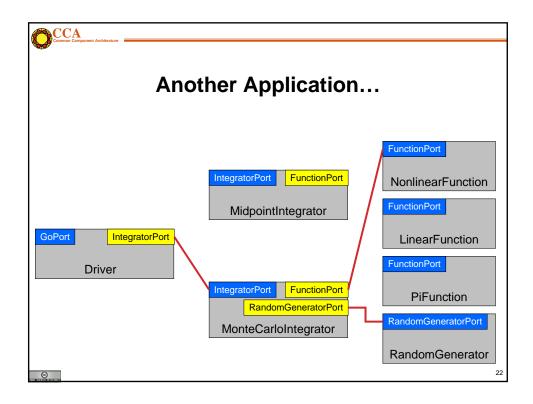
What is a Component Architecture?

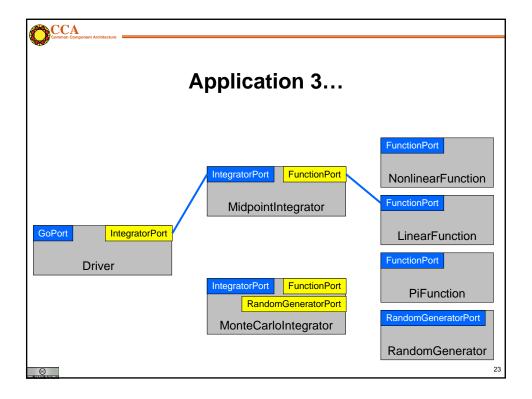
- A set of standards that allows:
 - Multiple groups to write units of software (components)...
 - And have confidence that their components will work with other components written in the same architecture
- These standards define...
 - The rights and responsibilities of a component
 - How components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

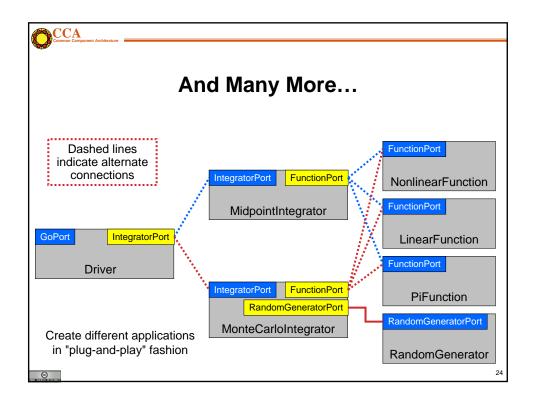
0













Comparison of Application Development Approaches

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

CCA

Be Aware: "Framework" Describes Many Things

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



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

2



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?

0

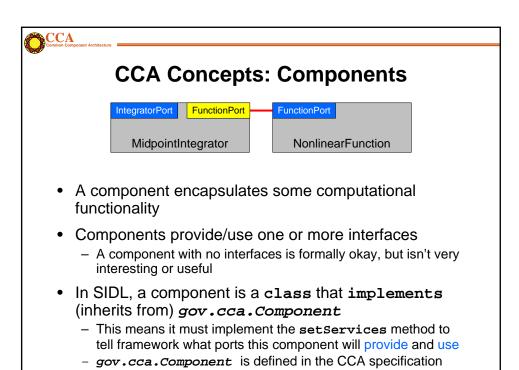
29



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

30



CCA Concepts: Ports

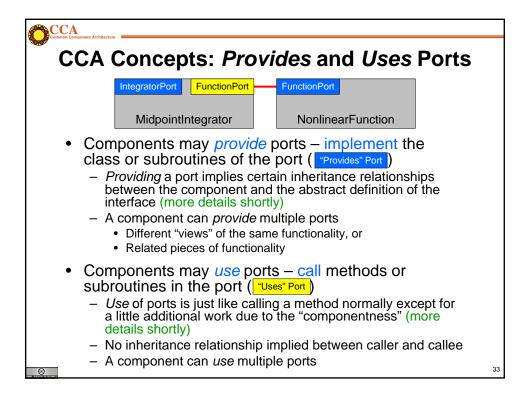
IntegratorPort FunctionPort FunctionPort
MidpointIntegrator NonlinearFunction

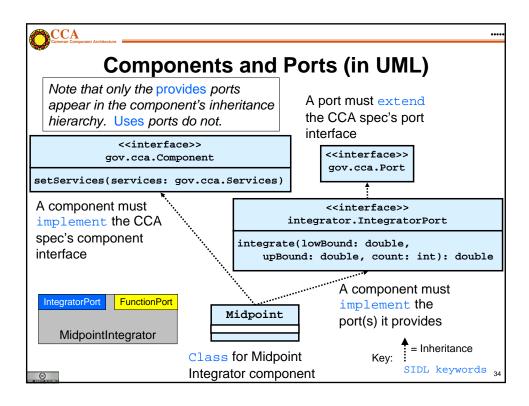
• Components interact through well-defined interfaces, or ports

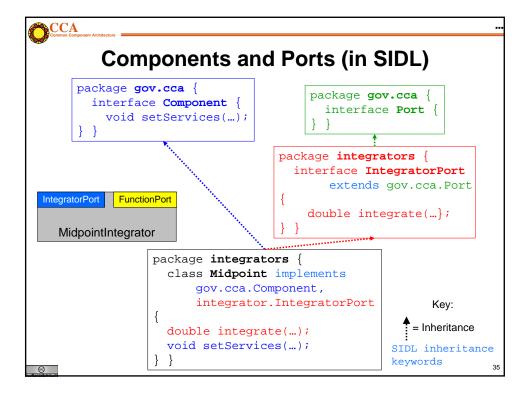
- A port expresses some computational functionality
- In Fortran, a port is a bunch of subroutines or a module
- In OO languages, a port is an abstract class or interface

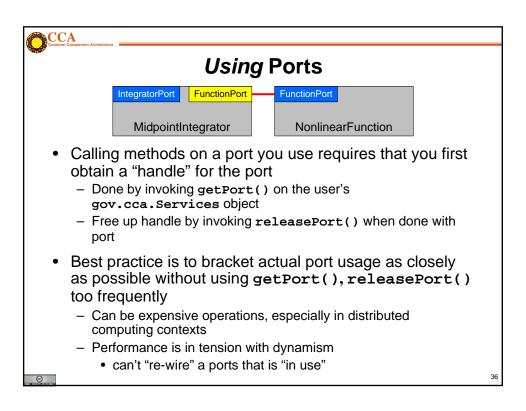
• Ports and connections between them are a procedural (caller/callee) relationship, not dataflow!

- e.g., FunctionPort could contain a method like evaluate(in Arg, out Result) with data flowing both ways











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

0

CCA Overture Interfaces are Key to **NWGrid** Reuse and MOAB Interoperability of Code Mesquite SuperLU Interoperability -- multiple GRUMMP implementations Frontier conforming to the same **FMDB** interface Reuse – ability to use a component in many Overture applications **NWGrid** The larger the community MOAB hypre that agrees to the Mesquite SuperLU TOPS Solver interface, the greater the PETSc **GRUMMP** opportunity for Frontier interoperability and reuse **FMDB**



Interfaces are an Investment

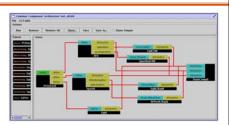
- The larger the community, the greater the time & effort required to obtain agreement
 - Equally true in component and non-component environments
 - MPI 1.0 (well understood at the start) took 8 months, meeting every six weeks
 - MPI 2.0 (not well understood at the start) took 1.5 years, meeting every 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

