



Components for Scientific Computing: An Introduction

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Goals of This Module

- Introduce basic **concepts and vocabulary** of component-based software engineering
- Highlight the special **demands of high-performance scientific computing** on component environments
- Provide a **unifying context** for the remaining talks
 - And to consider what components might do for your applications

Motivation: Modern Scientific Software Engineering Challenges

- **Productivity**
 - Time to first solution (prototyping)
 - Time to solution (“production”)
 - Software infrastructure requirements (“other stuff needed”)
- **Complexity**
 - Increasingly sophisticated models
 - Model coupling – multi-scale, multi-physics, etc.
 - “Interdisciplinarity”
- **Performance**
 - Increasingly complex algorithms
 - Increasingly complex computers
 - Increasingly demanding applications

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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

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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

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Some Observations About Software...

- “The complexity of software is an essential property, not an accidental one.” *[Brooks]*
 - **We can't get rid of complexity**
- “Our failure to master the complexity of software results in projects that are late, over budget, and deficient in their stated requirements.” *[Booch]*
 - **We must find ways to manage it**

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More Observations...

- “A complex system that works is invariably found to have evolved from a simple system that worked... A complex system designed from scratch never works and cannot be patched up to make it work.” *[Gall]*
 - Build up from simpler pieces
- “The best software is code you don’t have to write” *[Jobs]*
 - Reuse code wherever possible

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Not All Complexity is “Essential”

- An example of how typical development practices can exacerbate the complexity of software development...
- At least 41 different Fast Fourier Transform (FFT) libraries:
 - see, <http://www.fftw.org/benchfft/doc/ffts.html>
- Many (if not all) have different interfaces
 - different procedure names and different input and output parameters
- Example: SUBROUTINE FOUR1(DATA, NN, ISIGN)
 - “Replaces DATA by its discrete Fourier transform (if ISIGN is input as 1) or replaces DATA by NN times its inverse discrete Fourier transform (if ISIGN is input as -1). DATA is a complex array of length NN or, equivalently, a real array of length 2*NN. NN MUST be an integer power of 2 (this is not checked for!).”

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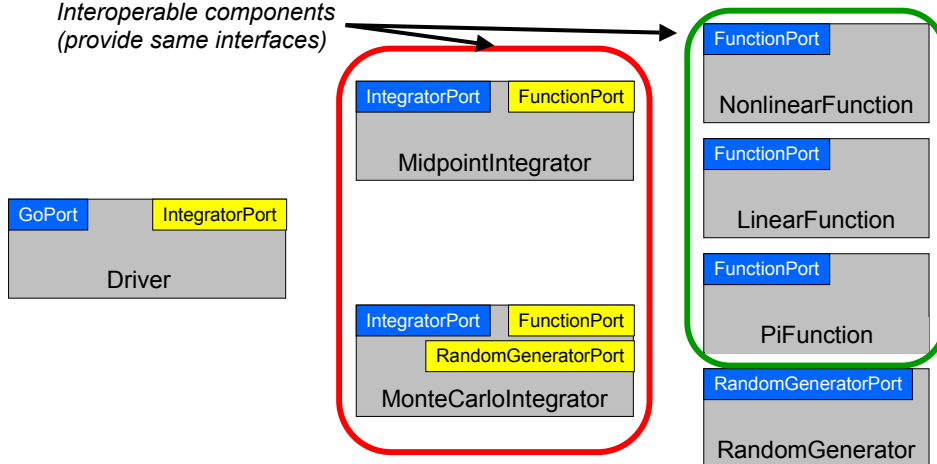
Component-Based Software Engineering

- CBSE methodology is emerging, especially from business and internet areas
- **Software productivity**
 - Provides a “**plug and play**” application development environment
 - Many components available “off the shelf”
 - Abstract interfaces facilitate **reuse and interoperability** of software
- **Software complexity**
 - Components **encapsulate** much **complexity** into “black boxes”
 - Plug and play approach simplifies applications
 - **Model coupling** is natural in component-based approach
- **Software performance** (indirect)
 - Plug and play approach and rich “off the shelf” component library simplify changes to **accommodate different platforms**

