The Missing Features of Workflow Systems for Scientific Computations

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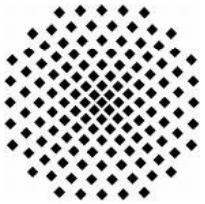


Universität Stuttgart
Germany

SimTech Stuttgart

- Cluster of projects with subject simulation technology
  - > 72 PhD projects
  - Systems biology, engineering, mathematics, philosophy, …
- Research topic of IAAS
  - Workflow management system for simulations
  - Based on business workflow technology

Agenda

- Introduction
  - Business and scientific workflow management (WFM)
- Discussing missing features
  - Tool integration
  - Deployment
  - Execution
  - Monitoring
  - Flexibility
  - Provenance
- Conclusion and outlook

Business Workflow Management

- Support of business processes since the 90s
- Nowadays established and well-proven
- General purpose systems
  - Universally designed
  - Independent of concrete business area
- High complexity
  - Lots of configuration options
- Process = product
- Exemplary systems
  - Commercial: IBM WebSphere family, Oracle SOA Suite, …
  - Open Source: Apache ODE, Bexee, Freeflou, …

Scientific Workflow Management

- Young research field
- Used to support scientists
  - Workflows implement experiments, simulations, computations
- Usually built from scratch
- Tailored to particular domains
- Exemplary systems
  - Kepler, Taverna, Triana, Pegasus, SEGL, e-BioFlow

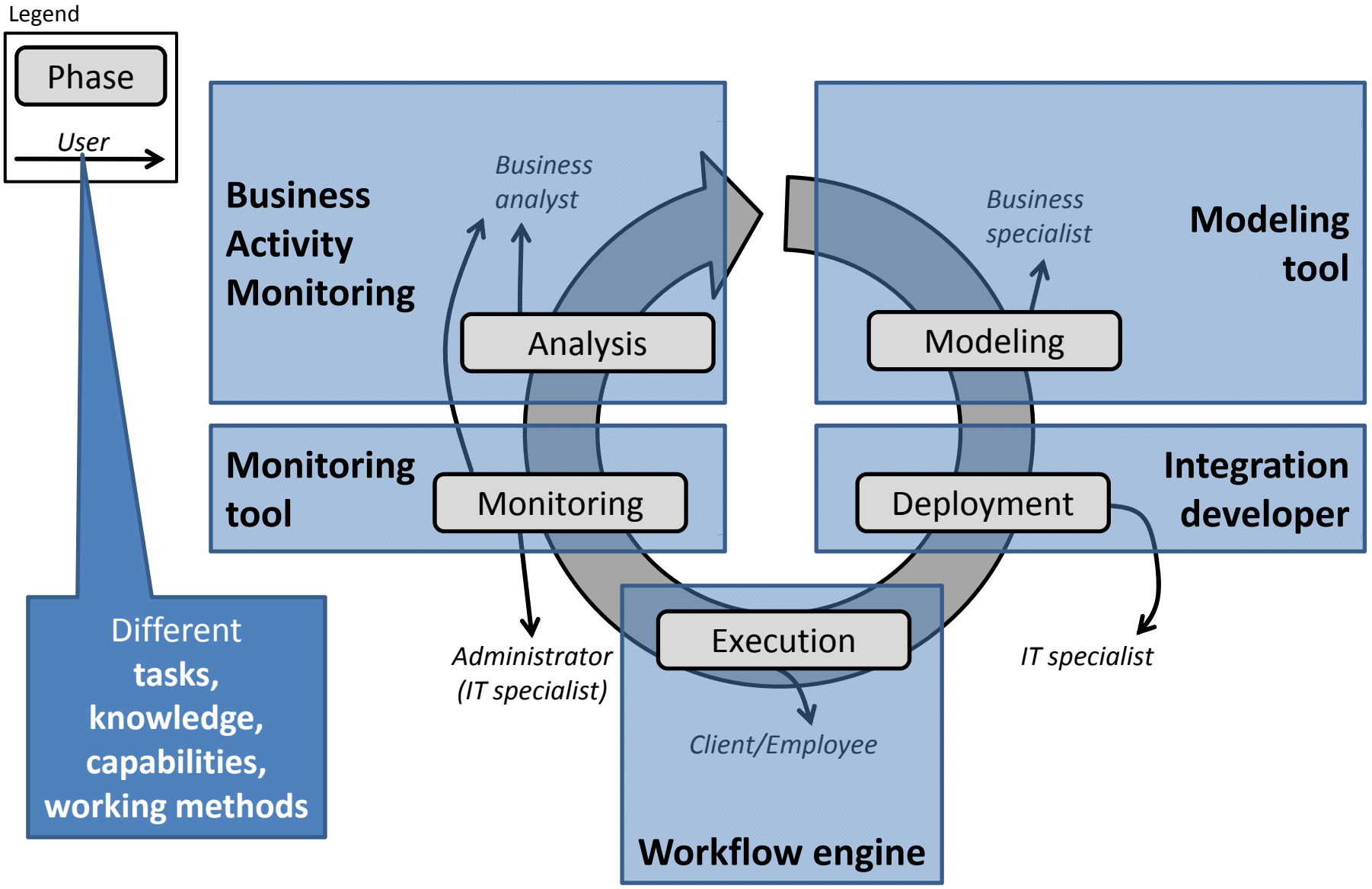
Business Workflow Technology for e-Science

