Orchestration and Choreography:
Standards, Tools and Technologies for Distributed Workflows

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Agenda

- What are Workflow, Orchestration and Choreography?
- What is SOA?
- How do all of these fit together?
- WS-CDL and bioinformatics
- WS-CDL under the hood
- Formalisms and what they mean
- WS-CDL in practice (lets look at tools)
- What can I do with it
- Summary

What is a workflow?

The automation of business processes, in whole or in part, during which documents, information or tasks are passed from one participant to another for action according to a set of procedural rules

WFMC

What is orchestration?

orchestration [of web service] is a technique to recursively compose and orchestrate web services to provide a new composite web service

WS-BPEL

What is choreography?

A choreography is a global behavioral contract that describes (and therefore can be used to constrain) the valid ordering of messages between services that make up some flow that meets some [business] objective

WS-CDL

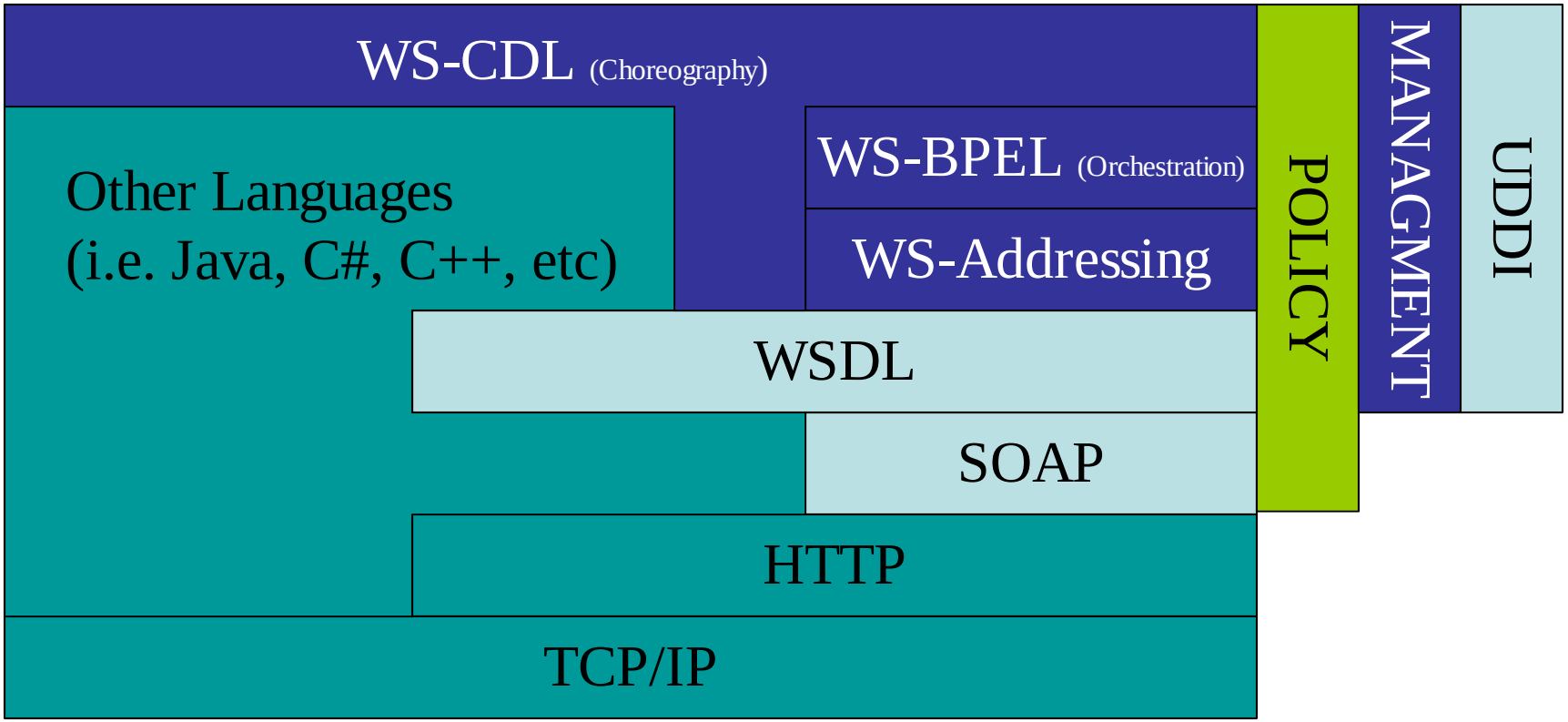
What is SOA?

- Service Oriented Architecture is a way of building distributed systems.
  - A service is a computational process with a WSDL interface.
  - A service may interact with other services through any communication mechanism (HTTP is but one).
  - Services are discovered at runtime.
  - SOA encourages document centric rather/messaging passing than function-centric programming (see WSDL2.0)

How does it fit together?

- An SOA is just a grid of services. Something has to give the grid and the services meaning.
- Meaning can be thought of as some notion of the common behavior of the services in achieving some goal. We might call this a workflow description.
- Distributed (peer to peer) workflows may be described using WS-CDL and executed at the peers using WS-BPEL. Thus orchestration is an execution idiom and choreography a description one.

How does it fit together?

