A Practical Introduction to Kepler

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Scientific Workflows

- Goals:
  - automate a scientist's repetitive data management and analysis tasks
- Typical phases:
  - data access, scheduling, generation, transformation, aggregation, analysis, visualization
  - design, test, share, deploy, execute, reuse, … SWFs

SWF Systems Requirements

USER REQUIREMENTS:

- **Design tools**-- especially for non-expert users
  - Need to look into how scientist's define their processes
- **Ease of use**-- fairly simple user interface having more complex features hidden in the background
- **Reusable generic** features
- Generic enough to serve to **different communities** but specific enough to serve one domain (e.g. geosciences, molecular biology)
- **Extensibility** for the expert user-- almost a visual programming interface
- **Registration** and **publication** of data products and "process products" (=workflows); **provenance**

SWF Systems Requirements

TECHNICAL REQUIREMENTS:

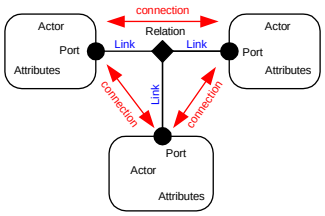
- Error detection and recovery from failure
- Logging information for each workflow
- Allow data-intensive and compute-intensive tasks (Maybe at the same time)
- HPC + Data management/integration
- Allow status checks and on the fly updates
- Visualization
- Semantics and metadata based dataset access
- Certification, trust, security…

Kepler based on Ptolemy II


- A set of Java packages for heterogeneous, concurrent modeling, design and execution.
- Strengths include:
  - Precisely defined **models of computation** and **component interaction**
    - e.g. Process Networks (PN) – data-flow oriented
  - An intuitive GUI that lets rapid workflow composition
  - A modular, reusable and extendable object-oriented environment
  - An XML based workflow definition – MoML
    - Workflows defined in Ptolemy II MoML XML schema
    - Easily exchangeable

Abstract Syntax of PTII Models

•Hierarchical Entities, Ports, Connections and Attributes



Abstract syntax defines the structure of a model, but says little about what it means.

Abstract syntax choices:

- Hierarchy is tree structured (like XML).
- A *relation* mediates connections.
- Ports can link multiple relations and relations can link multiple ports.
- Ports mediate connections across levels of the hierarchy (no statecharts-style level-crossing links)
- …

Adapted from the *.ppt slides by Edward A. Lee (See References)

The GUI -- Vergil

The rest… outline

- How to get and install Kepler
- Designing a Kepler workflow
  - HOW TO best do it?
- Some demos
- Building actors

Installing Kepler

- Kepler website: http://kepler-project.org
- Latest alpha release at:
  http://kepler-project.org/Wiki.jsp?page=Downloads
  Installers for Windows, MacOSX and Linux
  Install and run Kepler's *.exe file* in the Kepler directory it was installed.
- Issues:
  - Some workflows don't run on the fly
    - Local files dependencies, username/password requirements, broken
- Alternative installation for a more recent version:
  - Contact the Kepler cvs admin
  - Get a read-only account
  - Build it from scratch
    - Eclipse instructions at:
      http://kepler-project.org/Wiki.jsp?page=UsingEclipseForKeplerDevelopment
    - Command line building using Ant
      Tutorial: http://kepler-project.org/Wiki.jsp?page=Presentations

Designing Your Workflows in Kepler

- Write down the problem
- Generate a conceptual design of the workflow
  - *Data flow: Task1 -> Task2->..->Taskn*
  - *Data requirements: Types of data, I/O for each task*
- Look for existing Kepler actors for each task
- If there are related tasks, think how to use them; If not, design the stub actors
- Design the workflow using existing and stub actors
- Specify parts that can be sub-workflows and create hierarchies (composite actors)
- Implement the missing actors
- Run tests on the wf for a set of inputs and many times;
  - to check if it executes correctly, and if it produces the same results for the same inputs
- Annotate your workflow and improve usability

Building Kepler Extensions

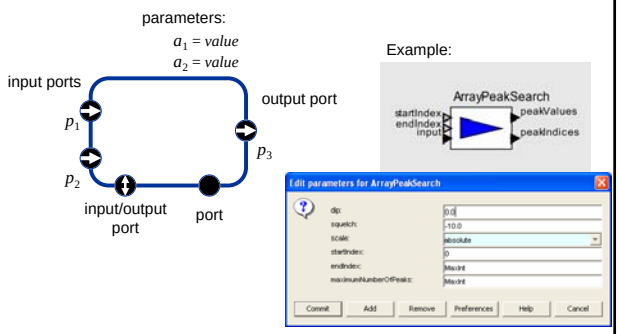
FOCUS: How to build actors?

