Overview of the Systems Biology Workbench

Michael Hucka, Andrew Finney,
Herbert Sauro, Hamid Bolouri

ERATO Kitano Systems Biology Project
California Institute of Technology, Pasadena, CA, USA

***Principal Investigators*: John Doyle, Hiroaki Kitano**

***Collaborators*: Adam Arkin (BioSpice), Dennis Bray (StochSim), Igor Goryanin (DBsolve), Les Loew (Virtual Cell), Pedro Mendes (Gepasi/Copasi), Masaru Tomita (E-Cell)**

Background

- **Modeling, simulation & analysis are critical**
  - Huge volumes of data
  - Many disparate findings
- **Rapid rate of software tool development**
  - Roles: data filtering, model creation, model simulation
  - Many groups are creating many tools
    - Different packages have different niche strengths reflecting expertise & preferences of the group
    - Strengths are often complementary to those of other packages

Problems

- **No single package answers all needs of modelers**
- **No single tool is likely to do so in the near future**
  - Range of capabilities is large
  - New techniques (⇒ new tools) evolving too rapidly
- **Researchers are likely to continue using multiple packages for the foreseeable future**
- **Problems in using multiple tools:**
  - Simulations & results often cannot be shared or re-used
  - Duplication of software development effort

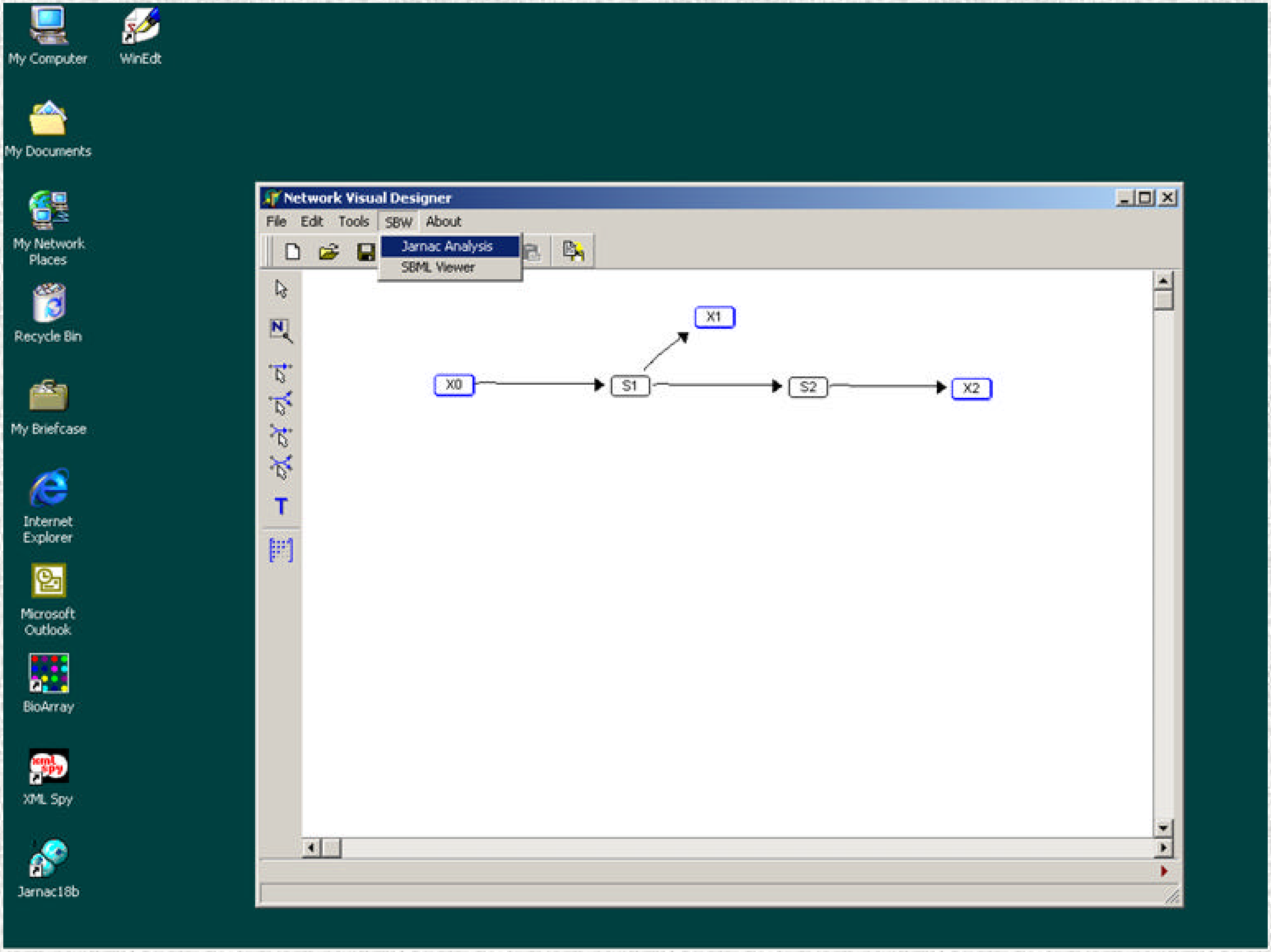
Goal & Approach

- **Systems Biology Workbench project goal: provide software infrastructure that**
  - Enables sharing of simulation/analysis software & models
  - Enables collaboration between software developers
- **Two-pronged approach:**
  - Develop a common model exchange language
    - SBML: Systems Biology Markup Language
  - Develop an environment that enables tools to interact
    - SBW: Systems Biology Workbench