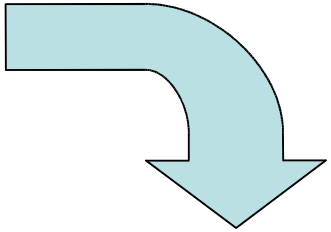


Legacy
Available
Nascent
Missing

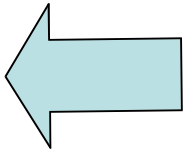
Relevance to Bioinformatics

- Formalism

Agents	Communication Events
Small molecules	Electron Sharing
Proteins	Protein-protein interaction, binding, phosphorylation, methylation, etc
Cells	Material consumption, environmental sensing, etc



Common formalisms



Agents	Communication Events
Network service	TCP/IP read/write
Email client/server	SMTP read/write
Browser server	HTTP read/write
WS-CDL service	send/receive

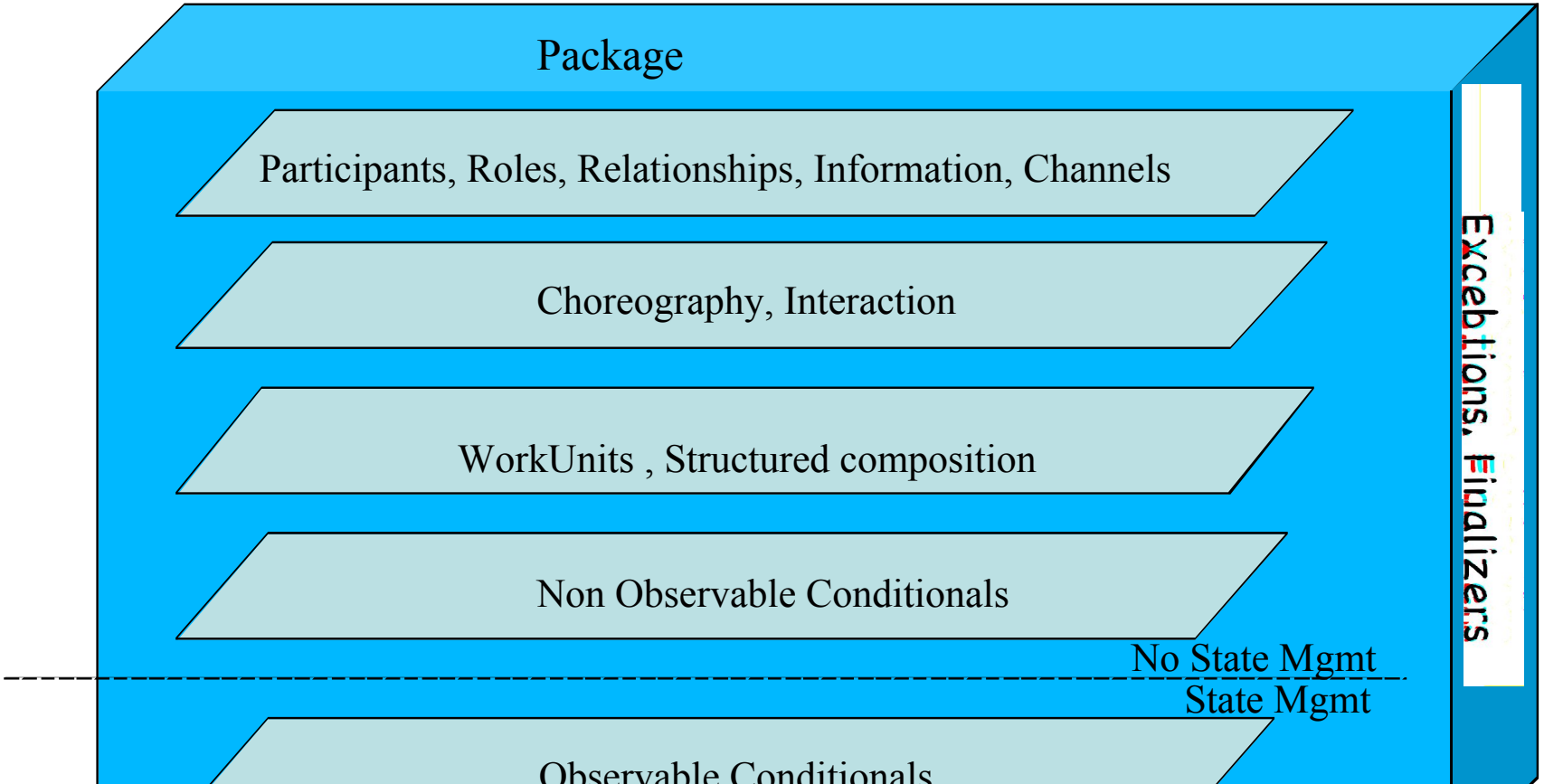
Relevance to Bioinformatics

- SOA
  - Emergence of WSDL described services (KEGG, BLAST, FASTA, Swiss-Prot, … etc)
  - Componentization for reuse and greater availability
  - Decrease in costs and complexity of data integration
  - WSDL, SOAP, Java, .NET, …. and the rest of the stack presented in the context of a service grid.