0

39



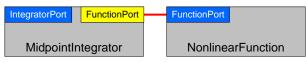
CCA Concepts: Frameworks



- 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

40





- 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

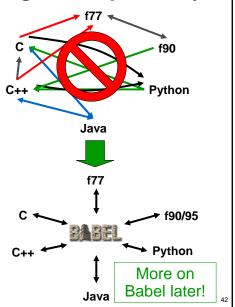
0

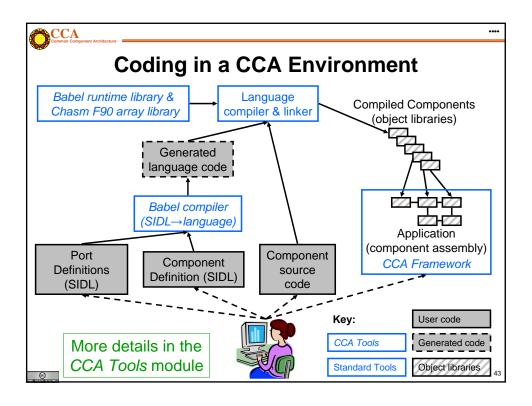
CCA

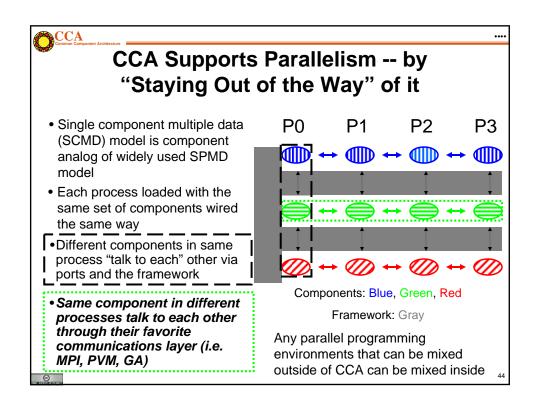
41

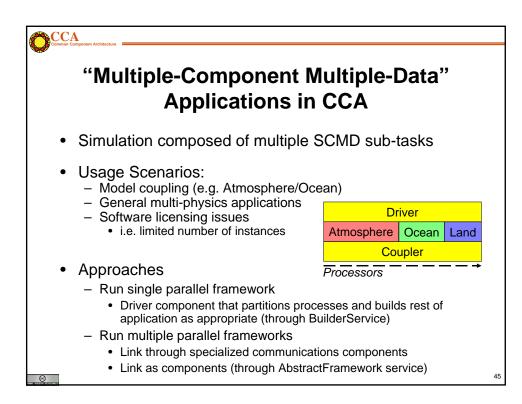
CCA Concepts: Language Interoperability

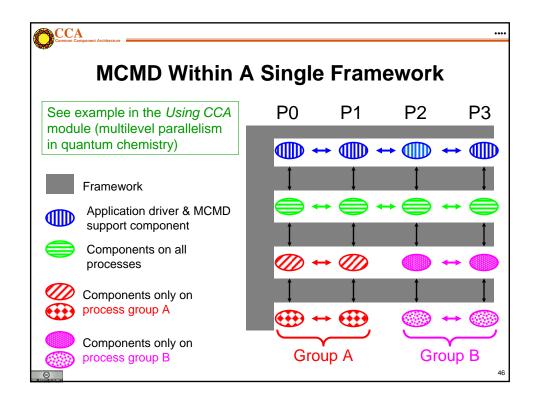
- Scientific software is increasingly diverse in use of programming languages
- In a component environment, users should not care what language a component is implemented in
- "Point-to-point" solutions to language interoperability are not suitable for a component environment
- The Babel language interoperability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

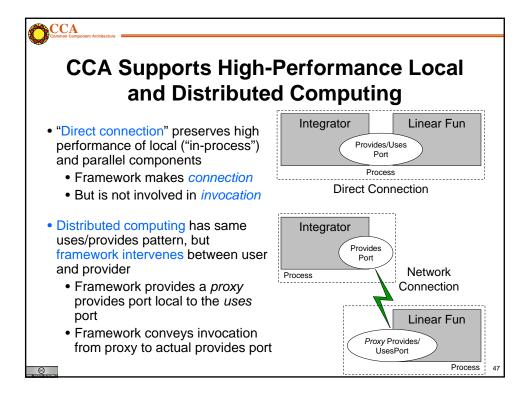








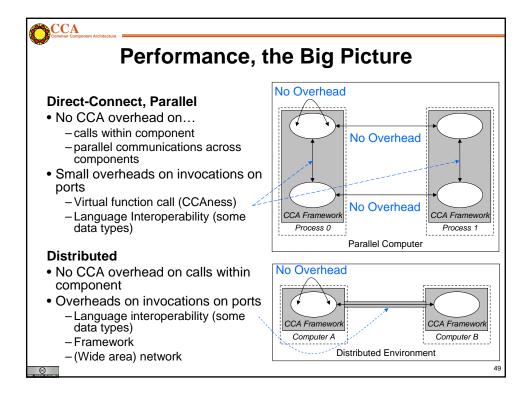






"Direct Connection" Details

- 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





Maintaining HPC Performance

 The performance of your application is as important to us as it is to you

More about performance in notes

- 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



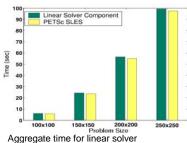
Some Performance Results and References

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



Supplementary material for handouts

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

51

MAN STOCKED OF BUILDING



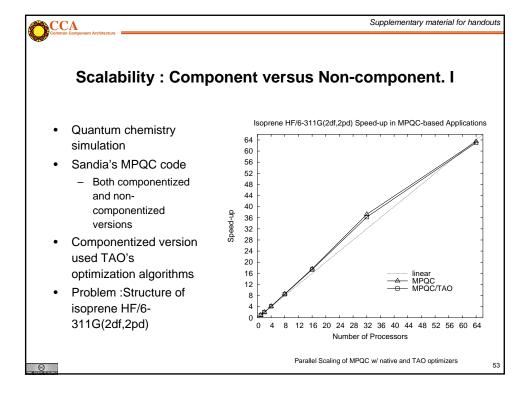
Supplementary material for handouts

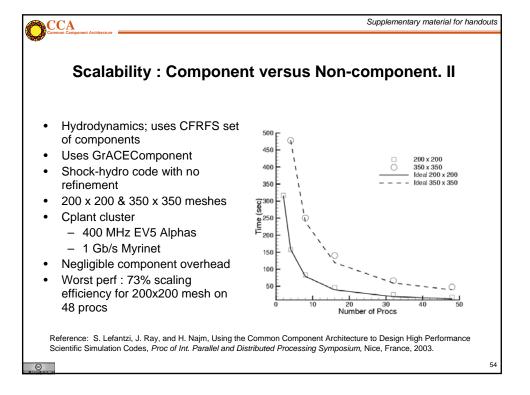
Overhead from Component Invocation

- Invoke a component with different arguments
 - Array
 - Complex
 - Double Complex
- Compare with f77 method invocation
- Environment
 - 500 MHz Pentium III
 - Linux 2.4.18
 - GCC 2.95.4-15
- Components took 3X longer
- Ensure granularity is appropriate!
- Paper by Bernholdt, Elwasif, Kohl and Epperly

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

⊚__







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)

0

55

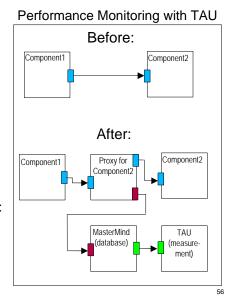


The Proxy Component Pattern

- 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



(6)



Component Lifecycle

Additional material in notes

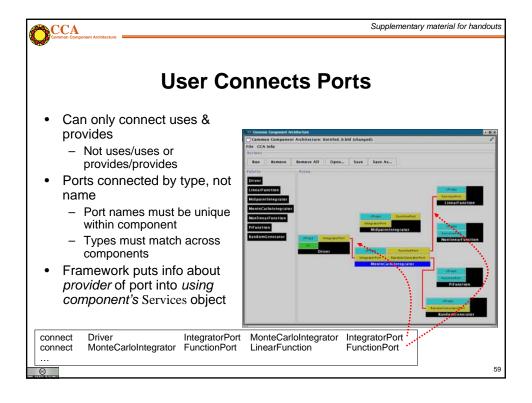
- Composition Phase (assembling application)
 - Component is instantiated in framework
 - Component interfaces are connected appropriately
- Execution Phase (running application)
 - Code in components uses functions provided by another component
- Decomposition Phase (termination of application)
 - Connections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

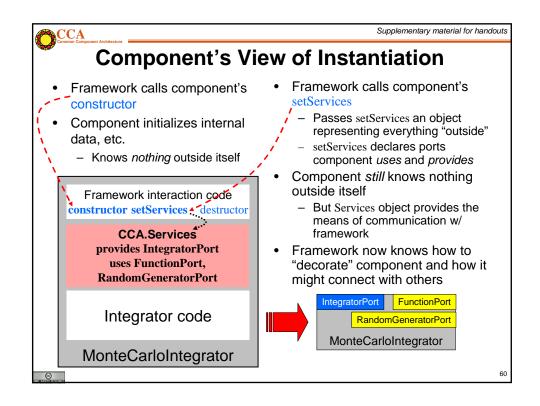
In an application, individual components may be in different phases at different times

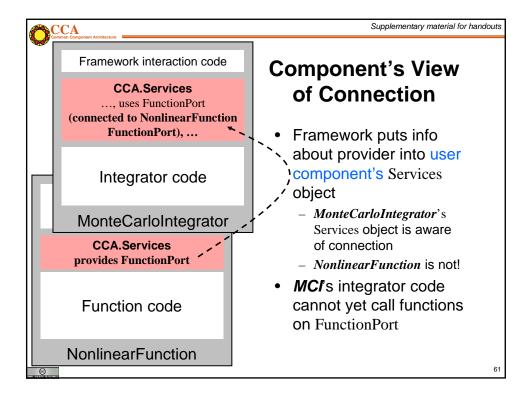
Steps may be under human or software control

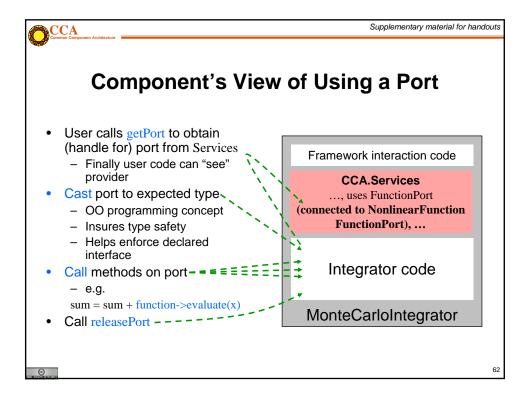
0

Supplementary material for handouts **User Viewpoint: Loading and Instantiating Components** Details are framework-specific! Components are code + metadata Ccaffeine currently provides both Using metadata, a Palette command line and GUI approaches of available components is constructed Components are instantiated by user action (i.e. by dragging from Palette into Arena) Framework calls component's constructo then setServices create Driver create LinearFunction (LinearFunction create MonteCarloIntegrator MonteCarloIntegrator ...