- Endeavor to join the business and scientific WF community
  - i.e. to use business WfMSs in the scientific domain
- Advantages
  - Collaboration through use of standards
  - Existing tools as development basis
  - Robustness
  - Scalability (w.r.t. resources, workflow models, workflow instances)
  - …

Requirements on Scientific WfMSs

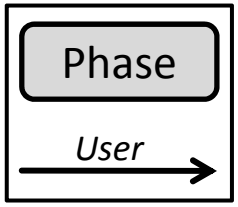
- Non-computer experts as users → high usability
- Long-running simulations
  - Can take hours, weeks or even months
- Importance of Data
  - Scientists think and model data-oriented
- Trial-and-error approach
  - Experiment design is an evolving process
- Grid support
  - To decrease run time of simulations + resource sharing
- Provenance
  - Reproducibility and trust

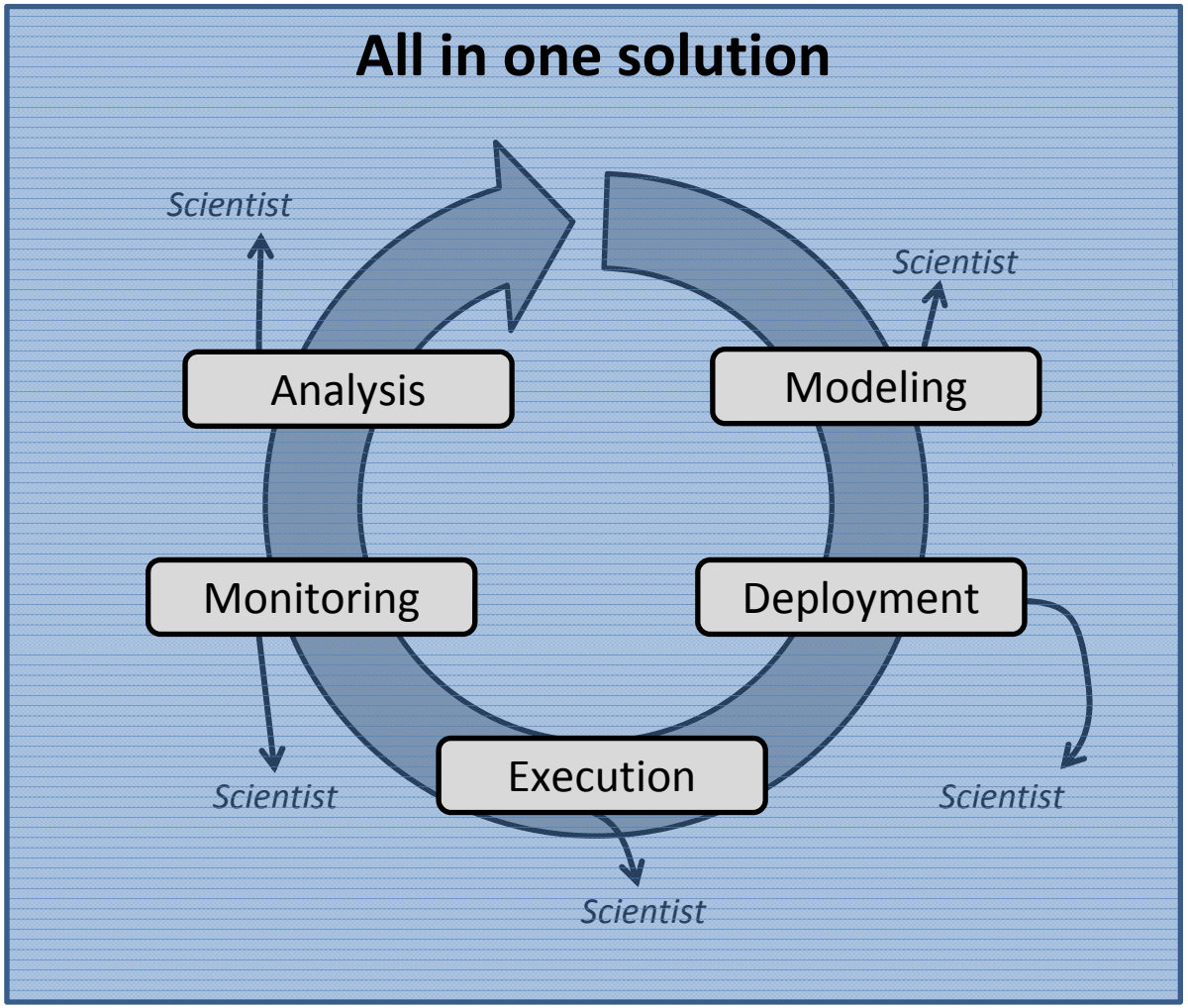
Life Cycle and Tool Integration



Life Cycle of Scientists

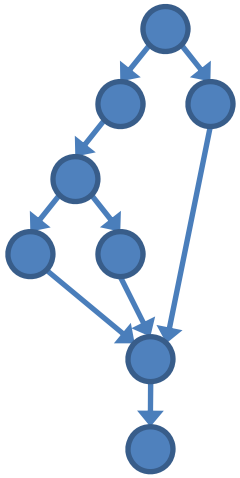
Legend





Deployment

Reuse of workflow parts



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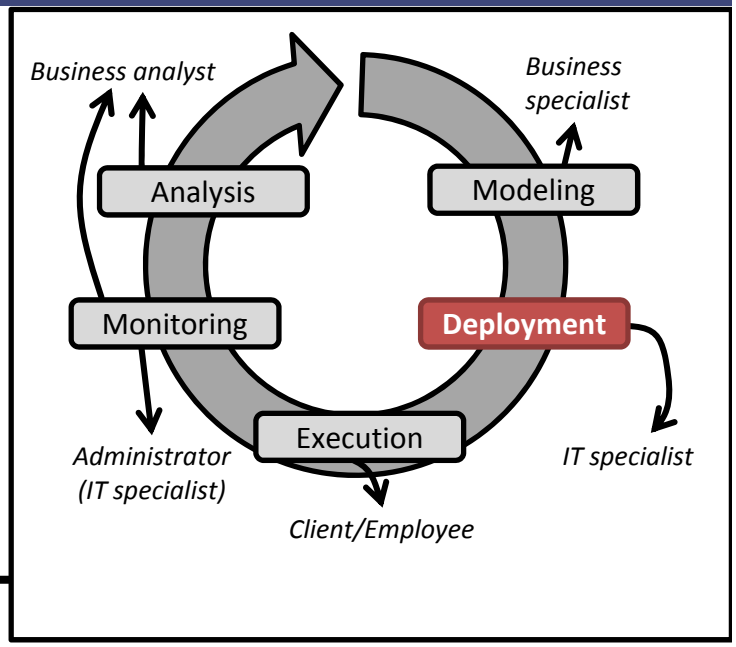