Ingredients:
- Java 1.4.2
- Cygwin for Developers (for Windows users)
- Ant 1.5 or higher

Adding Actors

- Domain and/or data polymorphic actors
- Use object-oriented inheritance to avoid code duplication
  - 3 base classes: Source, Sink, Transformer
- To use the actors in Vergil
  - Add them to one of the actor libraries
  - Most libraries are under $PTII/ptolemy/actor/lib
  - Libraries are XML files
  - In Kepler, this needs to be done through the actor ontology!!!
- The basic structure of an actor:
  - See http://www.sdsc.edu/~altintas/KeplerTutorial/ActorStructure.txt

Actor Interfaces: *Ports & Parameters*



Anatomy of an Actor: Ports

- Used for "message transport", can be an input, an output, or both.
- Key class: *IOPort* (Can be connected to other IOPort instances via IORelations.)
- Use *TypedIOPort* in order to benefit from the type system! (Domain specific: *DEIOPort*)
- Receiver and Sender interfaces depending on the usage of the port.
- Public members of the actors!!!

Ports: Introduction to the API

public TypedIOPort *portName;* //Definition
//Create the port
portName = new TypedIOPort(this, "*portName*", true, false);
portName.setMultiport(true); //Can support more than one link
int width = *portName*.getWidth(); //0 or 1 if single port
//Reading and Writing
portName.send(channelNumber, token);
Token token = *portName*.get(channelnumber);
//Setting the type of the port
portName.setTypeEquals(BaseType…a type in the type system…);
portName.setTypeAtLeast(…must be a port or parameter…);

Anatomy of an Actor: Parameters

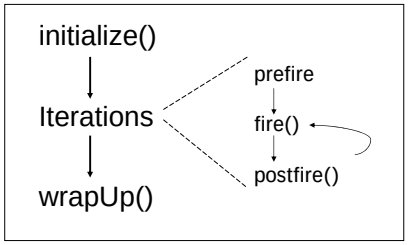
- Public members of the actors!
- Similar API with ports…

public Parameter *parameterName;* //Definition
//Creation and setting the initial value: 2-ways
parameterName = new Parameter (this, "*parameterName*",
new Token(…token value…));
OR
parameterName = new Parameter (this, "*parameterName*");
parameterName.setExpression(…tokenValue…);

Anatomy of an Actor: Constructors

- The major task:
  - To create and configure ports and parameters
- super(container, name);
  - Carries the NameDuplication and IllegalAction exceptions from the super class.
- The icon for the actor can be set here.

Execution of an actor



Action Methods

- *initialize():* Initialize the state variables of an actor.
- *prefire():* Returns a boolean which indicates if the actor wants to fire.
  - Can also be used to perform an operation that will happen exactly once per iteration.
- *fire():* The main point of execution.
  - For reading inputs, producing outputs, read the current parameter values.

Action Methods (cont.)

- *postfire():* Has two tasks:
  - Updating persistent state
  - Determining whether the execution of an actor is complete.
- *wrapUp():* For displaying final results.

Things to remember when implementing a fire() method

- Use the methods of the Token class for arithmetic whenever possible (to get data polymorphism)
- If data-polymorphism is not necessary, set the type to a base type then cast the token to that type.
- Cannot assume that there is be data available at all the input ports (for domain-polymorphism)
- Do not update the persistent state in fire() (use postfire())

Implementing Polymorphism

- Class: PortParameterFunction

- A *PortParameterFunction* object will be returned as a function of two objects.
- Set the type of the output equal to the type of this object.
- Type system will compute the type of the *PortParameterFunction* object and use it as the type of the output when necessary.

The manager

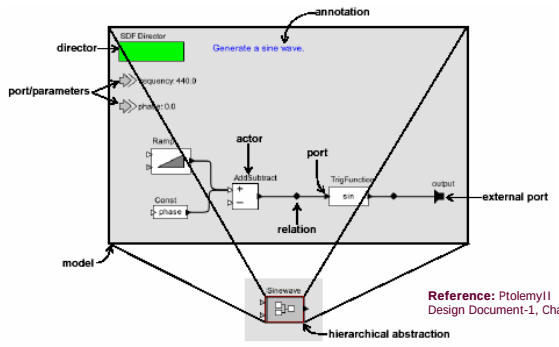
- Controls the overall execution of a model.
- Interacts only with the "*top-level composite actor*"
- startRun() -> run() -> execute()
- ExecutionListener interface provides the manager with info on the events generated during execution.

Ptolemy design doc... show how Ptolemy II handles mixing models of computations hierarchically.