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

(6)

63



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

64



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

⊚

6



CCA is Still Under Development

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

68



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

0

69



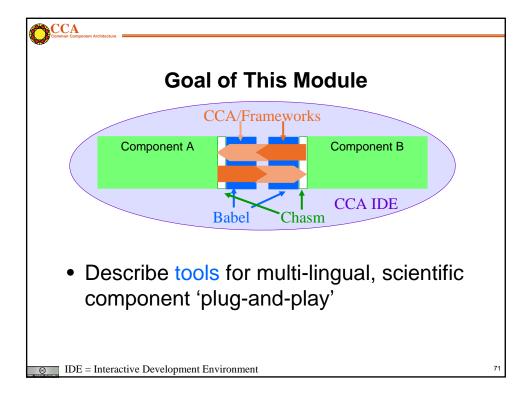
CCA Tools – Language Interoperability and Frameworks

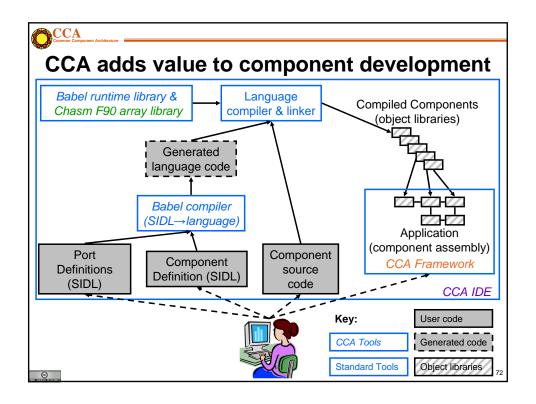
CCA Forum Tutorial Working Group

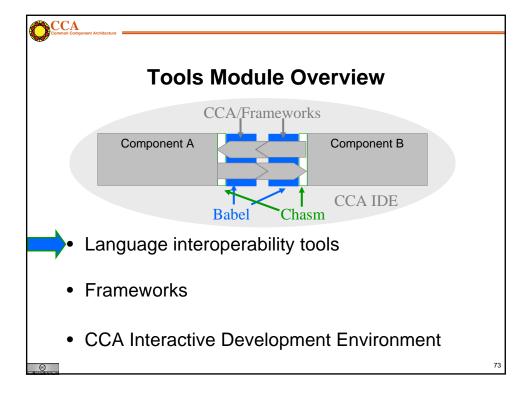
http://www.cca-forum.org/tutorials/ tutorial-wg@cca-forum.org

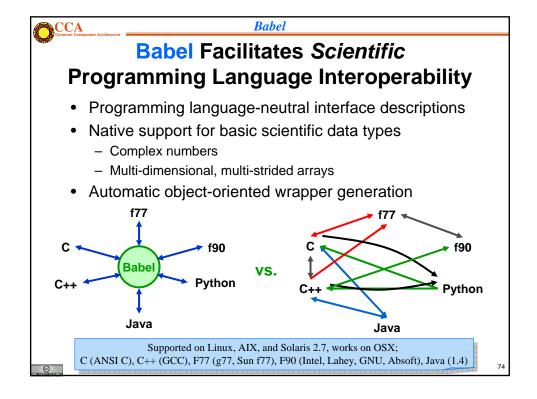
@

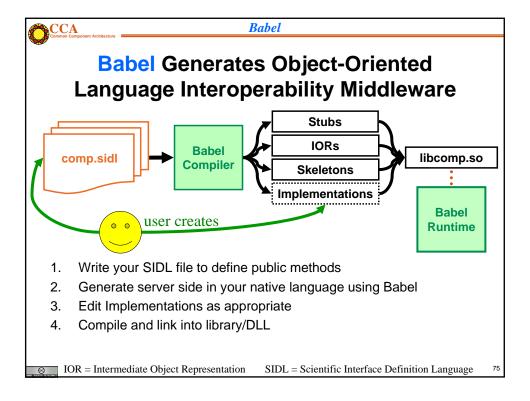
This work is licensed under a Creative Commons Attribution 2.5 License

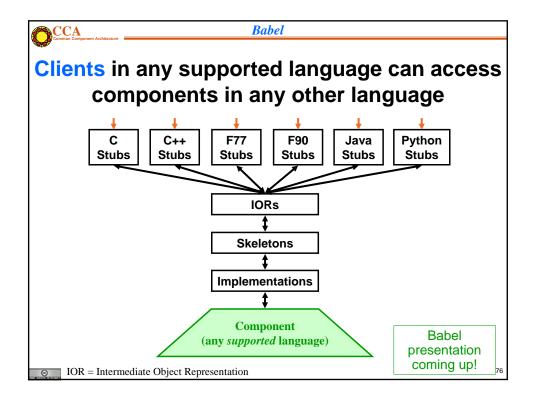














Babel

Supplementary material for notes

Recent and Upcoming Features

- Remote Method Invocation (BabelRMI) ALPHA
- Design-by-Contract ALPHA
- Pre- and post-method invocation hooks ALPHA

0

77



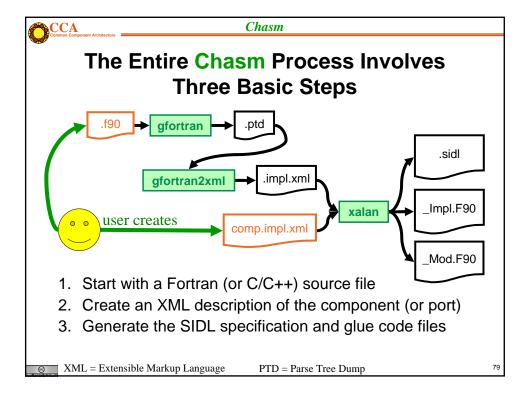
Chasm

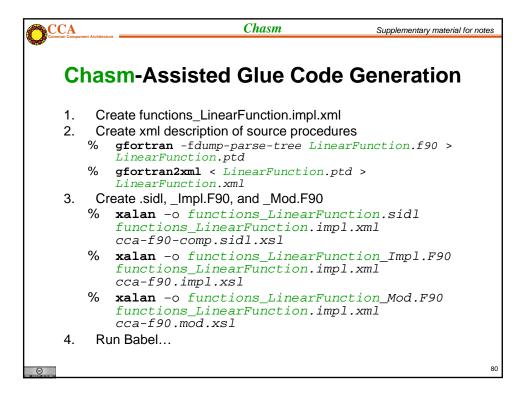
Chasm Provides Language Interoperability for Fortran, C, and C++

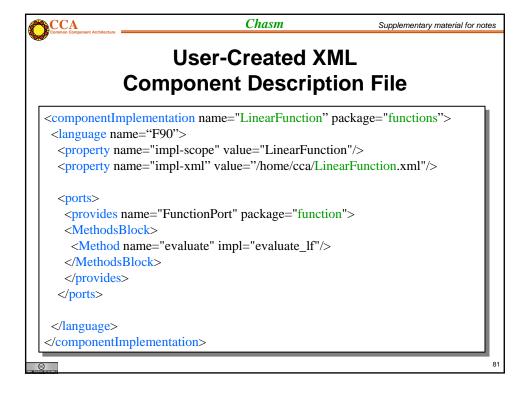
- Extracts interfaces from C/C++ and Fortran90 codes
- Uses library of XSLT stylesheets for language transformations → easily extended
 - Generates XML and SIDL representations
 - Generates Fortran90 Babel implementation glue
- Provides Fortran array descriptor library used by Babel

Supported on Linux, AIX, and Solaris 2.7, works on OSX; C (ANSI C), C++ (GCC), F90 (Intel, Lahey, GNU, Absoft)