Modeling

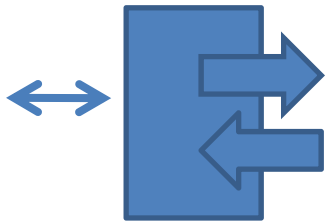
Execution

Efficient execution

Engine

Database

Robustness



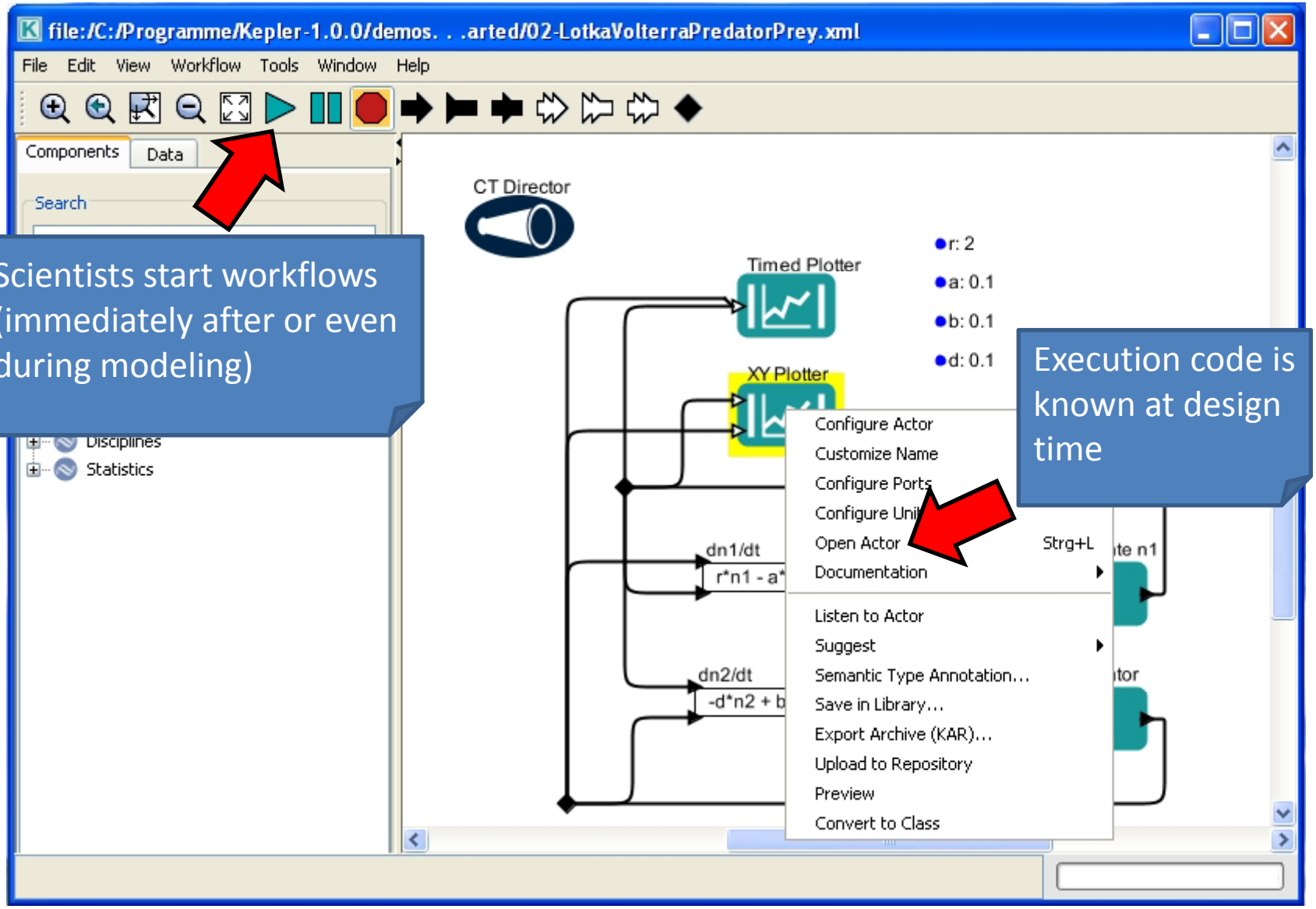
Web Service

Collaboration

Deployment Descriptor of Apache ODE

```
<deploy xmlns=„…" …>
  <process name="main:MagicSessionMain">
    <in-memory>true</in-memory>
    <active>true</active>
    <provide partnerLink="executePartnerLink">
      <service name="mws:MSMainExecuteService" port="MSExecutePort"/>
    </provide>
    <invoke partnerLink="responderPartnerLink">
      <service name="mws:MSResponderService" port="MSResponderPort"/>
    </invoke>
    <process-events generate="none">
      <enable-event>activityLifecycle</dd:enable-event>
      <scope-events name="aScope">
        <enable-event>dataHandling</bpel:enable-event>
        <enable-event>scopeHandling</bpel:enable-event>
      </scope-events>
    </process-events>
  </process>
</deploy>
```

Deployment in Scientific WFM – Kepler

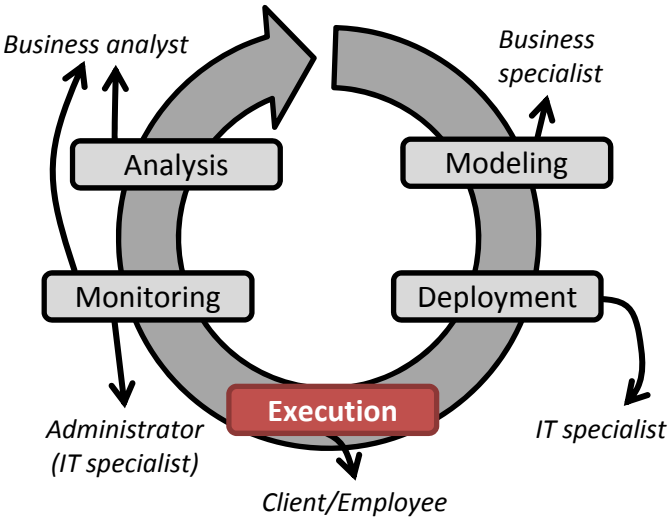


Deployment Specific Information in Kepler's MoML

```
<entity name="Open Database Connection" class="org.geon.OpenDBConnection">
  <property name="databaseFormat"
      class="ptolemy.data.expr.StringParameter" value="MySQL" />
  <property name="databaseURL"
      class="ptolemy.kernel.util.StringAttribute" value="jdbc:mySql://localhost:3306/" />
  <property name="username"
      class="ptolemy.data.expr.StringParameter" value="admin" />
  <property name="password"
      class="ptolemy.data.expr.StringParameter" value="password" />
</entity>
<entity name="Web Service Actor" class="org.sdm.spa.WebService">
  <property name="wsdlUrl" class="ptolemy.data.expr.StringParameter"
      value="http://localhost:8080/ode/testservice?wsdl" />
  <property name="methodName" class="ptolemy.data.expr.StringParameter"
      value="testOperation" />
  <property name="userName" class="ptolemy.data.expr.StringParameter"
      value="admin" />
  <property name="password" class="ptolemy.data.expr.StringParameter"
      value="password" />
</entity>
```