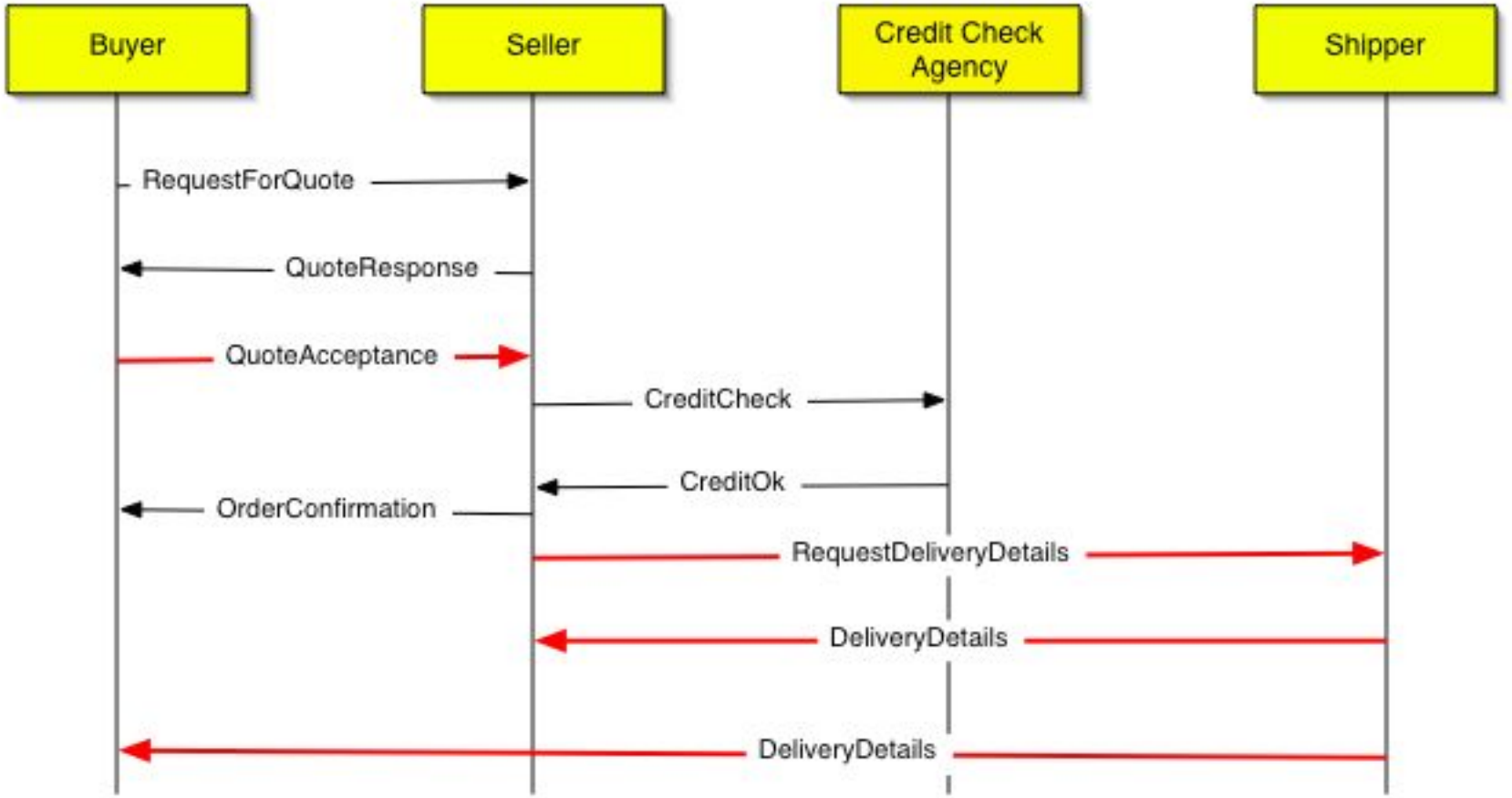
Relevance to Bioinformatics

- Process volatility
  - In-silico experimentation as workflows across a peer to peer SOA
  - Contractual descriptions for clinical trial protocols (Vioxx) that can be proven to have been followed
  - Outsourcing and yet remaining in control
  - WS-BPEL and WS-CDL

WS-CDL under the hood



WS-CDL under the hood



Normal Collaboration

WS-CDL under the hood

```
<interaction name="                                          " operation="          ÓchannelVariable="              ">
Ê  <description type="          ">            </description>
Ê  <participateRelationshipType="          " fromRole="              " toRole="              " />
   <exchange name="            " informationType="              " action="       "></exchange>
</interaction>

<interaction name="                                          " operation="          " channelVariable="             ">
   <description type="          ">                                  </description>
Ê  <participateRelationshipType="          " fromRole="              " toRole="              " />
    <exchange name="            " channelType="              " action="       ">
      send variable="                                " />
      receivevariable="                                " />
    </exchange>
</interaction>


<interaction name="                                                  " operation="              Ó
channelVariable="              ">
   <description type="          ">                                </description>
   participateRelationshipType="          " fromRole="              " toRole="              " />
   <exchange name="                      " informationType="                  " action="       "></exchange>
   <exchange name="                     " informationType="                 " action="       "></exchange>
</interaction>


<interaction name="                                  " operation="          " channelVariable="             ">
   <description type="          ">                                </description>
   participateRelationshipType="          " fromRole="              " toRole="              " />
   <exchange name="                " channelType="              " action="       ">
Ê    <send variable="                                " />
Ê    <receivevariable="                                " />
Ê  </exchange>
</interaction>

<interaction name="                                      " operation="          " channelVariable="             ">
   <description type="          ">                                </description>
   participateRelationshipType="          " fromRole="              " toRole="              " />
   <exchange name="                    " informationType="                  " action="       "></exchange>
</interaction>
```

WS-CDL under the hood

```
<?xml version="1.0" encoding="UTF-8" ?>
<package name="                " author="                "
version="    "targetNamespace ="                                  "
xmlns="http://www.w3.org/2004/12/ws-chor/cdl"
xmlns:bs="http://www.pi4tech.com/ cdl/BuyerSellerExample-1">
<description type="            ">                                                </description>

ÉÉÉÉ

 <choreography name="     " root="     ">
Ê<description type"          ">                                                  </description>

   ÉÉÉÉ

  <sequence>
   <interaction name"                                    "  operation"              "channelVariable"            " initiate    ">
Ê    <description type"          ">                 </description>

Ê    <participateRelationshipType"          "fromRole="              "toRole="              " />
     <exchange name ="       "informationType"                    " action"       ">
Ê      <description type"          ">                 </description>
Ê    </exchange>
       exchange name ="        "informationType"          " action"       ">
Ê      <description type"          ">                 </description>
Ê    </exchange>
     </interaction

    ÉÉÉÉ

  </sequence>
 </choreography>
</package>
```