0





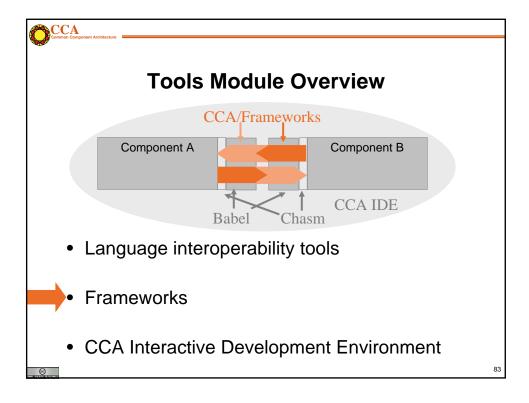


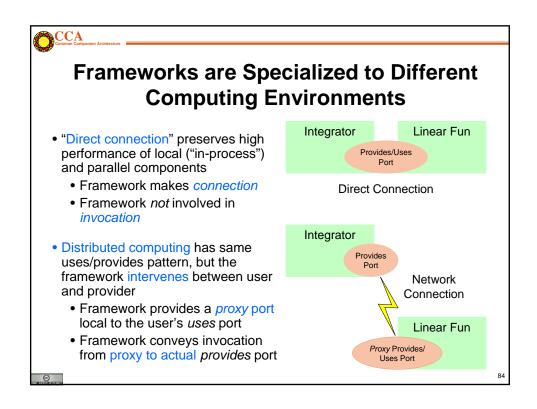
CCA Chasm Supplementary material for notes

Recent and Upcoming Features

- Generate Fortran 2003 MPI Bindings 1Q 2006
- Update XML processor and generator to new PDToolkit releases 1Q 2006

8:







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, SciRUNVisualization: SciRUN

None of these (yet) plug into your favorite Integrated Development Environment (e.g., Eclipse, MS Dev. Studio, Java Studio, ...).

⊚___

A CCA

Ccaffeine Framework

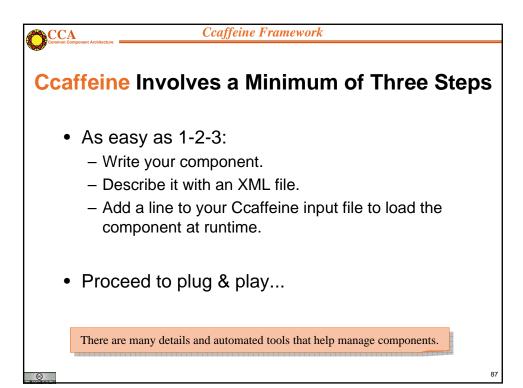
Ccaffeine is a *Direct-Connect*, Parallel-Friendly Framework

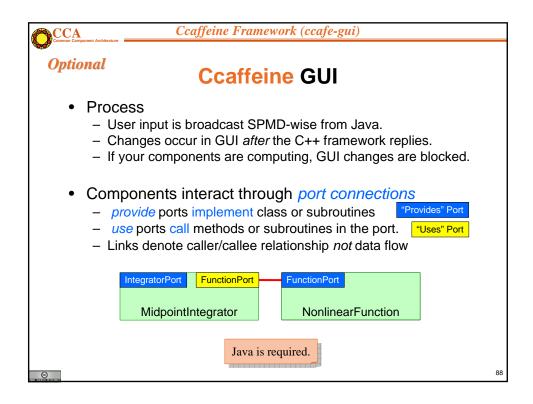
- Supports SIDL/Babel components
 - Conforms to latest CCA specification (0.7)
 - Also supports legacy CCA specification (0.5)
 - Any C++ allowed with C and Fortran by C++ wrappers
- Provides command-line and GUI for composition
 - Scripting supports batch mode for SPMD
 - MPMD/SPMD custom drivers in any Babel language

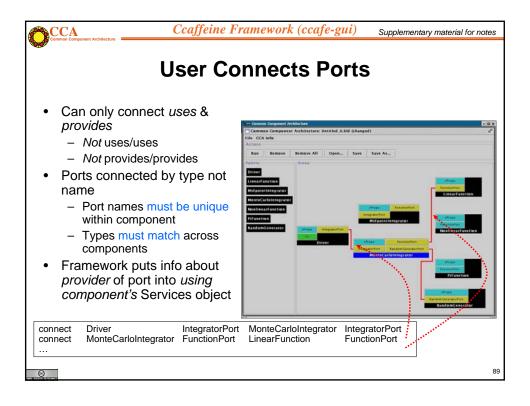
Supported on Linux, AIX, OSX and is portable to modern UNIXes.

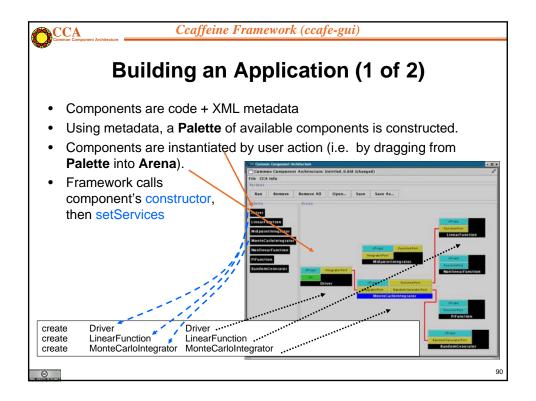
86

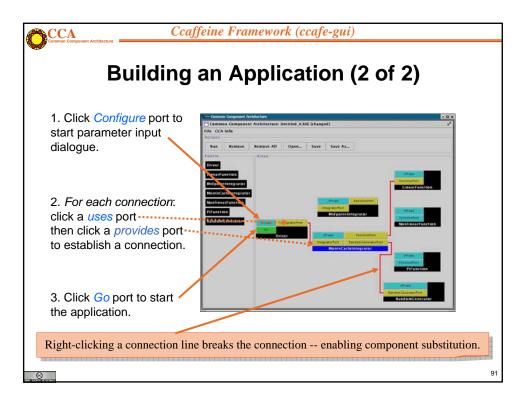
@

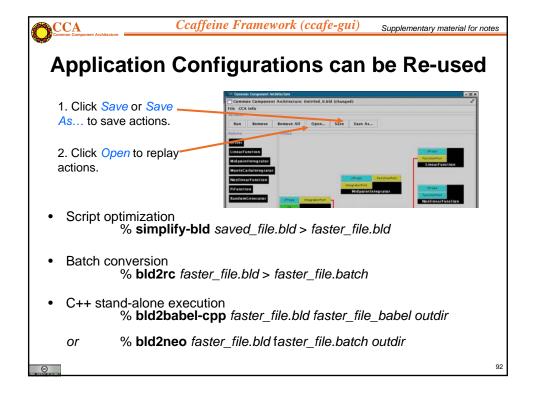














Ccaffeine Framework

Supplementary material for notes

Recent and Upcoming Features

- Interoperate with other CCA frameworks
 - Via Babel RMI 2H 2006



XCAT-C++ Framework

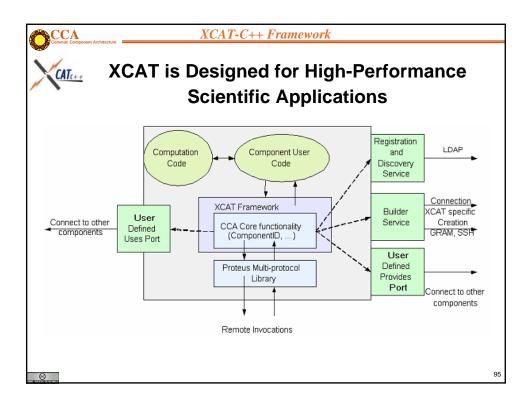


XCAT is a Web-services based **Distributed Component Framework**

- Remote references
 - Port types described in C++ header files or in WSDL documents
- User Interface
 - C++ and Python interface to CCA BuilderServiceUses 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-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)



XCAT-C++ Framework

Supplementary material for notes



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

 $GRAM = Grid \ Resource \ Allocation \ Management \quad \ UDT = UDP\text{-}based \ Data \ Transfer \ protocol$



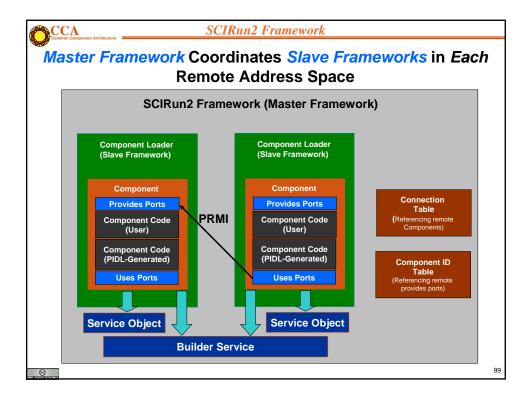
SCIRun2 Framework

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

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

SCIRun2

Supported on Linux.