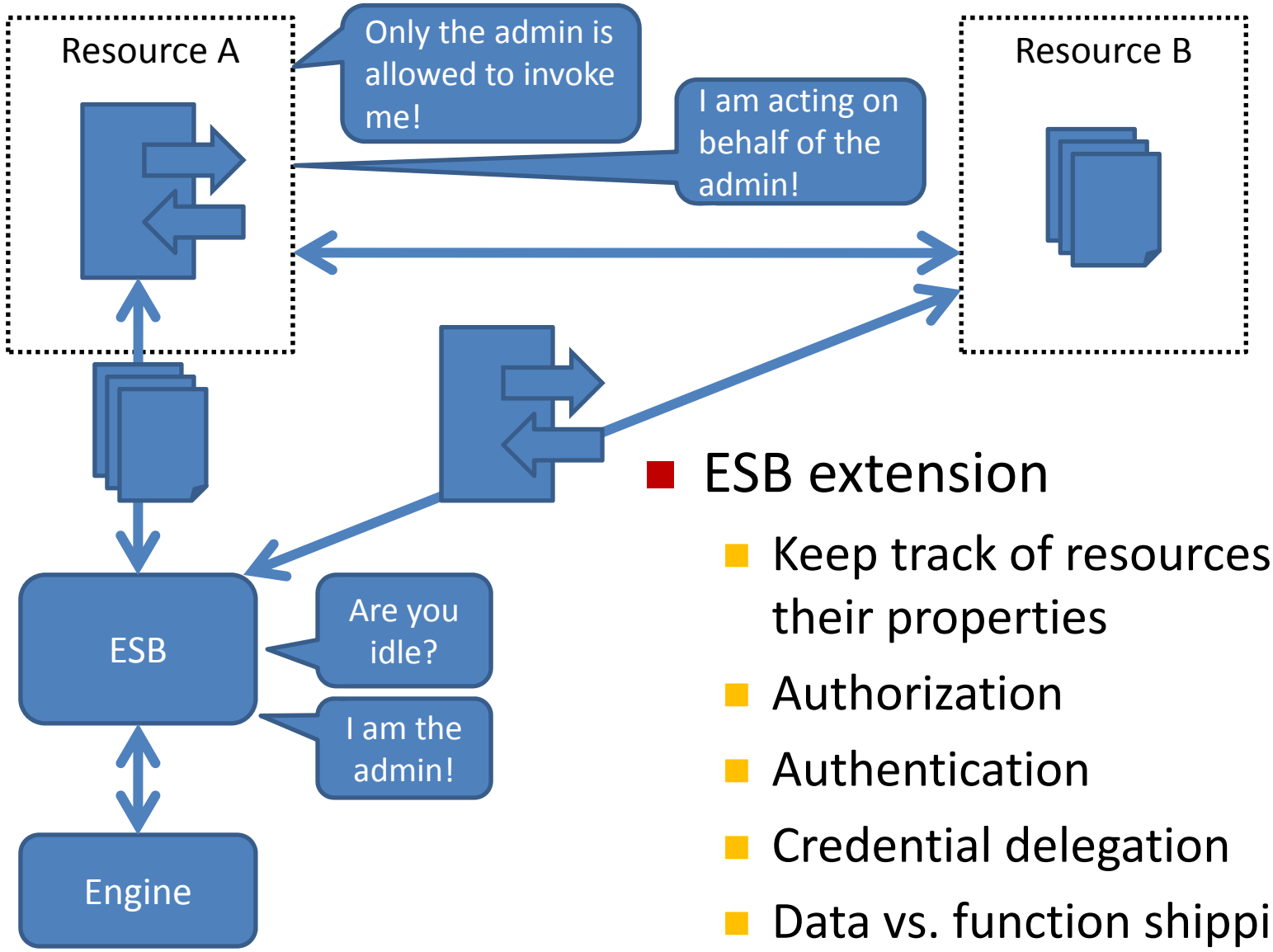
Execution

- Grid-awareness in business WfMSs via OGSA and WSRF
  - Resources can be accessed as stateful WSs