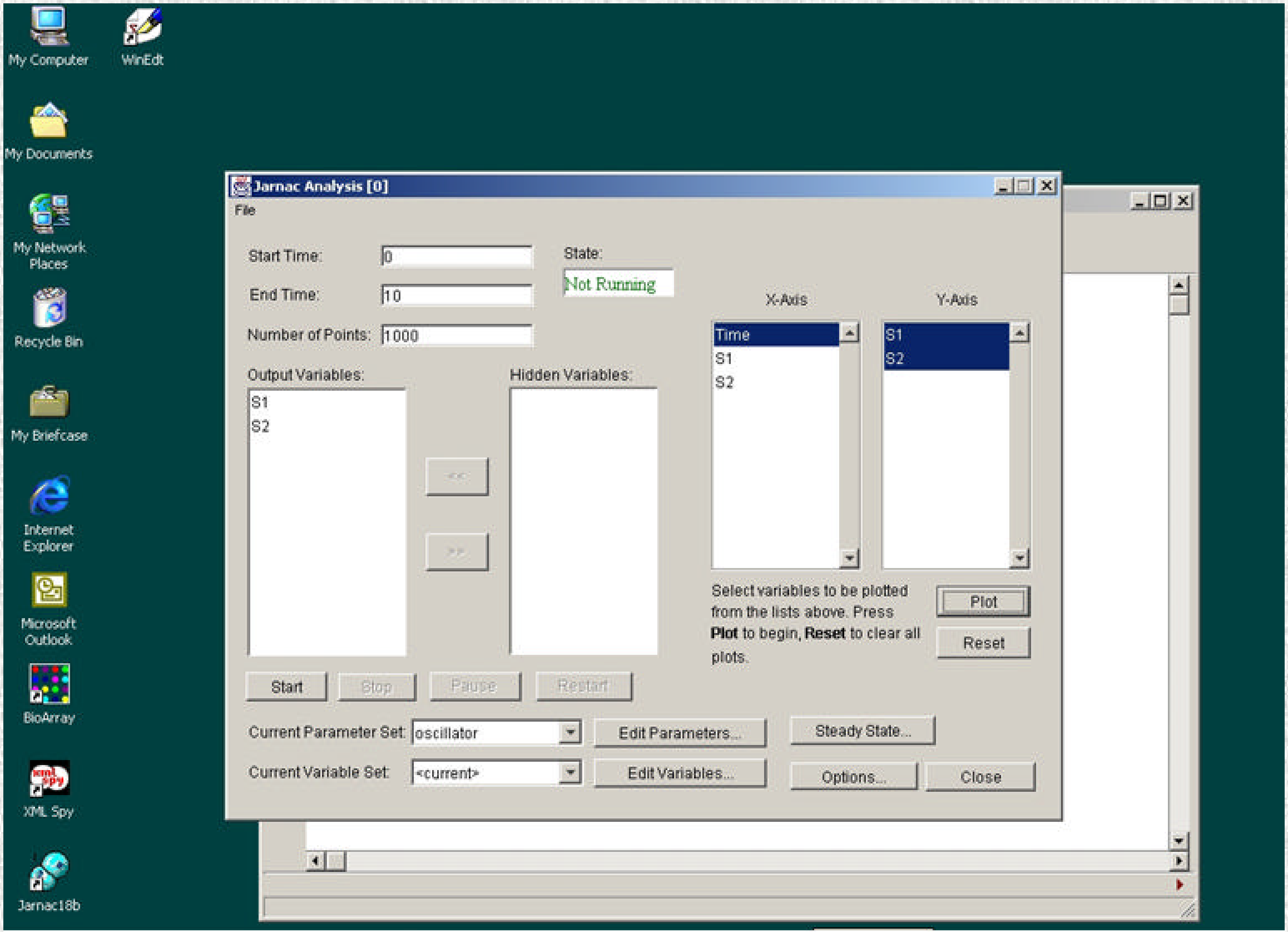
Systems Biology Workbench

- **Open-source, integrated software environment that enables sharing of computational resources**
  - Allows software developers to build interprocess communications facilities into their applications
- **From the user's perspective:**
  - One SBW-enabled application can interact with another
  - Each application or module offers services to others
    - E.g.: ODE solution, time-based simulation, visualization, etc.

From the User’s Perspective



From the User’s Perspective



Start Time: 0

End Time: 10

Number of Points: 1000

State: Not Running

Output Variables:
S1
S2

Hidden Variables:

X-Axis
Time
S1
S2

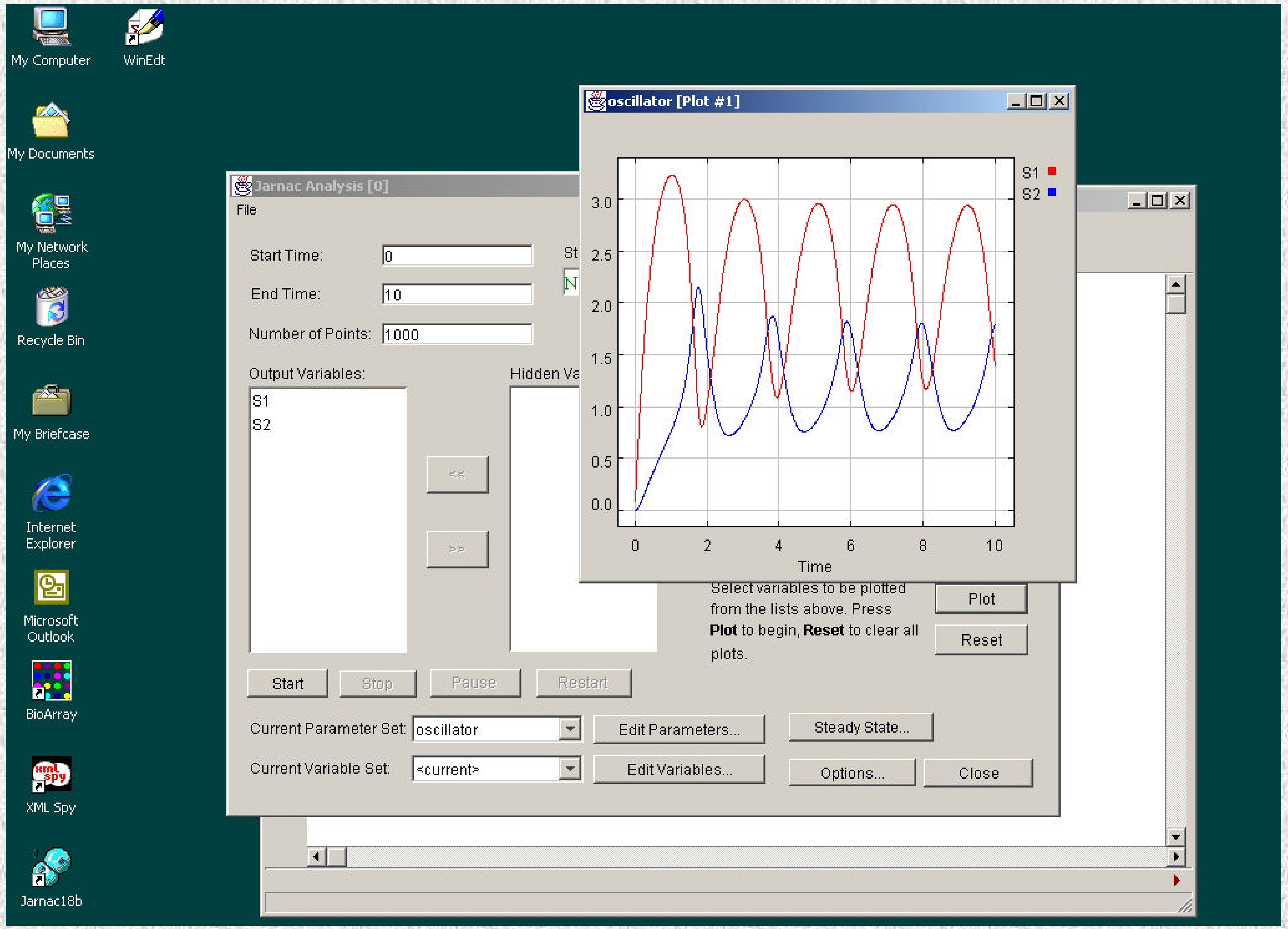
Y-Axis
S1
S2

Select variables to be plotted from the lists above. Press **Plot** to begin, **Reset** to clear all plots.

Current Parameter Set: oscillator

Current Variable Set: <current>

From the User’s Perspective



Start Time: 0

End Time: 10

Number of Points: 1000

Output Variables:

S1

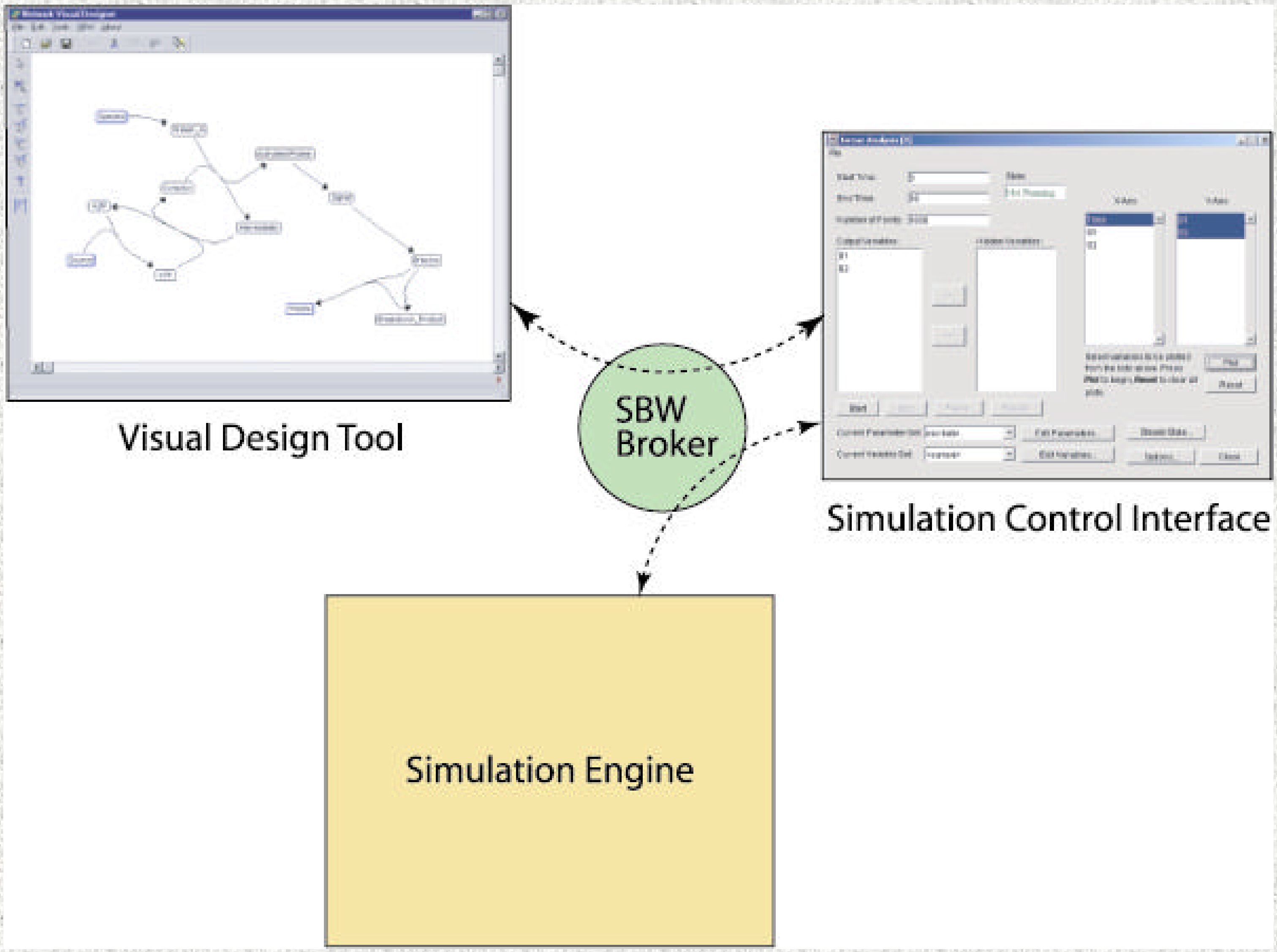
S2

Select variables to be plotted from the lists above. Press **Plot** to begin, **Reset** to clear all plots.