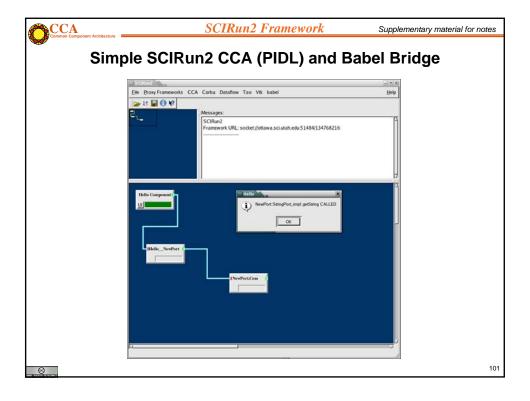


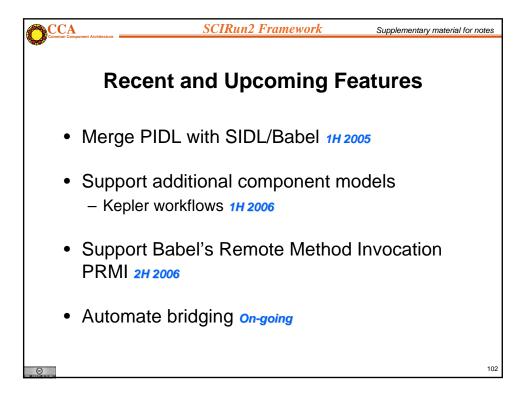


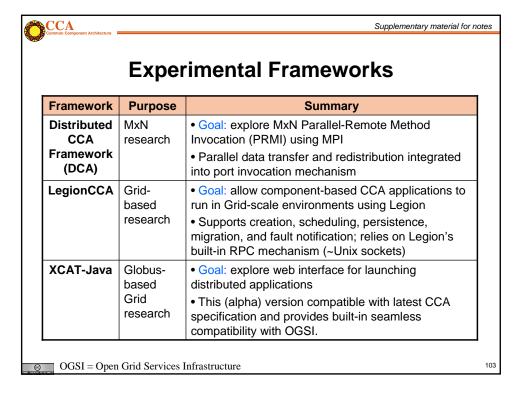
SCIRun2 Framework

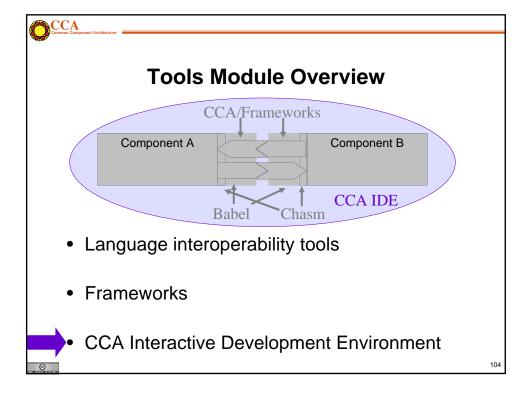
Basic How-To

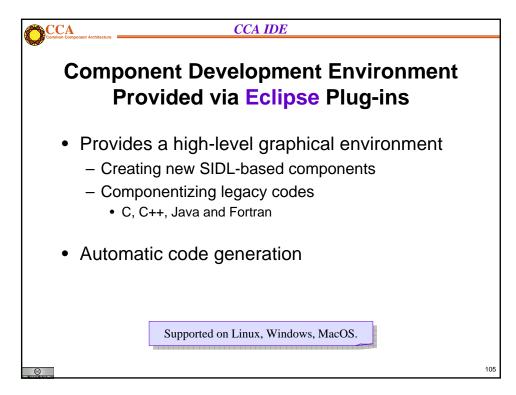
- Add component source files and makefile to SCIRun2 sources
 - May need to define ports in SIDL
- Add component information to the component model xml file
- 3. Build component using SCIRun2 make scripts
 - Alternatively, build component using Babel
- Start the framework and graphical (default) or text builder
- 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

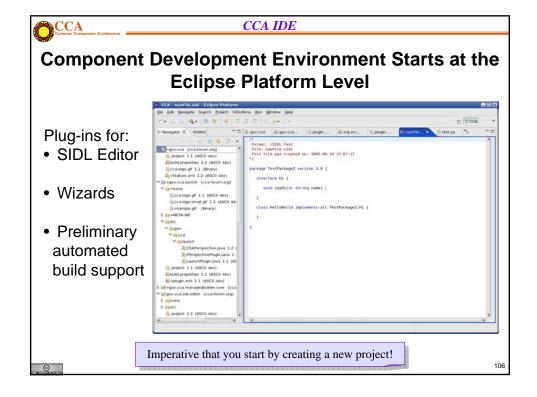


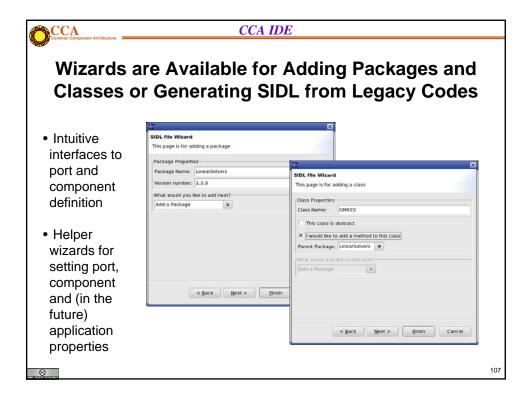


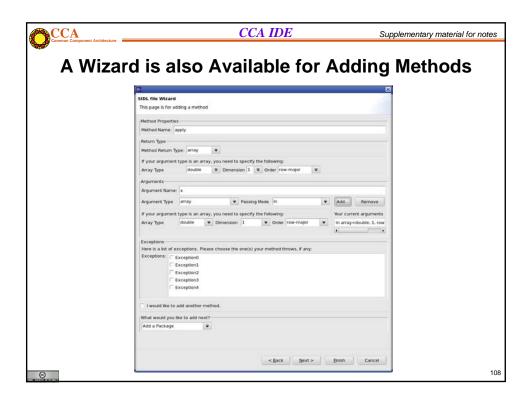














CCA IDE

Supplementary material for notes

Recent and Upcoming Features

- Provide automated build support 1H 2005
- Launch application via GUI 1H 2006

0

109



Supplementary material for notes

CCA Tools Contacts (1 of 2)

Tool	Purpose	More information
Babel	Scientific language interoperability tool kit	URL: www.llnl.gov/CASC/components Email: components@llnl.gov or babel-users@lists.llnl.gov
Ccaffeine	Direct-connect, parallel-friendly framework	URL: www.cca-forum.org/software/ Email: Ben Allan, ccafe-help@z.ca.sandia.gov Wiki: https://www.cca-forum.org/wiki
Chasm	Fortran90 interoperability wrapper	URL: chasm-interop.sourceforge.net Examples: chasm/example/cca-tutorial
DCA	MxN research framework	URL: www.cs.indiana.edu/~febertra/mxn Email: Felipe Bertrand, febertra@cs.indiana.edu
CCA IDE	CCA development environment	Email: usability@cca-forum.org

0



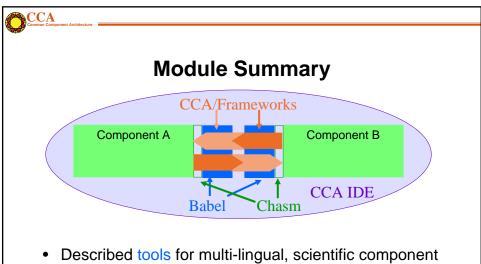
Supplementary material for notes

CCA Tools Contacts (2 of 2)

Tool	Purpose	More information
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

0

111



- 'plug-and-play'
- Language interoperability through Babel and Chasm
- CCA Frameworks provide mechanisms for composition
- CCA Interactive Development Environment via Eclipse plug-in

0





CCA Forum Tutorial Working Group

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



113



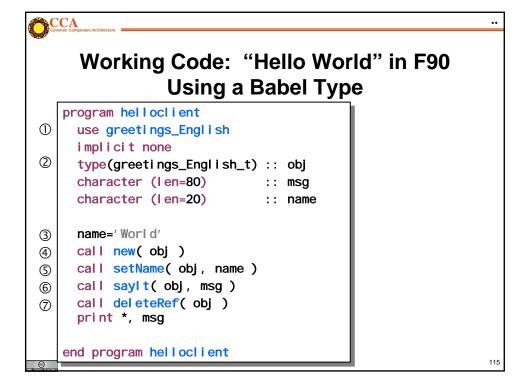
Goal of This Module

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

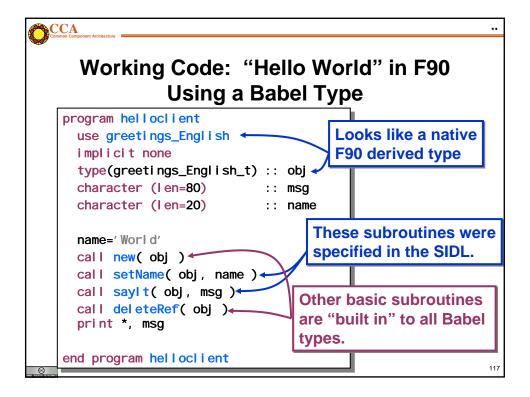




Handout Material: Code Notes

- ① Use statement for the greetings. English type
- ② 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
- ③ 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".
- ④ 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.
- S setName() puts data into the obj. It sets its state.
- Saylt() returns the entire greeting including the aforementioned name.
- ② 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.