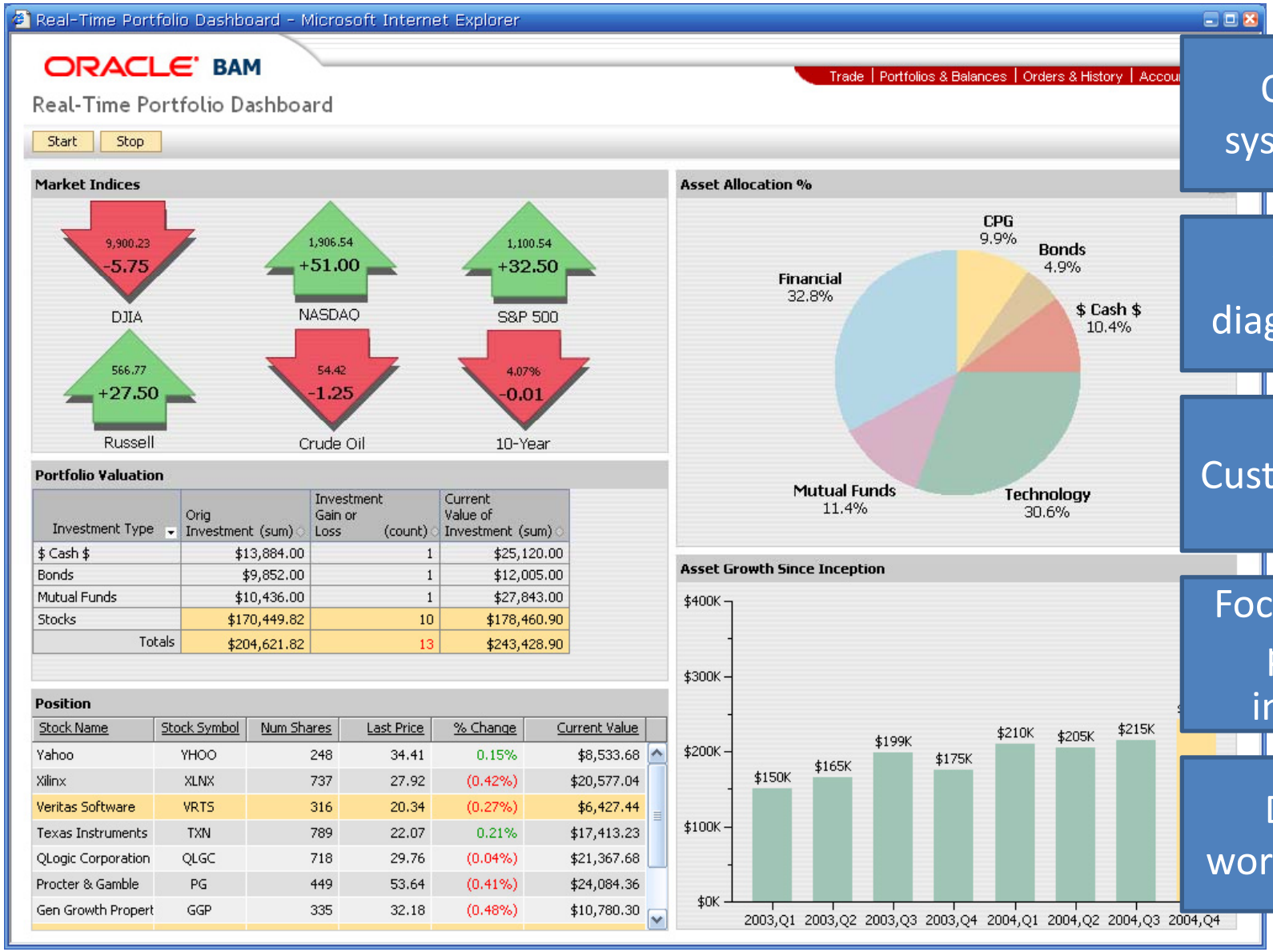
- Enterprise service bus (ESB) can be used to keep track of resources
  - Policy negotiation, finding, selecting, binding of services/resources

Recommendation for Execution



- ESB extension
  - Keep track of resources and their properties
  - Authorization
  - Authentication
  - Credential delegation
  - Data vs. function shipping

Monitoring & Analysis – Oracle BAM



Observe system state

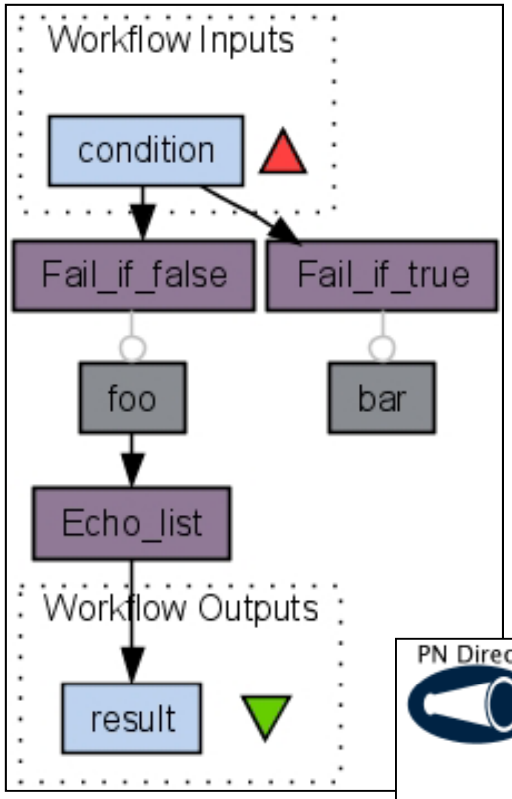
Tables, diagrams, etc.