Exceptions

- A uniform mechanism for reporting errors
- Base class: *KernelException*
- Exception chaining re-implemented since Java versions < 1.4 doesn't support it.
  - The detail message includes the detail message from the cause argument.
  - A protected _setCause() method is implemented, but not the public initCause() method that JDK1.4 has.
- Non-severe exceptions: *IllegalActionException, NameDuplicationException, NameDuplicationException.*
- Severe-exceptions: *KernelRuntimeException, InvalidStateException, InternalErrorException.*

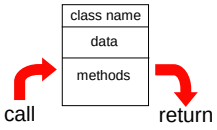
Actor-Oriented Design



Reference: PtolemyII Design Document-1, Chapter 1

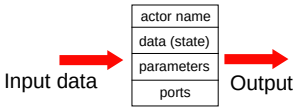
Focus on Actor-Oriented Design

Object orientation:



What flows through an object is sequential control

Actor orientation:

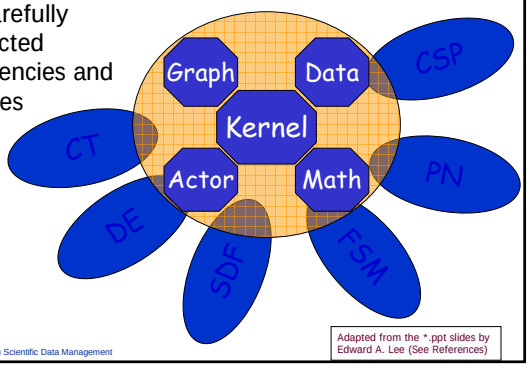


What flows through an object is streams of data

Adapted from the *.ppt slides by Edward A. Lee (See References)

Layered Software Architecture

Ptolemy II packages have carefully constructed dependencies and interfaces



Adapted from the *.ppt slides by Edward A. Lee (See References)

Ptolemy II Architecture

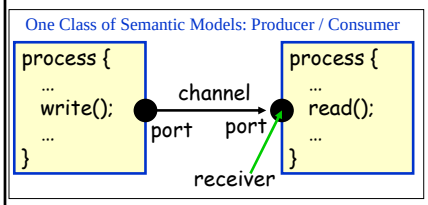
- Core packages (actor, data, kernel, math, util)
  - The data model(--abstract syntax) of the models
  - Abstract semantics
- User Interface (UI) packages
  - MoML and visual interface support
- Library packages
  - Domain polymorphic actors
- Domain packages
  - Implementations of different models of computation

Overview of the Key Classes

Models of Computation

- Semantic interpretations of the abstract syntax

Different models <=> Different semantics <=> Different execution



- Are actors active? passive? reactive?
- Are communications timed? synchronized? buffered?

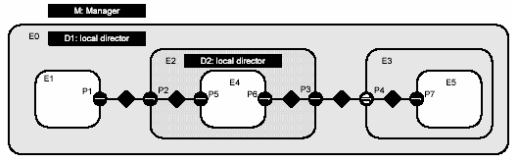
Models of Computation:

- continuous-time
- dataflow
- rendezvous
- discrete events
- synchronous
- time-driven
- publish/subscribe
- …

Adapted from the *.ppt slides by Edward A. Lee (See References)

Director

- Governs the execution of a composite entity.
  - Scheduling, dispatching threads, generate code, etc.
- A composite entity is called *opaque* if it doesn't have a local director.
  - An opaque composite entity inherits the director of its container as its *executive director*.



MoML

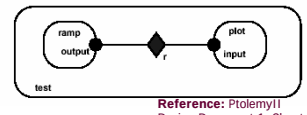
- Modeling Markup Language
- A primary persistent XML file format for Ptolemy II.
  - ptolemy *filename*.xml
  - ptexecute *filename*.xml
  - vergil *filename*.xml
  - moml *configuration*.xml *filename*.xml

An Example MoML File

```
<?xml version="1.0" standalone="no"?>
<!DOCTYPE entity PUBLIC "-//UC Berkeley//DTD MoML 1//EN"
"http://ptolemy.eecs.berkeley.edu/xml/dtd/MoML_1.dtd">
<entity name="test" class="ptolemy.actor.TypedCompositeActor">
<property name="director"
class="ptolemy.domains.sdf.kernel.SDFDirector"/>
<entity name="ramp" class="ptolemy.actor.lib.Ramp"/>
<entity name="plot" class="ptolemy.actor.lib.gui.SequencePlotter"/>
<relation name="r" class="ptolemy.actor.TypedIORelation"/>
<link port="ramp.output" relation="r"/>
<link port="plot.input" relation="r"/>
</entity>
```

Top-level entity

SDF domain



Reference: PtolemyII Design Document-1, Chapter 6

Type System

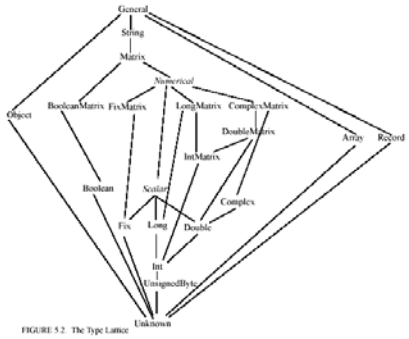


FIGURE 5.2. The Type Lattice