0



```
The SIDL File that defines the "greetings.English" type

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

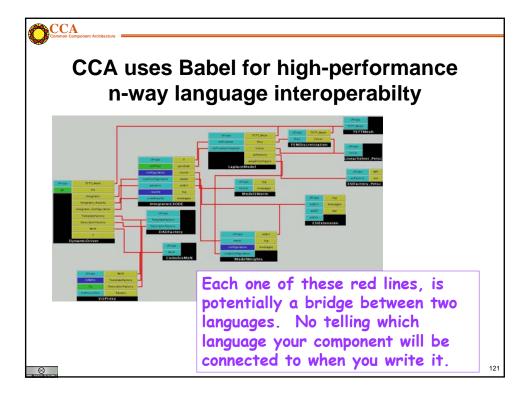


Handout Material: Code Notes

- 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.
- S 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".
- 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.

⊚

```
CCA
 Question: What language is "obj" really
                 implemented in?
  program helloclient
    use greetings_English
    implicit none
    type(greetings_English_t) :: obj
    character (len=80)
                              :: msg
    character (len=20)
                              :: name
                                Answer: Can't Know!
    name=' Worl d'
    call new(obj)
                                With Babel, it could be C.
                               C++, Python, Java, Fortran77,
    call setName( obj, name )
                               or Fortran90/95
    call sayIt(obj, msg)
    call deleteRef( obj )
                               In fact, it could change on
    print *, msg
                                different runs without
                               recompiling this code!
  end program helloclient
```

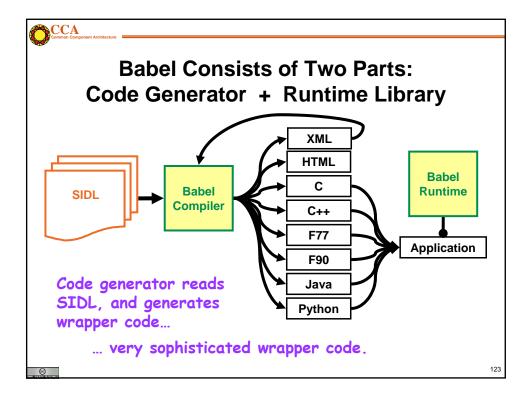


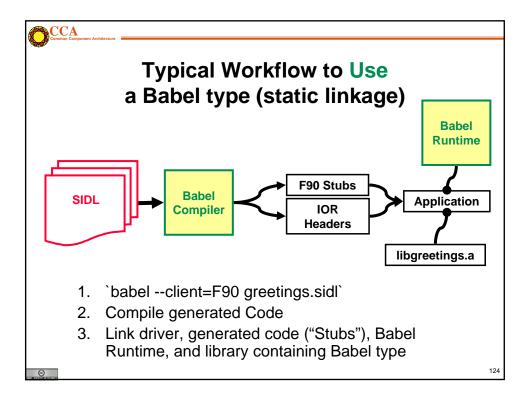


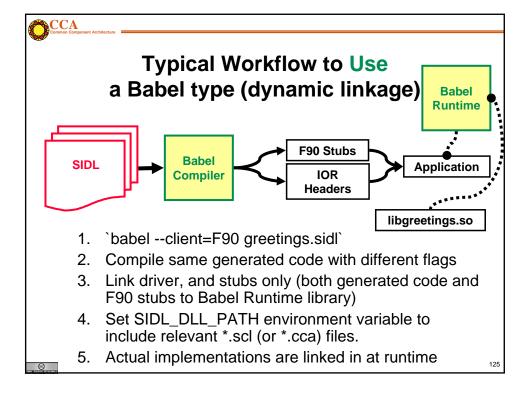
CCA uses SIDL to specify APIs and Type Hierarchy for Frameworks, Services, Components, & Ports

- A CCA framework must
 - implement gov. cca. AbstractFramework,
 - provide a gov. cca. ports. Bui I derServi ce,
 - 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.



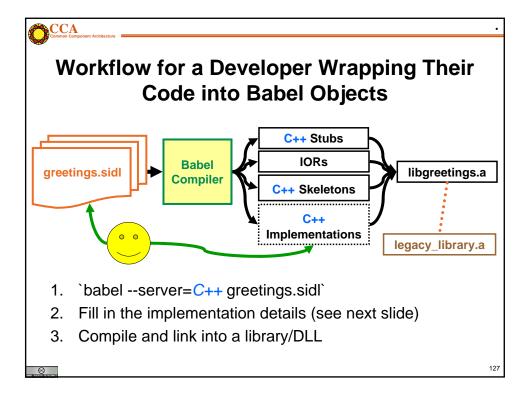


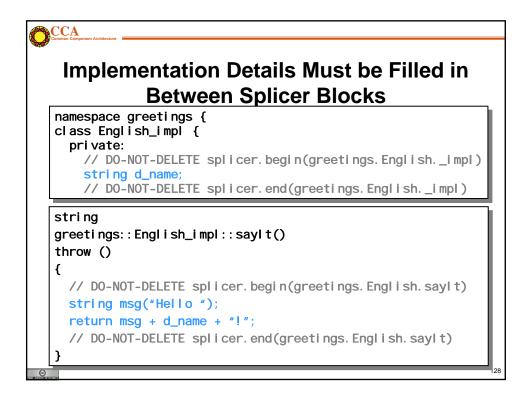




Static vs. Dynamic Linkage

- 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







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)

0

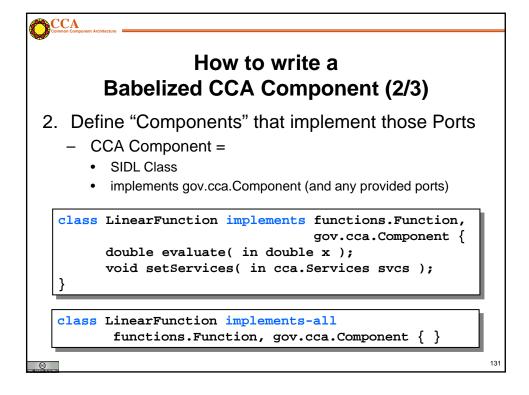
129

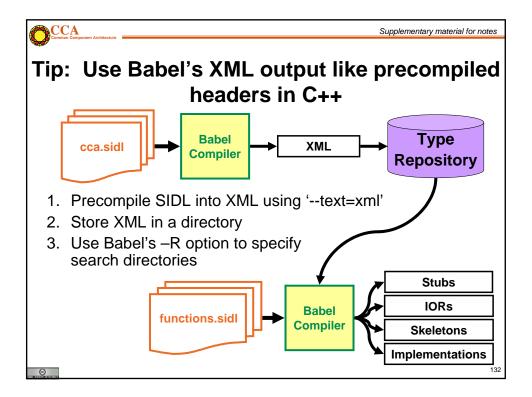


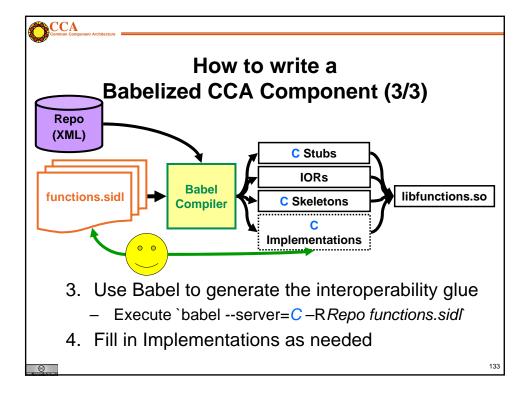
How to write a Babelized CCA Component (1/3)

- 1. Define "Ports" in SIDL
 - CCA Port =
 - · a SIDL Interface
 - extends gov.cca.Port

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









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

0

135



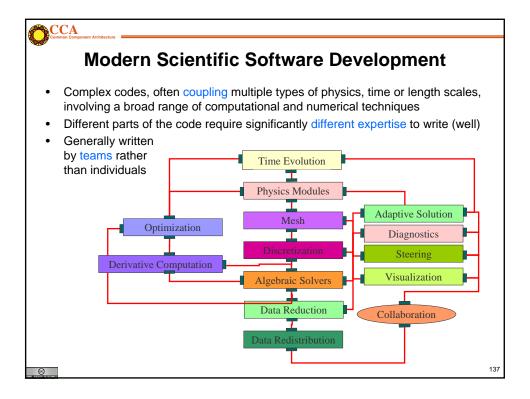
Using CCA: Approaches & Experience

CCA Forum Tutorial Working Group

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

CC)

This work is licensed under a Creative Commons Attribution 2.5 License





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

0

139



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 welldefined, lasting components
- Wrapped legacy portions need not be reimplemented or reverified

0

141