Customizability

Focus: Lots of process instances

Data on workflow level

Monitoring and Analysis in Scientific WFM



Taverna

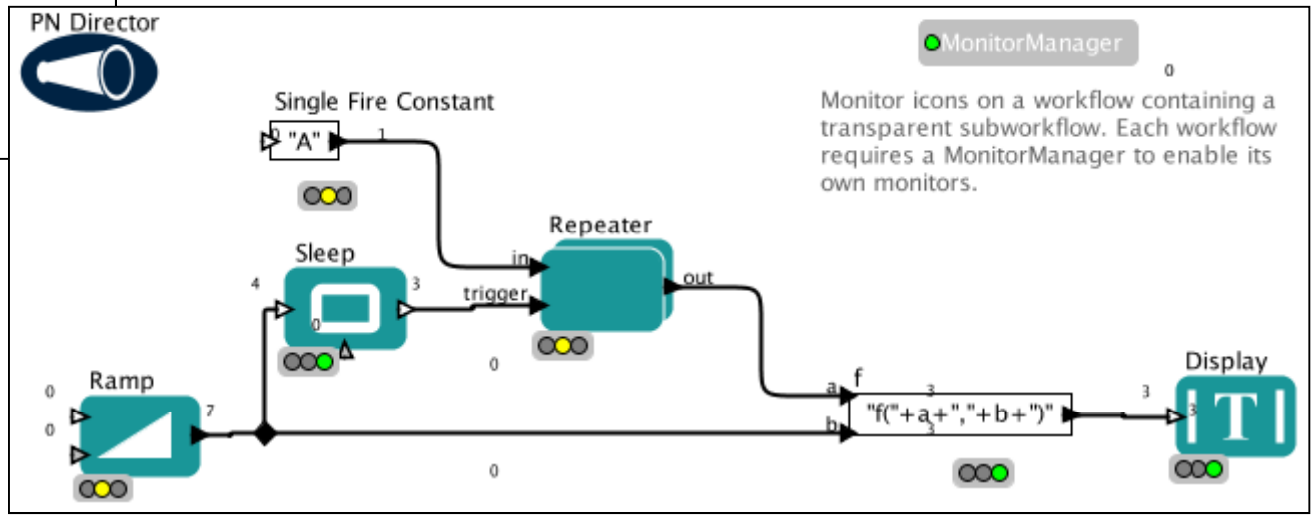
Scientists follow their experiments, simulations, …

Graph-oriented

Focus: single instances

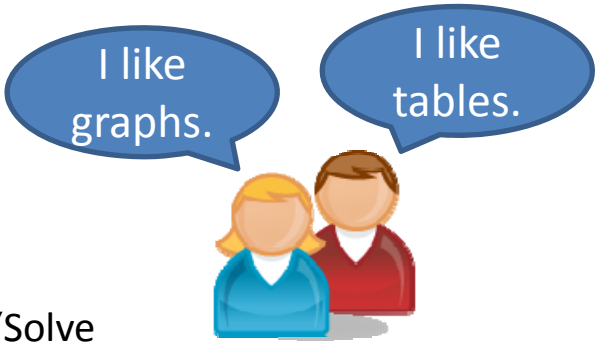
Restricted customizability

Kepler



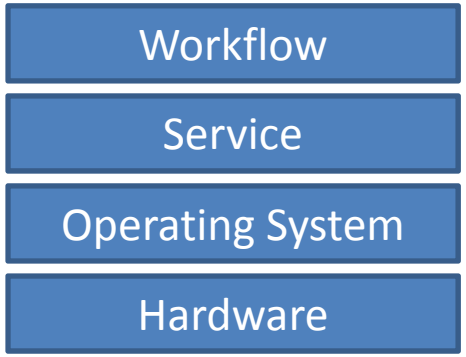
Recommendation for Monitoring and Analysis

- Adopt concepts
  - User notification
  - Customizability
  - Event model



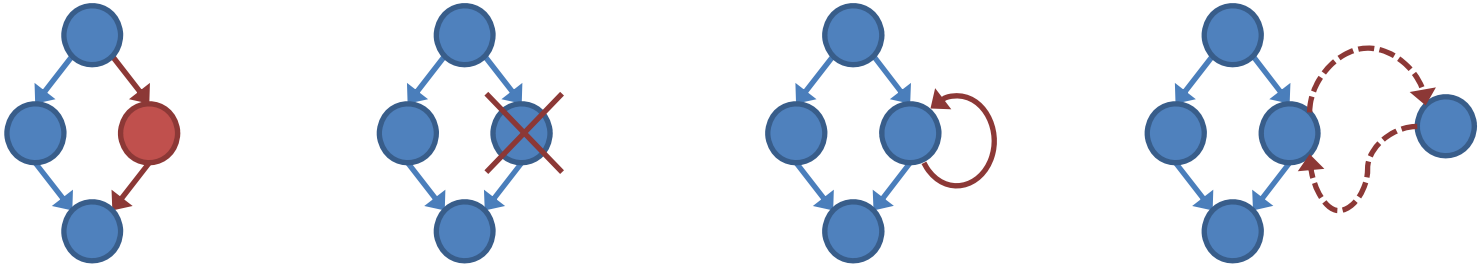
Activity “Solve equation system” has started

- Extensions needed
  - Focus on single instances
  - Monitoring in Grid environments