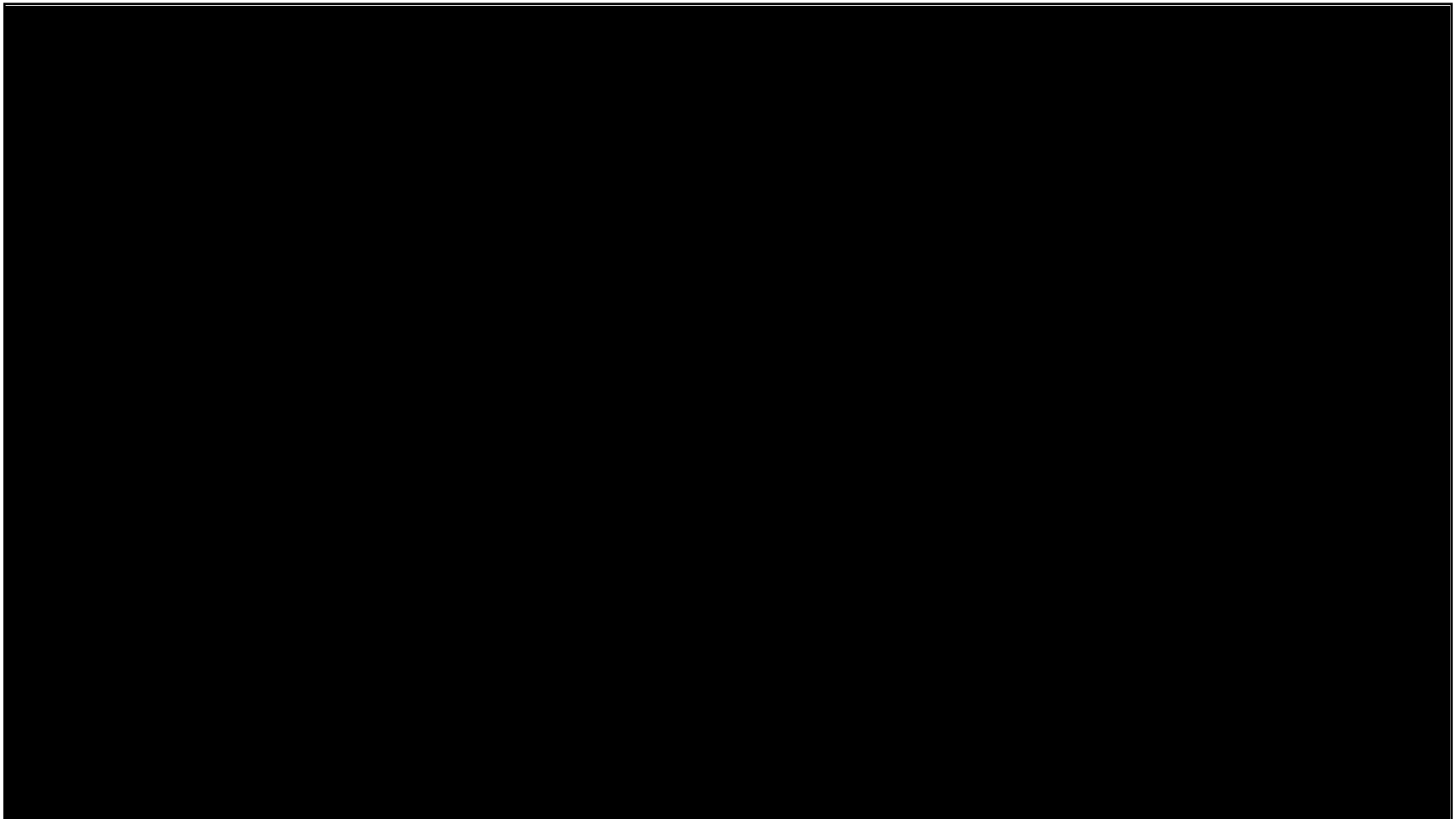
WS-CDL under the hood

```
<workunit name="                                    " repeat="                  ">
  <choice>
    <silentAction roleType="                ">
      <description type="          ">                              </description>
      silentAction>

    <sequence>
      <interaction name="                                                  " operation="           "channelVariable="            ">
        <description type="          ">           </description>
        <participateRelationshipType="          " fromRole="             "toRole="              " />
        <exchange name="            "informationType="                " action="       ">
        </exchange>
      </interaction>
      <interaction name="                                                  " operation="           "channelVariable="            ">
        <description type="          ">                              </description>
        <participateRelationshipType="          " fromRole="             "toRole="              " />
        <exchange name="            "channelType="                " action="       ">
          <send variable="                                  " />
          <receive variable="                                 " />
        </exchange>
      </interaction>
      <assignroleType="              ">
        <copy name="     ">
          <sourceexpression="     " />
          <targetvariable="                                 " />
        </copy>
      </assign>
    </sequence>

    <sequence>
      <interaction name="                                                  " operation="           "channelVariable="            ">
        <description type="              ">           </description>
        <participateRelationshipType="          " fromRole="             "toRole="              " />
        <exchange name="            " informationType="                " action="       ">
        </exchange>
        exchange name="                  " informationType="                " action="       ">
          <description type="             ">                    </description>
```