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

0

143



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

14

⊚



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?

0

145



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.

0

escal for the



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-specbabel-config and if possible compile & link with babellibtool

450



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

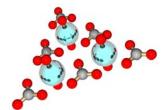
0

151



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)



152



CCA-Chemistry Project Participants

Pacific Northwest National Laboratory

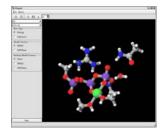
Theresa L. Windus Yuri Alexeev Manojkumar Krishnan Jarek Nieplocha Carl Fahlstrom Elizabeth Jurrus

Sandia National Laboratory

Curtis L. Janssen Joseph P. Kenney

Argonne National Laboratory

Steve Benson Lois Curfman McInnes Jason Sarich











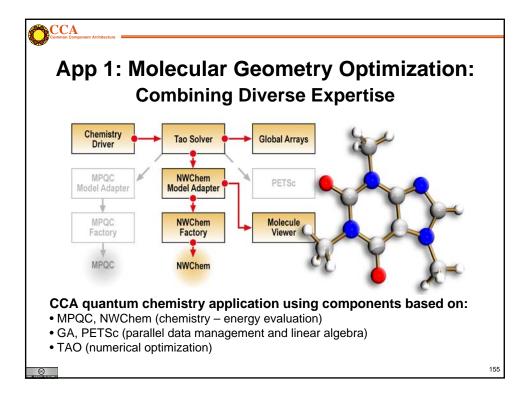


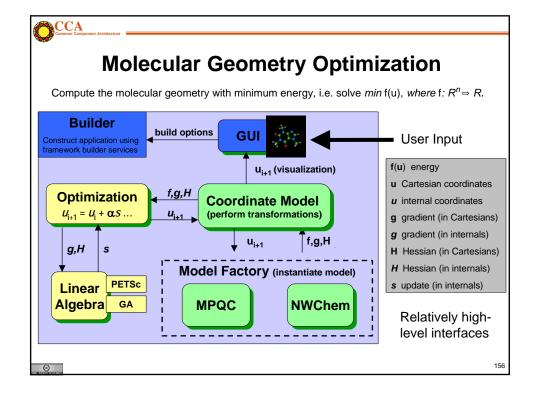
CCA Impacts in Computational Chemistry

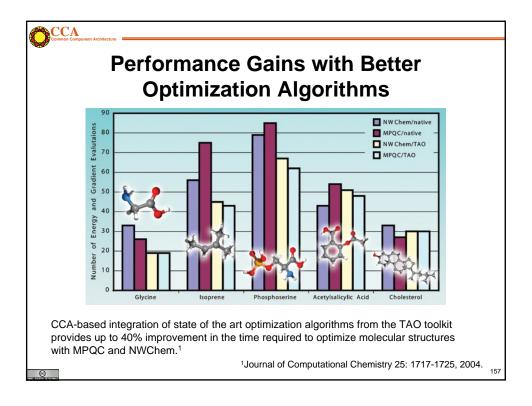
Through 4 chemistry applications we consider different facets of CCA functionality:

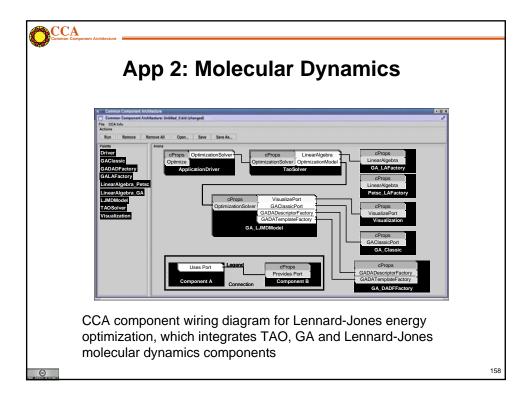
- Molecular Geometry Optimization

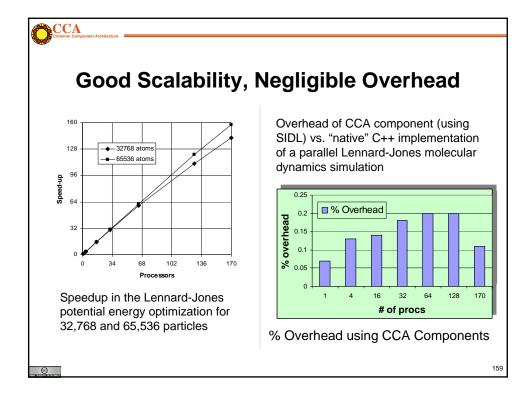
 Combining diverse expertise of 5 different research groups
- **Lennard-Jones Molecular Dynamics**
 - Achieving good scalability and low CCA overhead
- Multi-level Parallelism in Computational Chemistry
 - Combining SPMD and MPMD parallelism
- **Molecular Integral Evaluation**
 - Component interoperability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







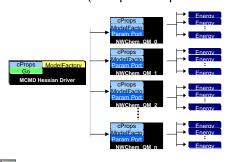






App 3: Multilevel Parallelism Using CCA

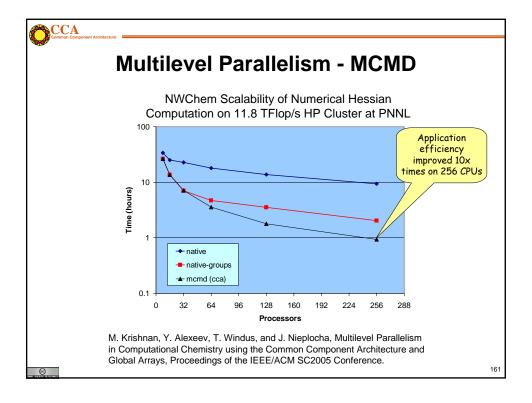
- Massive numbers of CPUs in future systems require leading edge tools to exploit all available parallelism
- GA helps exploit multi-level parallelism
- Multi-level parallelism using CCA and GA processor groups: Combining SCMD (Single Component Multiple Data) and MCMD (Multiple Component Multiple Data)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

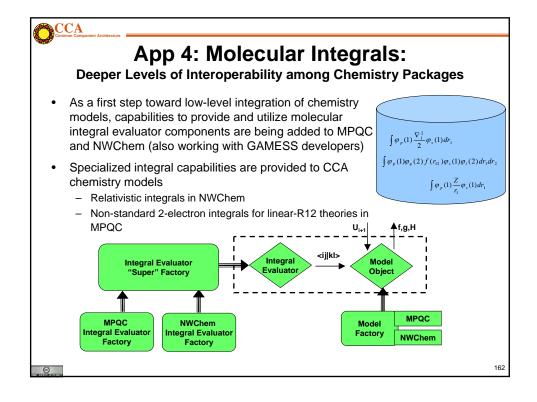


The MCMD Driver launches multiple instances of NWChem components on subsets of processors (also assigns a GA communicator for every instance). Each NWChem QM component does multiple energy computations on subgroups.

160

(0)







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

0

163



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

164



Case Study 2: Combustion Project

- Computational Facility for Reacting Flow Science (CFRFS)
 - http://cfrfs.ca.sandia.gov
 - Funded via SciDAC initiative (PI: H. Najm)