Current Parameter Set: oscillator

Current Variable Set: <current>

Behind the Scenes



Visual Design Tool

SBW Broker

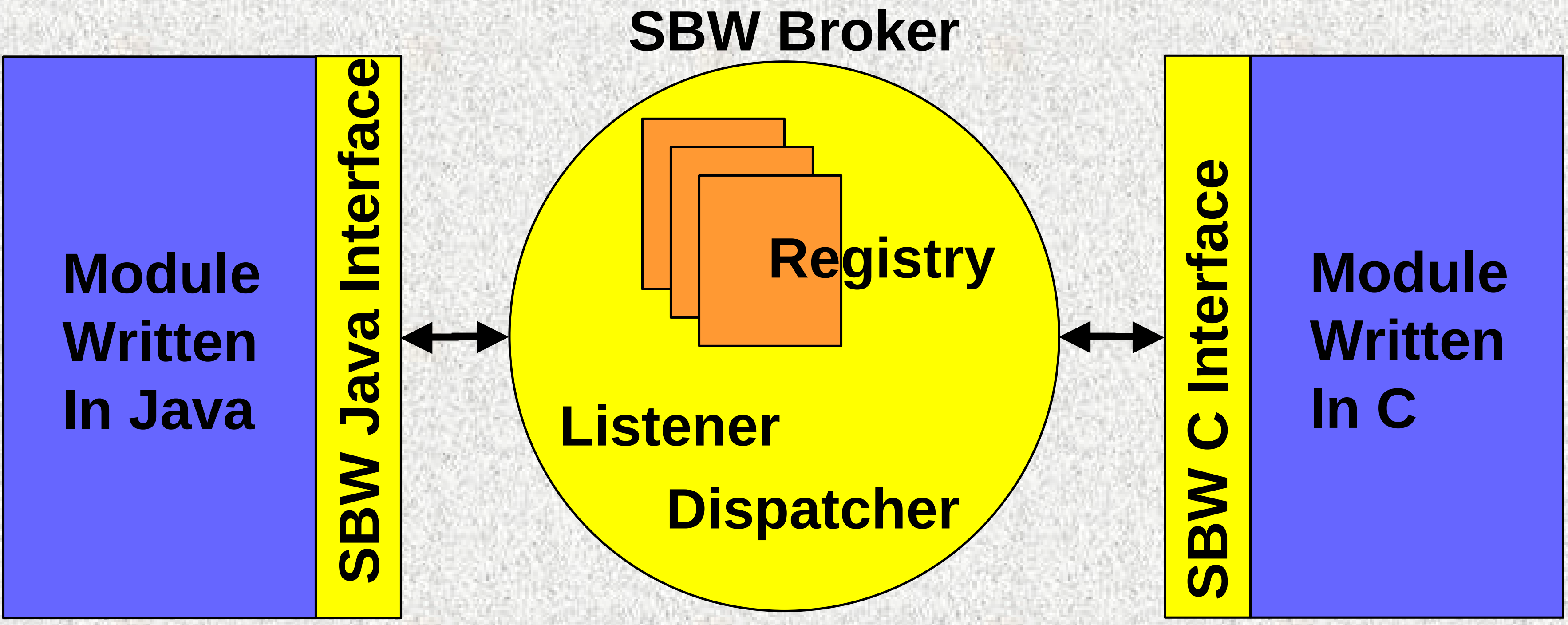
Simulation Control Interface

Simulation Engine

From the Programmer’s Perspective

- **Numerous desirable features**
  - Small application programming interface (API)
  - Simple message-passing architecture
    - Easy to make cross-platform compatible
    - Easy to make distributed
  - Language-neutral architecture
    - We’ll provide C, C++, Java, Delphi, Python libs for Windows & Linux
    - … but libs can be implemented for any language
  - A registry of services for applications to query
  - Use of well-known, proven technologies

The SBW Framework



- **SBW libraries implement RPC mechanisms**
  - – Provide language bindings for SBW
    - C, C++, C++ Builder, Java, Delphi, Python, etc.
  - – Implement underlying message-passing protocols

Communications in SBW

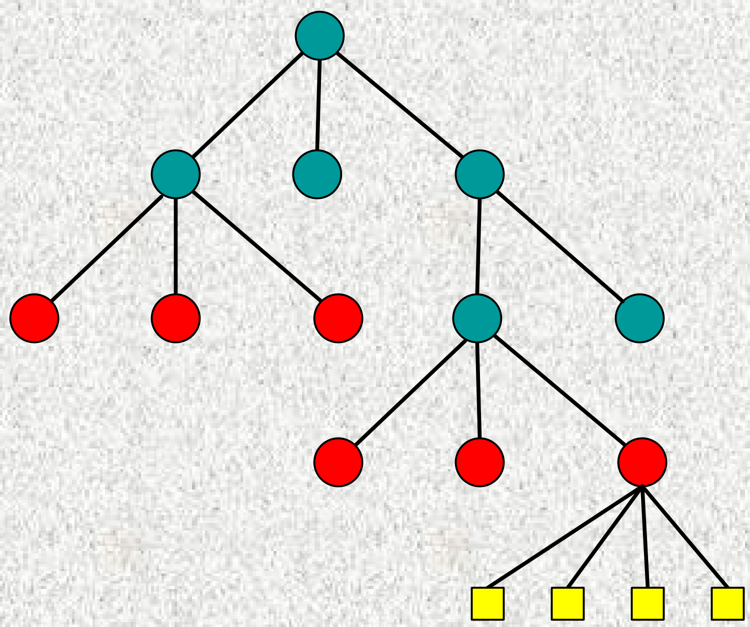
- **Message types:**
  - Call: blocking
  - Send: non-blocking
  - Reply: reply to a call
  - Error: exception handling
- **Message payloads:**
  - Call, send, reply: one or more data elements
  - Error: error code and diagnostic messages
- **Data elements are tagged with their types**
- **Supported data types:**

  Byte Boolean Integer Double String

  List (heterogeneous) Array (homogeneous)

The SBW Registry

- **Registry records info about modules**
  - Module name
  - How to start module
  - Which service categories the module provides
- **Hierarchy of service categories**



Service Categories **(Interface Hierarchy)**

Services **(Interfaces)**

Methods **(Methods)**

Why?

- **Why not use CORBA?**
  - Complexity, size, compatibility
  - SBW scheme does not require IDL
- **Why not use SOAP or XML-RPC?**
  - Performance, data type issues, quality of implementations
- **Why not Java RMI?**
  - Java-specific
- **Why not COM?**
  - Microsoft-specific, low portability
- **Why not MPI?**
  - Designed for homogeneous distributed systems rather than heterogeneous

Summary & Availability

- **Preliminary test implementation completed**
- **Production version is now in development**
  - Draft API definition & other info available
    - Your hand-outs
    - http://www.cds.caltech.edu/erato/sbw/docs
- **Expect first public beta release in November at ICSB 2001 (http://www.icsb2001.org)**