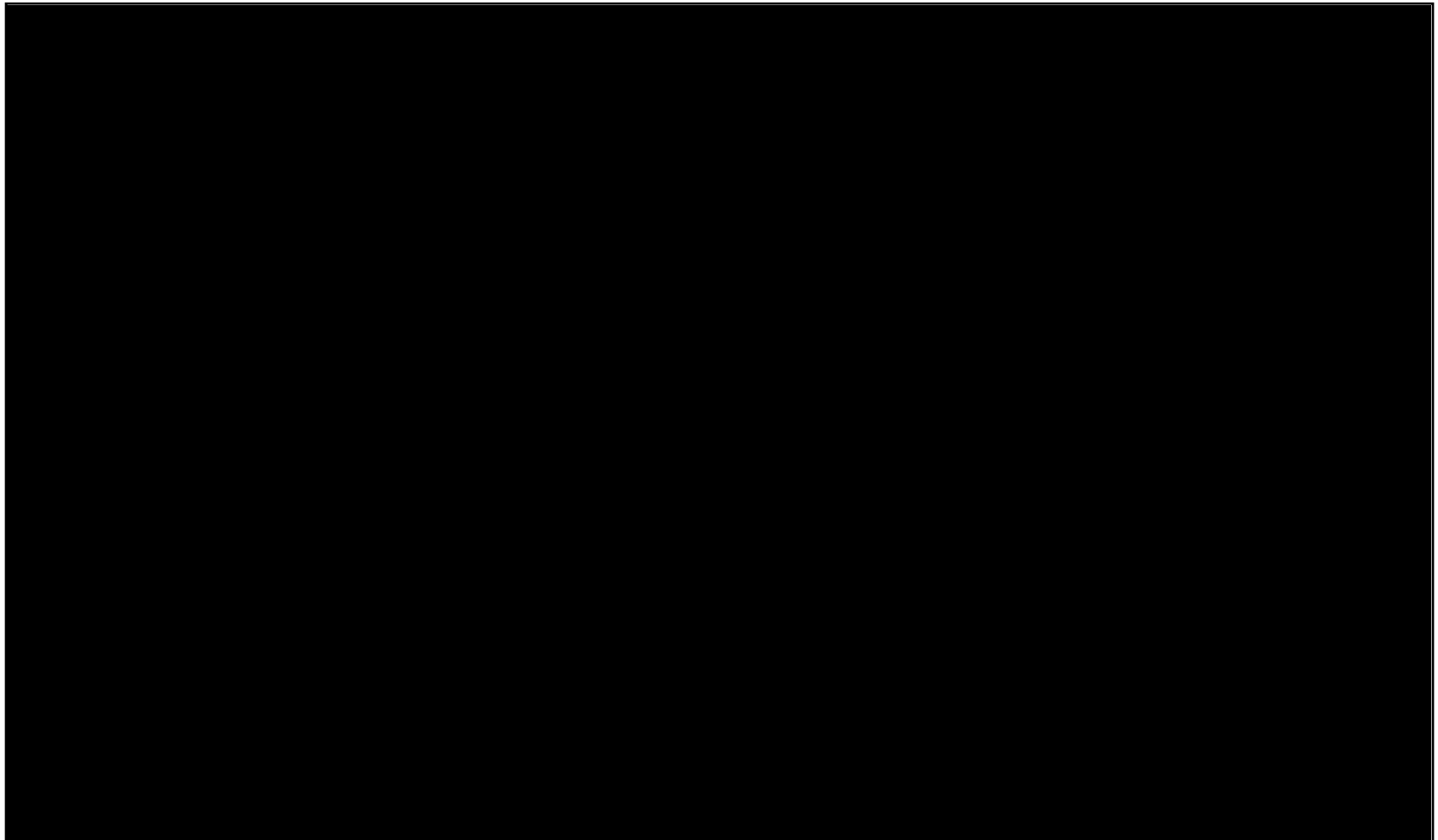
WS-CDL under the hood

```
<parallel>
  <workunit name="                    ">
    <sequence>
      <interaction name="                                    " operation="          "channelVariable="                  ">
Ê       <description type="          ">                                                    </description>
Ê       <participateRelationshipType"                 " fromRole="              "toRole"                        " />
        exchange name="          "informationType"                " action"       "></exchange>
Ê     </interaction>

       choice>
         sequence>Ê
           interaction name"                              "  operation"           "channelVariable"                  ">
Ê        <description type"          ">                                                  </description>
Ê          <participateRelationshipType"                " fromRole="              "toRole"                        " />
           exchange name="               "informationType"                " action"       "></exchange>
Ê        </interaction>
           assignroleType"              ">
Ê            <copy name="     ">
Ê              <sourceexpression"     " />
Ê              <targetvariable"                                  " />
Ê            </copy>
Ê          </assign>
           sequence>Ê

         sequence>Ê
           interaction name"                           "  operation"        "channelVariable"                  ">
Ê        <description type"          ">                                                  </description>
Ê          <participateRelationshipType"                "fromRole="              " toRole"                        " />
           exchange name="                 " informationType"                " action"       "> </exchange>
Ê        </interaction>
           assignroleType"              ">
Ê            <copy name="     ">
             Ê  <sourceexpression"     " />
Ê              <targetvariable"                                  " />
Ê            </copy>
Ê          </assign>
           sequence>Ê
       choice>
     sequence>Ê
   workunit>


   workunitname ="               " guard"                   "blocking"    ">
     ÊÊ
Ê </workunit>
</parallel>
```

WS-CDL under the hood



WS-CDL under the hood



Formalisms

- Pi-calculus
  - Algebraic encoding of behavior
  - Reduction rules to show progress
- Static checking for liveness (livelock and deadlock)
- Composition
- Channel/port passing (dynamic topologies)
- Higher order calculii
  - Includes stochastic pi-calculus used for in-silco experiments to simulate interaction between molecules

Formalisms

Model	Completeness	Compositionality	Parallelism	Resources
Turing Machines	☑	☒	☒	☑
Lambda	☑	☑	☒	☒
Petri Nets	☑	☒	☑	☑
CCS	☑	☑	☑	☒
π	☑	☑	☑	☑

Formalisms

Operation	Notation	Meaning
Prefix	τ.P	Sequence
Action	$\bar{x}(y)$, $x(y)$	Communication
Summation	a.P + b.Q $\cdot_{i=1..n} P_i$	Distributed Choice
Recursion	P={É.. }.P	Repetition
Replication	!P	Repetition
Composition	P | Q	Concurrency
Restriction	(νx)P	Encapsulation
Nothing	0	Do nothing

System = (!Client | !IdleServer)

Client(o,c,req,rsp) = o.req_1.rsp1.req_2.rsp2.c.Client(o,c,res,rsp)

IdleServer(o,req,rsp,c) = o.BusyServer(o,req,rsp,close)

BusyServer(o,req,rsp,c) = req.rep.BusyServer(o,req,rsp,c) + c.IdleServer(o,req,rsp,c)