- Focus: A toolkit to perform simulations of lab-sized unsteady flames
 - Solve the Navier-Stokes 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:
 - J. Ray, S. Lefantzi, J. Lee, C. Kennedy, W. Ashurst, K. Smith, M. Liu, N. Trebon



165



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)

40



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

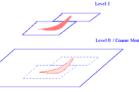
0

167



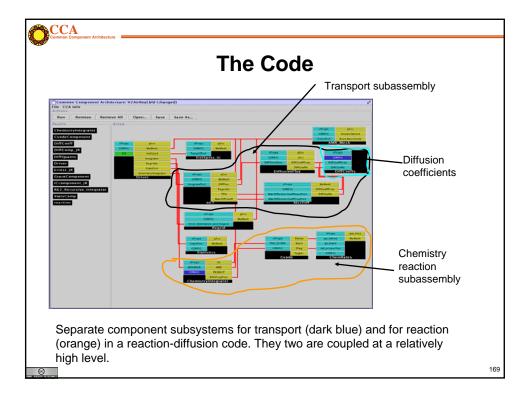
Design Principles of the Toolkit - 2

- 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

168

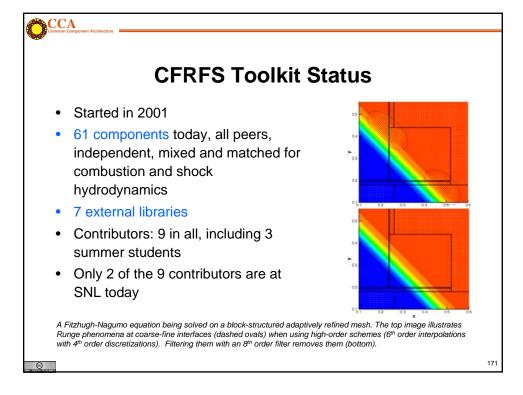


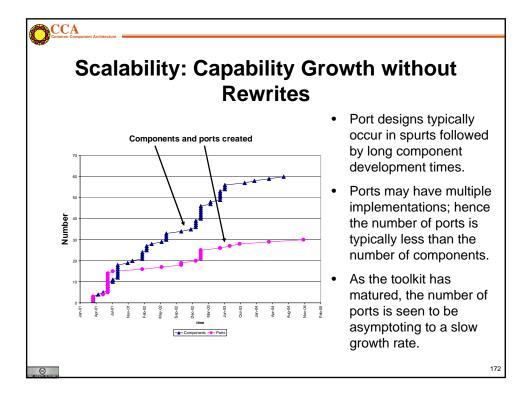


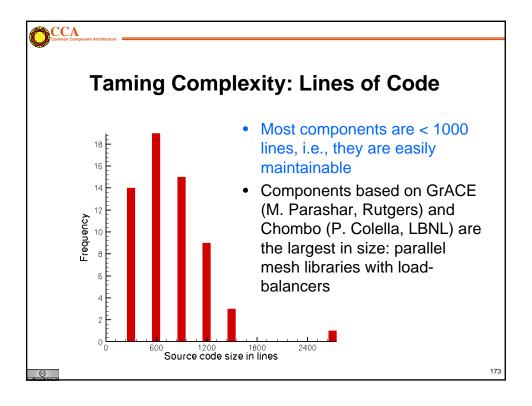
Has the Toolkit Approach Helped Tame Software Complexity?

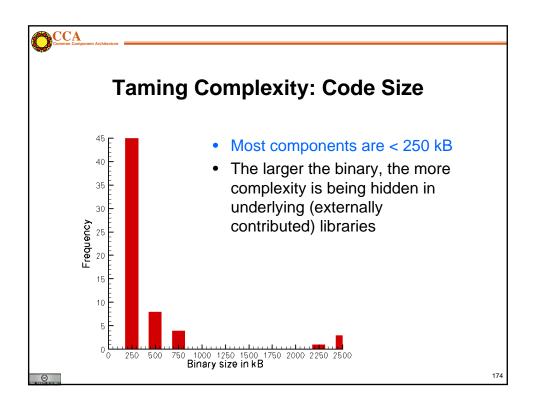
Questions to consider:

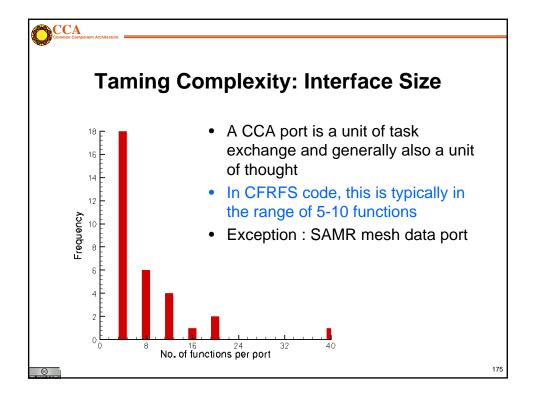
- How has the code evolved?
 - How often have new ports been added?
 - How many rewrites have been done?
- How large are the components?
- How many ports do they have?
 - How large are the ports?
- How many ports exist?
 - i.e., Is the design general enough to support many implementations?
- What is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

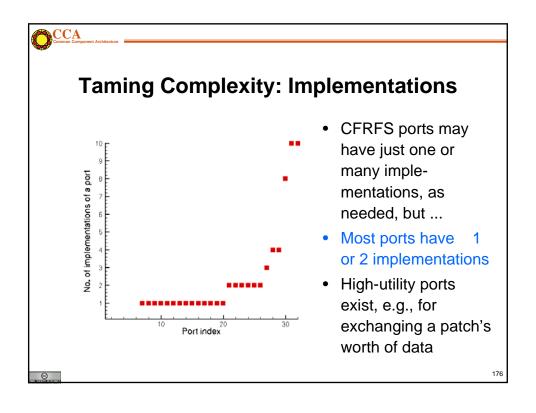


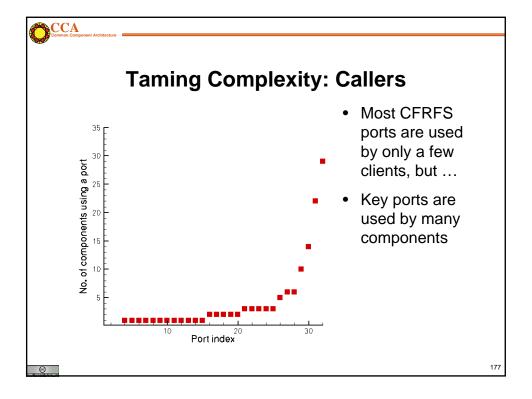


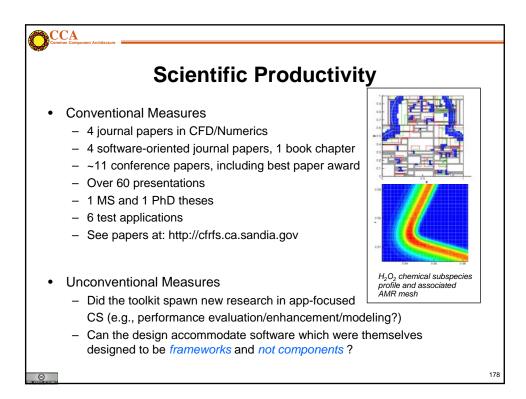














Adaptive Codes

- 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

0

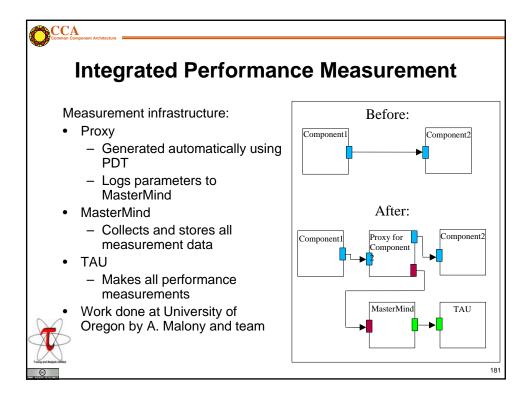
179

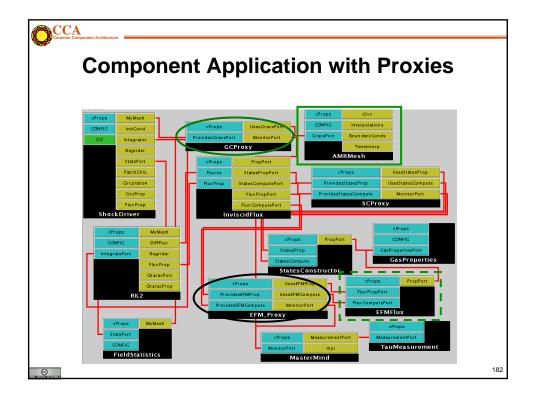


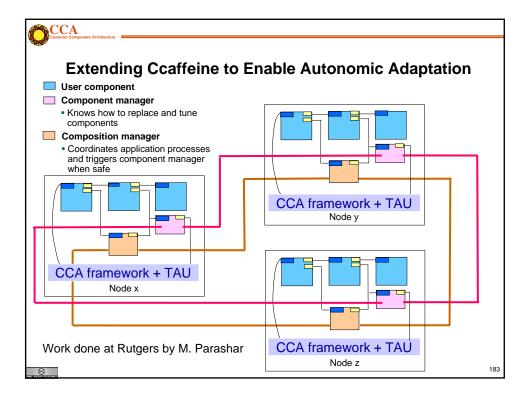
Performance Measurement in a Component World

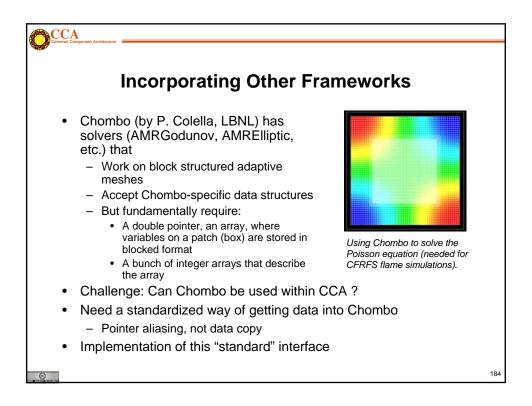
- · Different from traditional software
 - The researcher may not be the author of the component
 - Will need performance info on a component granularity
 - Will need a non-intrusive way of getting it.
- Proxies: Simple component to be inserted between a caller and a callee component
 - Intercepts and 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?

180











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:
 - Chemistry: http://www.cca-forum.org/~cca-chem
 - Combustion: http://cfrfs.ca.sandia.gov
- Different facets of CCA components may be useful within different projects ... What are your needs and priorities?

0

185



A Few Notes in Closing

CCA Forum Tutorial Working Group

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

@

This work is licensed under a Creative Commons Attribution 2.5 Licens



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

0

187



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

18



CCA is Interactive

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

0

189



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