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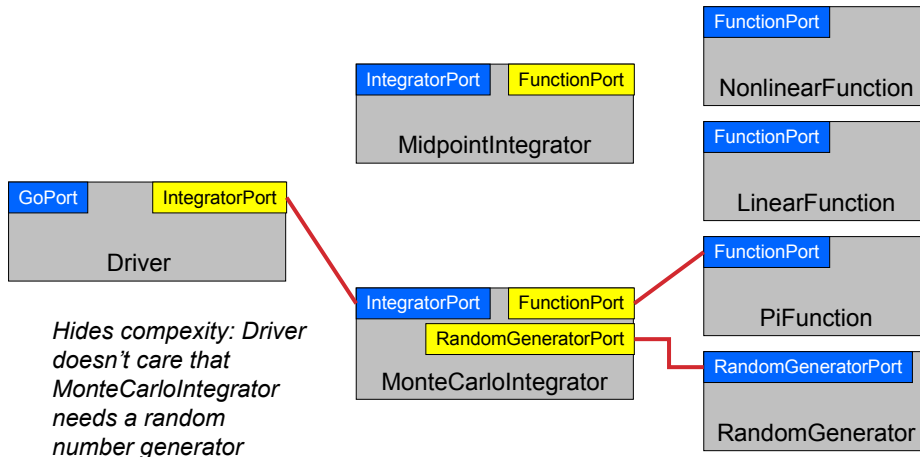
A Simple Example: Numerical Integration Components

*Interoperable components
(provide same interfaces)*



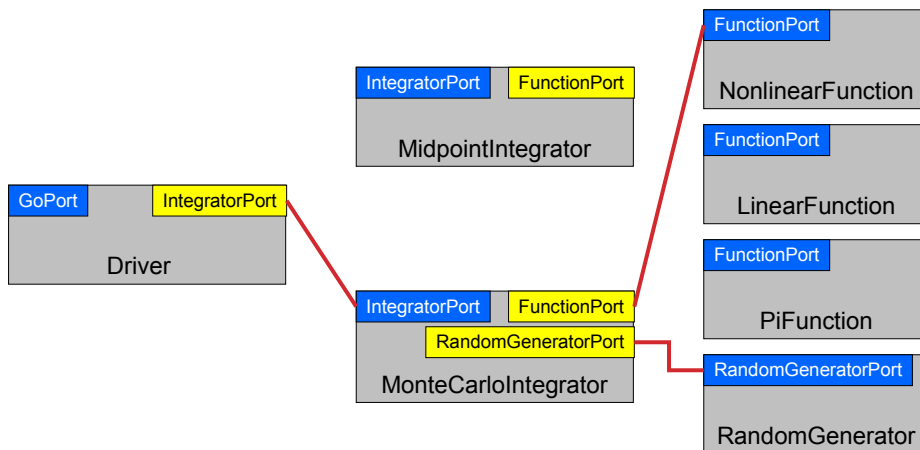
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An Application Built from the Provided Components



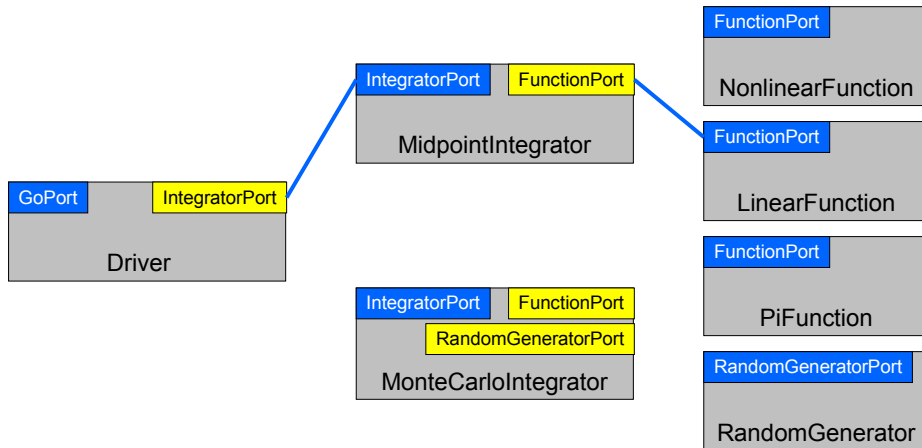
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Another Application...