Formalisms

WS-CDL	**The π-calculus**
The channels	a pair of "ports" in the π-calculus
An interaction	message exchange that occurs between paired ports
message	a polyadic message
type	sorts
Guarded workunit	Process pattern

WS-CDL in practice

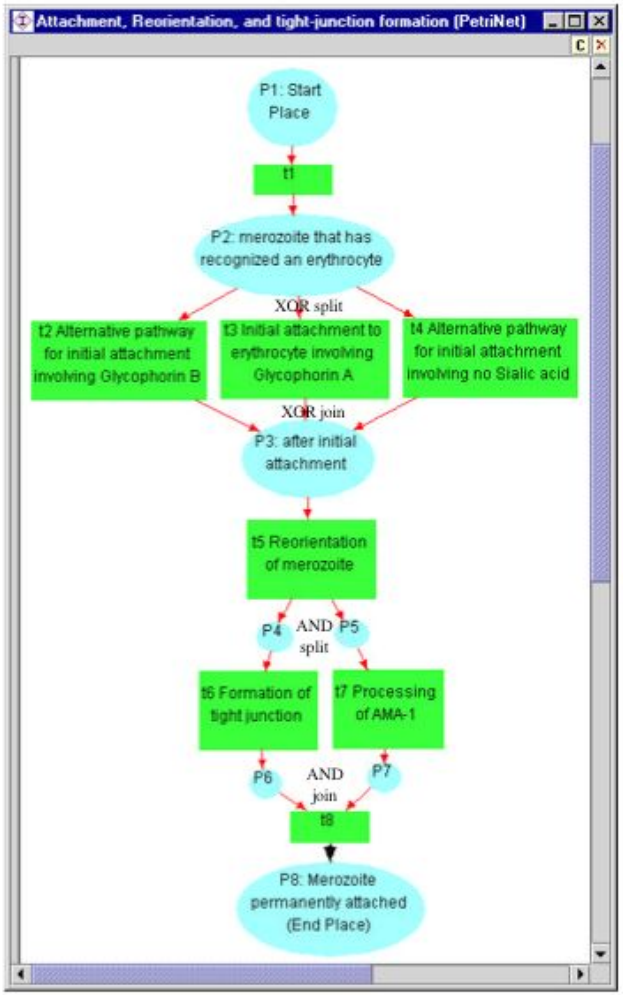
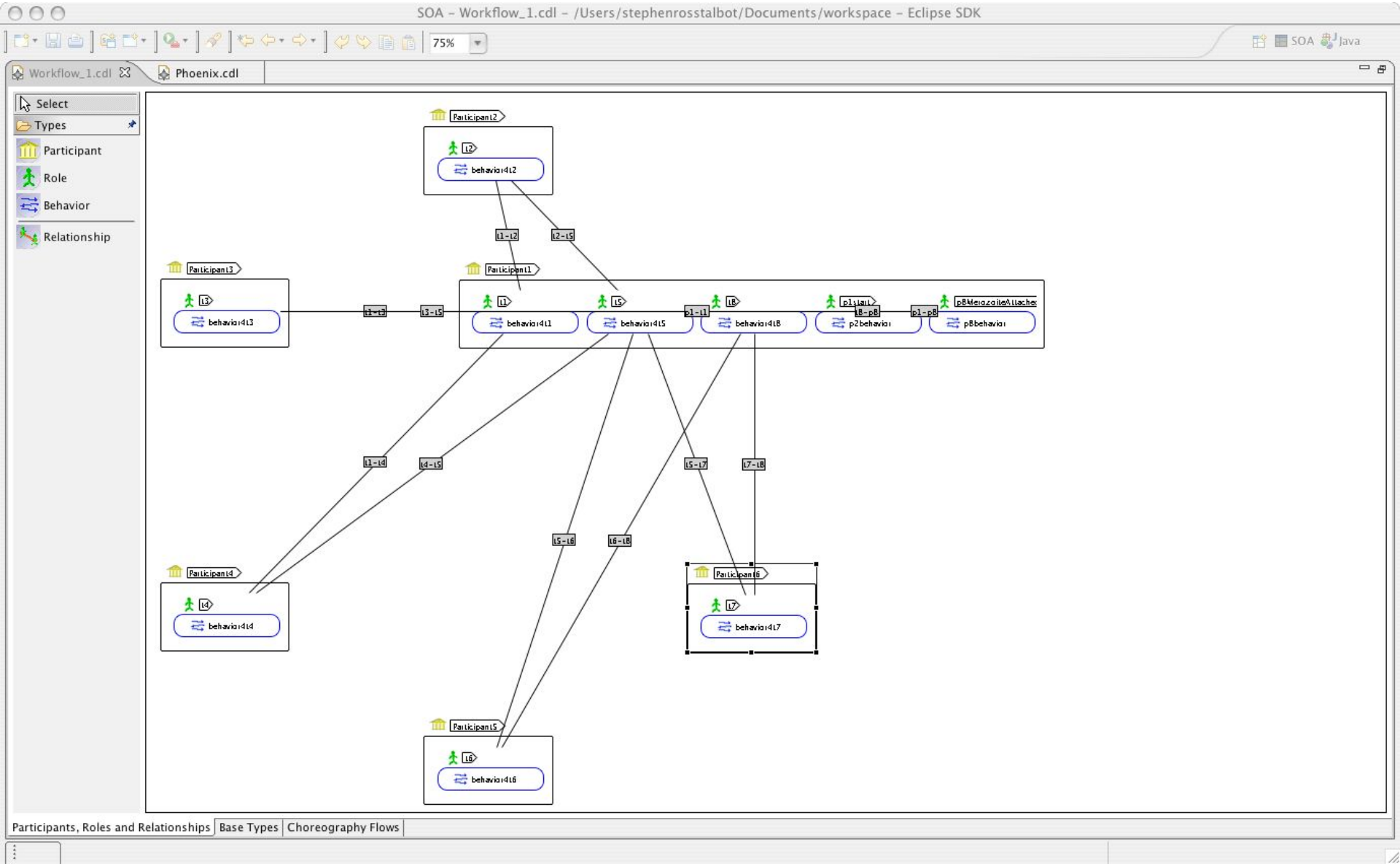