Flexibility in Business WFM

- Avoid change
- Workflow adaptation
  - Schema evolution
  - Ad hoc adaptation



Insert activity | Delete activity | Reiteration | Inquiry

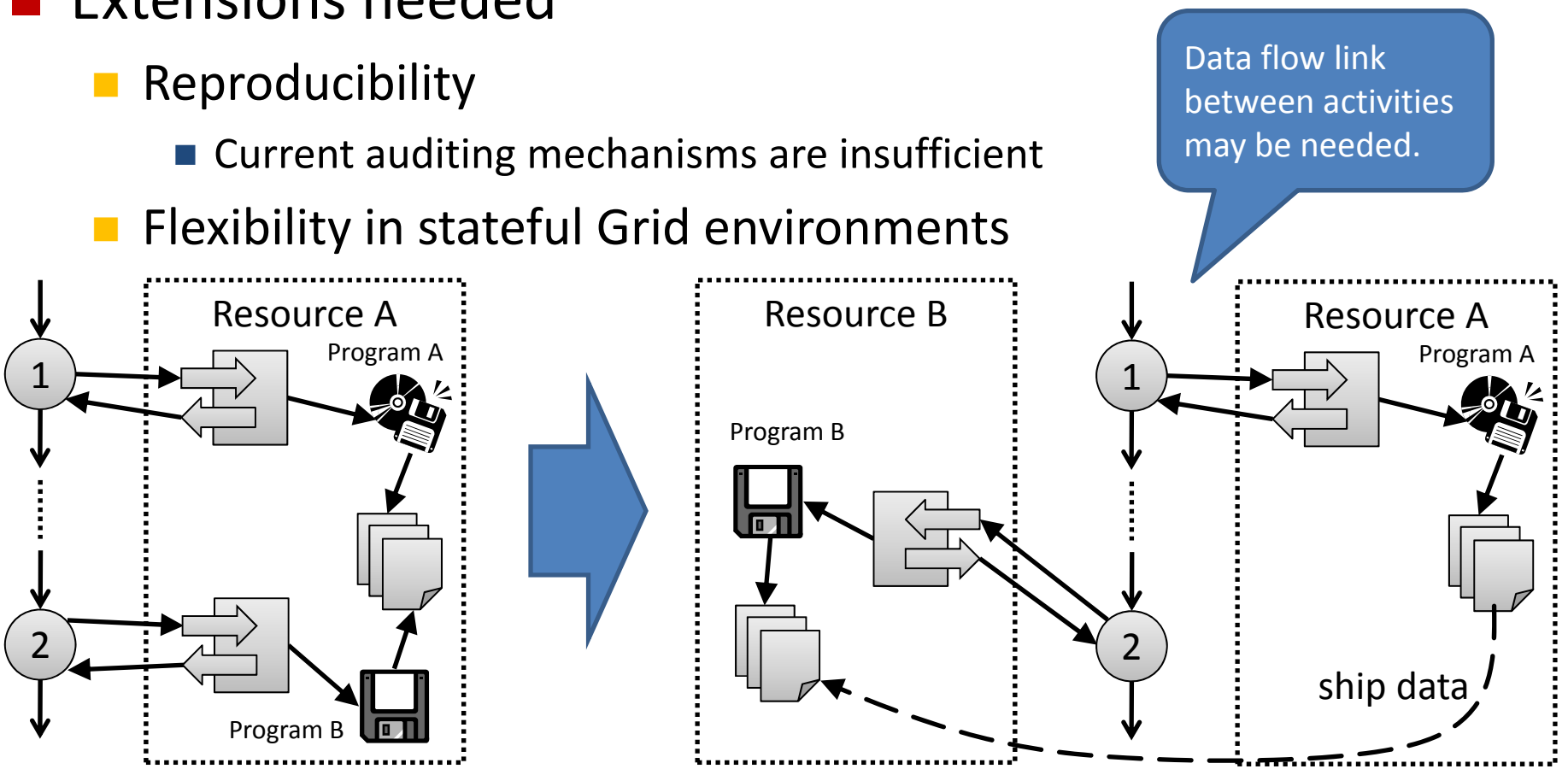
- Well-known, but insufficiently implemented
  - Versioning is typical approach

Flexibility in Scientific WFM

- Helps scientists to conduct experiments in a trial-and-error manner
- Currently almost unaddressed
  - Pegasus
    - Late binding of resources, workflow reduction, retry activities
  - Taverna
    - Retry activities, use alternative services
  - e-BioFlow
    - Re-execution of workflow fragments

Recommendation for Flexibility

- Adopt existing concepts from the workflow technology
  - Fortunately, instance migration is of minor importance
- Extensions needed
  - Reproducibility
    - Current auditing mechanisms are insufficient
  - Flexibility in stateful Grid environments



Provenance

- Guarantee reproducibility of results
- Current audit trails can contribute but are insufficient
  - On workflow level only
  - Information on tools, versions, operating systems, hardware needed
  - How were services found, selected, bound, invoked?
- ESB events are needed (at least)

Conclusion and Future Work

- There are reasons for the discrepancy between what business WfMSs deliver and what scientists need
- It is reasonable to apply the conventional WF technology to scientific applications
- But: we identified many missing features
- We provided recommendations how this can be done
  - And we know: this is hard work!
- Planned future work
  - Implement a scientific WfMS built on top of existing open-source WF engine, modeling tool, and service bus
  - Special attention on Grid awareness, monitoring, flexibility, data centrality

Questions ???

Thanks for your attention!
Any questions?