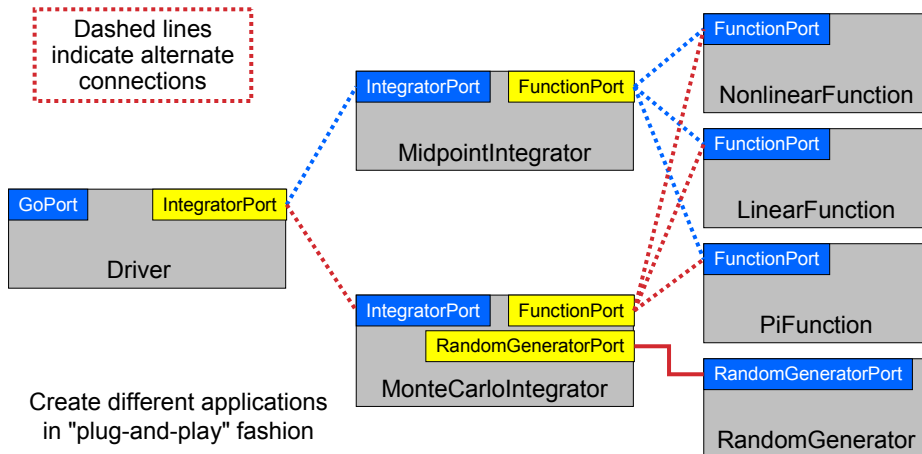
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Application 3...



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And Many More...



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What are Components?

- No universally accepted definition...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
 - Components *may* maintain state information
 - But external access to state info must be through an interface (*not a common block*)
 - File-based interactions can be recast using an “I/O component”
- **Can be composed with other components**
 - “Plug and play” model to build applications
 - **Composition based on interfaces**

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What is a Component Architecture?

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

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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...
- General plug and play interoperability requires **multiple implementations** providing the same interface
- Reuse of components occurs when they provide interfaces (functionality) needed in **multiple applications**

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Designing for Reuse, Implications

- Designing for interoperability and reuse requires **“standard” interfaces**
 - Typically domain-specific
 - “Standard” need not imply a formal process, may mean “widely used”
- Generally means **collaborating** with others
- *Higher* initial development cost (**amortized over multiple uses**)
- Reuse implies **longer-lived code**
 - thoroughly tested
 - highly optimized
 - improved support for multiple platforms

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Typical Component Lifecycle

- **Composition Phase**
 - Component is **instantiated** in framework
 - Component interfaces are **connected** appropriately
- **Execution Phase**
 - Code in components uses functions provided by another component
- **Decomposition Phase**
 - **Connections** between component interfaces may be **broken**
 - Component may be **destroyed**

In an application, individual components may be in different phases at different times
Steps may be under human or software control

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Relationships: Components, Objects, and Libraries

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

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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**

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
 - Commodity component models often not so useful in HPC scientific context

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Special Needs of Scientific HPC

- Support for legacy software
 - How much **change** required for component environment?
- Performance is important
 - What **overheads** are imposed by the component environment?
- Both parallel and distributed computing are important
 - What approaches does the component model support?
 - What **constraints** are imposed?
 - What are the **performance costs**?
- Support for **languages, data types, and platforms**
 - Fortran?
 - Complex numbers? Arrays? (as first-class objects)
 - Is it available on my parallel computer?

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Commodity Component Models

- CORBA, 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

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The “Sociology” of Components

- Components need to be shared to be truly useful
 - Sharing can be at several levels
 - Source, binaries, remote service
 - Various models possible for intellectual property/licensing
 - Components with different IP constraints can be mixed in a single application
- Peer component models facilitate collaboration of groups on software development
 - Group decides overall architecture and interfaces
 - Individuals/sub-groups create individual components

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Who Writes Components?

- “Everyone” involved in creating an application can/should create components
 - Domain scientists as well as computer scientists and applied mathematicians
 - Most will also use components written by other groups
- Allows developers to focus on their interest/specialty
 - Get other capabilities via reuse of other’s components
- Sharing components within scientific domain allows everyone to be more productive
 - Reuse instead of reinvention
- As a unit of publication, a well-written and –tested component is like a high-quality library
 - Should receive same degree of recognition
 - Often a more appropriate unit of publication/recognition than an entire application code

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Summary

- Components are a software engineering tool to help address software productivity and complexity
- Important concepts: components, interfaces, frameworks, composability, reuse
- Scientific component environments come in “domain specific” and “generic” flavors
- Scientific HPC imposes special demands on component environments
 - Which commodity tools may have trouble with

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