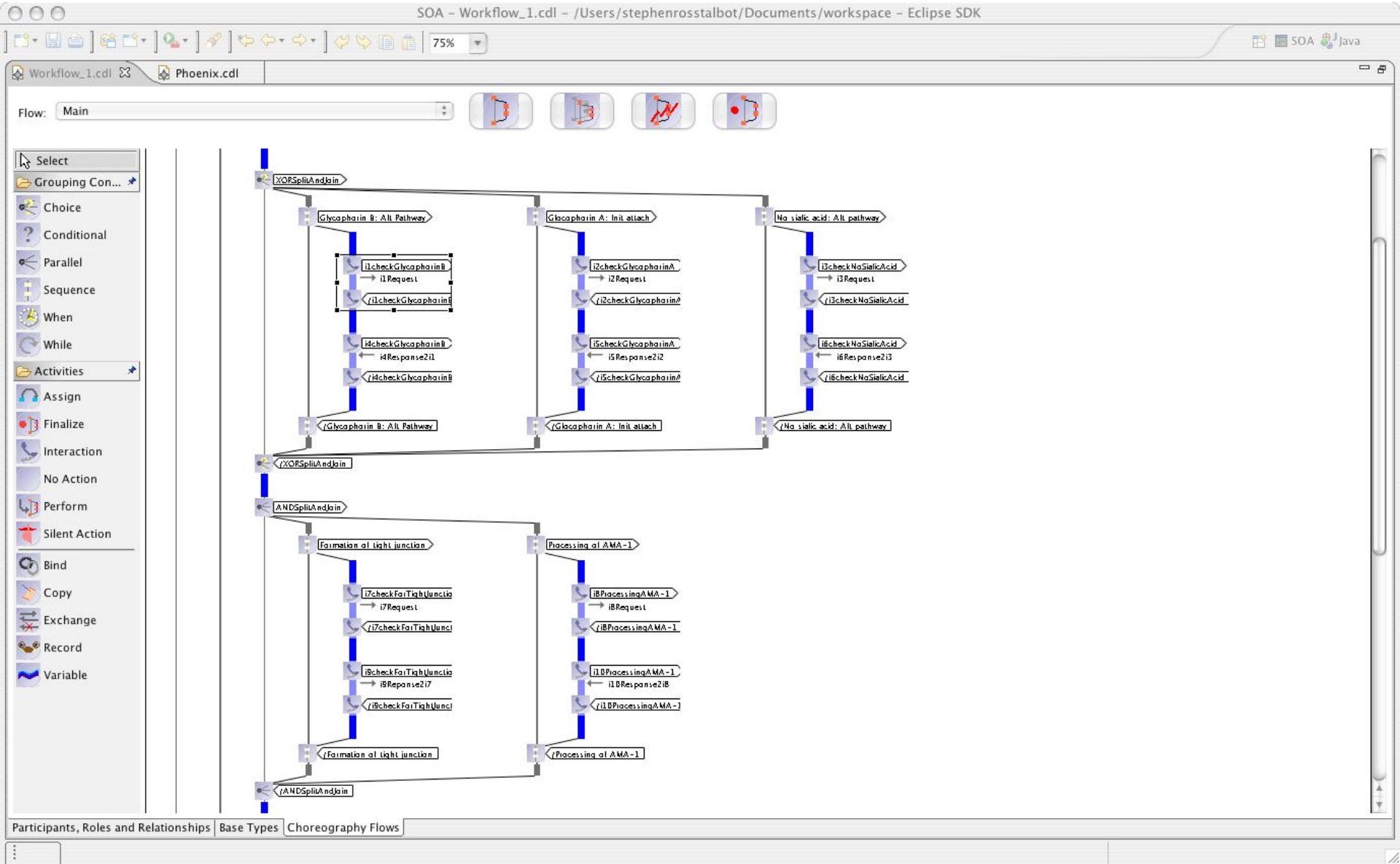
Figure 5. A Petri Net model of the invasion process, corresponding to the Workflow model shown in Figure 2. Places are shown as circles, and transitions as rectangles, and are labeled as $t_1..t_8$. The first and last places in the Petri Net are also labeled (as P_1 and P_8). Implicit XOR split and joins are marked as "XOR split" and "XOR join", respectively. AND split and joins are also marked.

Modeling biological processes using Workflow and Petri Net models
Mor Peleg, Iwei Yeh, Russ B. Altman
Standford Medical Informations, Standford Universirt, Stanford CA 94305, USA

WS-CDL in practice



WS-CDL in practice



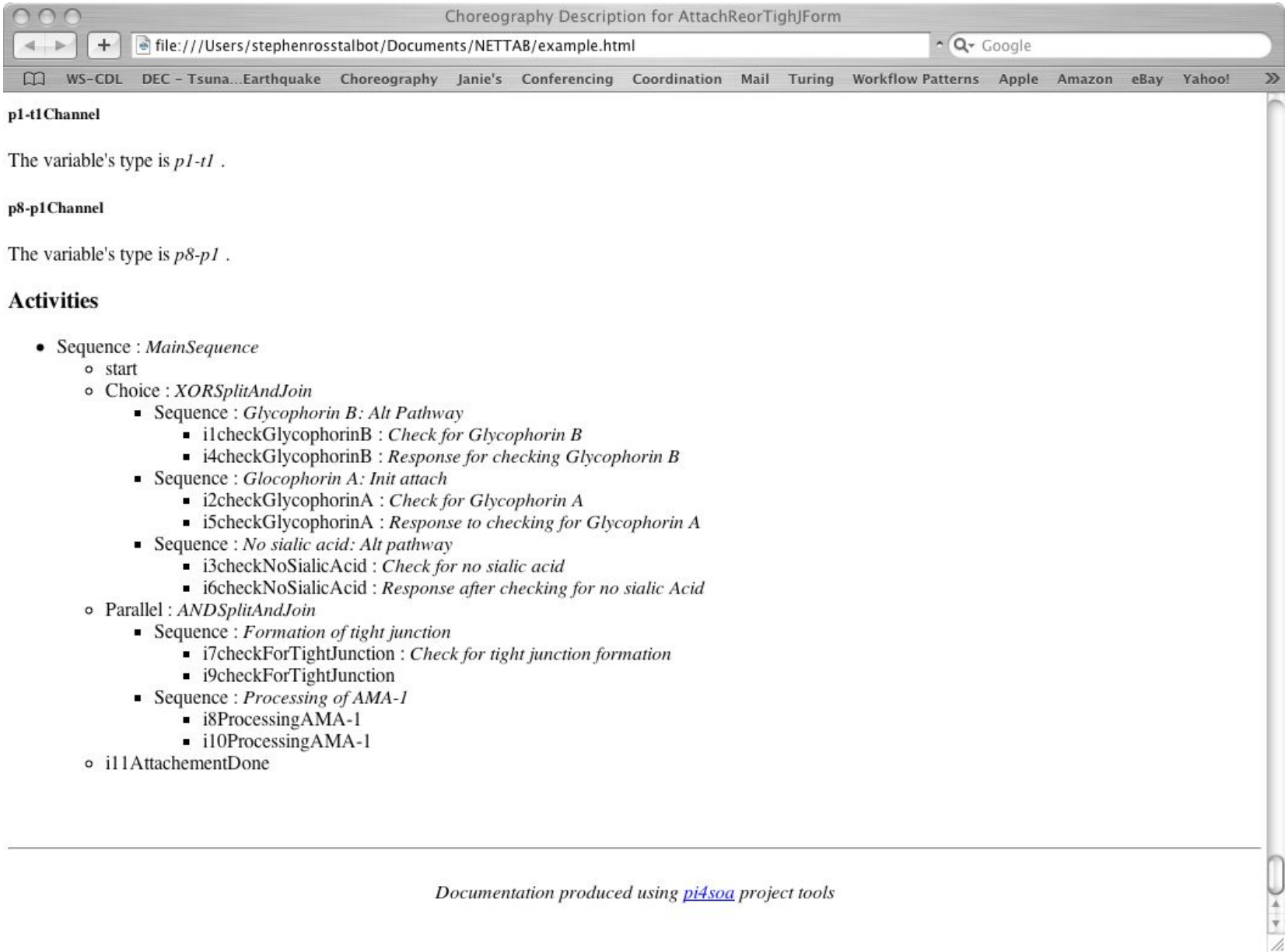
WS-CDL in practice

```
+ <variableDefinitions>
- <sequence>
    <description type="documentation">MainSequence</description>
  + <interaction name="start" operation="start" channelVariable="p1-t1Channel">
  - <choice>
      <description type="documentation">XORSplitAndJoin</description>
    - <sequence>
        <description type="documentation">Glycophorin B: Alt Pathway</description>
      + <interaction name="i1checkGlycophorinB" operation="checkGlycophorinB" channelVariable="t1-t2Channel">
      + <interaction name="i4checkGlycophorinB" operation="checkGlycophorinB" channelVariable="t2-t5Channel">
      </sequence>
    - <sequence>
        <description type="documentation">Glocophorin A: Init attach</description>
      + <interaction name="i2checkGlycophorinA" operation="checkGlycophorinA" channelVariable="t1-t3Channel">
      + <interaction name="i5checkGlycophorinA" operation="checkGlycophorinA" channelVariable="t3-t5Channel">
      </sequence>
    - <sequence>
        <description type="documentation">No sialic acid: Alt pathway</description>
      + <interaction name="i3checkNoSialicAcid" operation="checkNoSialicAcid" channelVariable="t1-t4Channel">
      + <interaction name="i6checkNoSialicAcid" operation="checkNoSialicAcid" channelVariable="t4-t5Channel">
      </sequence>
    </choice>
  - <parallel>
      <description type="documentation">ANDSplitAndJoin</description>
    - <sequence>
        <description type="documentation">Formation of tight junction</description>
      + <interaction name="i7checkForTightJunction" operation="checkForTightJunction" channelVariable="t5-t6Channel">
      + <interaction name="i9checkForTightJunction" operation="checkForTightJunction" channelVariable="t6-t8Channel">
      </sequence>
    - <sequence>
        <description type="documentation">Processing of AMA-1</description>
      + <interaction name="i8ProcessingAMA-1" operation="processAMA-1" channelVariable="t5-t7Channel">
      + <interaction name="i10ProcessingAMA-1" operation="processingAMA-1" channelVariable="t7-t8Channel">
      </sequence>
    </parallel>
  + <interaction name="i11AttachementDone" operation="start" channelVariable="p8-p1Channel">
  </sequence>
</choreography>
</package>
```

What can I do with it?

- Simulation:
  - I can test it (simulate the message exchanges)
- Generation:
  - I can generate Java or BPEL code, deploy and execute or run it as a set of peer services (no single point of control)
- Documentation:
  - I can produce documentation (html) to describe it
- Execution:
  - I can monitor the threads of execution through it

What can I do with it?



Summary

- WS-CDL is the Web Services Choreography Description Language (CDL for short)
- Common formalism (the pi-calculus) between SOA/WS-CDL and bioinformatics
- WS-CDL to describe workflow, Orchestration to execute workflow
- WS-CDL description for compliance

Acknowledgments

- Greg Meredith of Djinnisys
- Maria Mirto (for some example and early access to papers)
- Dr Gary Brown (pi4tech)

Grazie
Thank You

Q & A