Bridging the Gap Between Research and IT

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Productivity Continuum

Personal Productivity
- Self Service
- Captured Knowledge
- Data Discovery
- Process Verification

Workgroup
- Reusability
- Collaboration

Enterprise
- Integration
- SharePoint Management
- Scalability

- Consistency
- Security
Today’s Research Challenge

Drive Top Line Growth

More innovation
Increase R&D success rate
Re-user corporate knowledge
Improve data modeling and simulations
Increase time available for experiments

Reduce Costs

Reduce redundant experiments
Increase productivity
Increase R&D efficiency
Improve business processes
Automate key tasks

Companies with effective product innovation processes grow at three times the pace of those without (Source: PRTM Product Development Database).

Only 11% of R&D activities are related to innovation (Source: R&D Productivity Analysis, Yazdani, Holmes, A.D. Little)
## IT Strategic Priorities

<table>
<thead>
<tr>
<th>Strategy Expectations</th>
<th>Ranking of strategy priorities BU CIOs selected as one of their top 5 priorities in 2010 and 2013</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ranking</strong></td>
<td>2010</td>
</tr>
<tr>
<td>Reducing the cost of IT</td>
<td>1</td>
</tr>
<tr>
<td>Linking business and IT strategies and plans</td>
<td>2</td>
</tr>
<tr>
<td>Delivering projects that enable business growth</td>
<td>3</td>
</tr>
</tbody>
</table>

*Source: Gartner (February 2010)*
The Researcher’s Challenge

- Distribute & Report Results
- Present & Review Results
- Identify New Opportunity
- Gather Data
- Prepare Data for Experiment
- Import Data
- Build Model
- Validate Model
- Apply Model to Experiment
- Collate Results
- Reformat Results
- Generate Report
Pipeline Pilot Maturity Model

Enterprise
Data Integration
Visualization
Automation
Collaboration
Application Development & Deployment
Deployment of Best Practices

Biz Analyst  Project Mgr  Engineer/IT  Management

Work Group
Data Integration
Visualization
Automation
Collaboration

Biz Analyst  Engineer/IT  Project Mgr

Personal Productivity
Data Integration
Visualization
Automation

Scientist

Enterprise Adoption
Productivity Continuum

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Personal Productivity
Personal Productivity Challenges

- Lack of Developer Expertise
- Application Integration
- Code/Script Reusability
- Data Access

Personal Productivity
Pipeline Pilot: Protocols

- A highly efficient, flexible paradigm for data processing
- Pipelines guide the flow of data through a series of modular components
- Pipelines can perform:
  - Highly computational, batch processing tasks (millions of data rows)
  - Short-running integration and reporting tasks
Information Discovery & Access

Vendor

Corporate

Public

Web Services

Data Sources

Pipeline Pilot

SOAP

WSDL

REST

ODBC/JDBC

Files (Local/UNC)

SharePoint

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Workgroup
Workgroup Enablement

- Project Leader
- Developer
- Scientist
- Scientist
Workgroup Challenges

- Varied Expertise
- Academic/Contracting
- Global Resources
- Data Management
- Collaboration
- Workgroup Productivity
Pipeline Pilot Clients and User-types

Pipeline Pilot Professional Client

- Create and edit protocols
- Execute protocols
- Deploy / share protocols
- Develop Pipeline Pilot-based web applications

Pipeline Pilot Web Clients: Execute protocols, review results

Accelrys Web Port
Accelrys Custom Web Client
Microsoft SharePoint

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Many tasks require working across domain boundaries
Enterprise

- Consistency
- Security
Enterprise Enablement

Enterprise IT

Workgroup

Application Development

Support Services
Enterprise IT Challenges

- Increased Business Requirements
- Budget Constraints
- Resource Availability
- Data Management
- Collaboration
- Business Delivery
Pipeline Pilot - Scientific Informatics Platform

Scientist

Engineer

Biz Analyst

Management

Portal

Accelrys Apps

Reporting & Analytics

Text Mining

Image Analysis

Data Mining

3rd Party Algorithms

Chemistry

Biology

Materials

Engineering

Data Transformation & Modeling

Complex Data Integration

Numeric

Chemical Structures

Text

Biological Sequences

Corporate Data

Image

3rd Party Applications

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Pipeline Pilot SharePoint Bridge

- Pipeline Pilot provides the **science**
- SharePoint provides the **place to get it**
- Together they provide a **scientific collaboration and decision-support site**
Example SharePoint site

Shared Documents Web Part

Pipeline Pilot Web Parts
Consistency

• Validation
• Versioning
• Regression Testing
• Data Sources
• Role-based Security
Web Services Integration

Example
Publish Protocol as a Web Service
WSDL Endpoint

Execute

Launches a protocol job on the server with the given parameters. Provide a valid SessionID with each request. Use the Login method to get a valid SessionID.

Request:

- sessionID : xsd:string
- settings : JobExecutionSettings
- Source : xsd:anyURI
- X-Property : xsd:string
- Y-Property : xsd:string

Response:

- ExecuteResponse : return : JobExecutionOutcome

DeleteJob

Deletes the job directory from the server.

Request:

- jobID : xsd:string

Response:

- DeleteJobResponse
To see a list of available services on a specific server, enter a service URL and click Go. To browse for available services, click Discover.

Address:
http://ace:9944/scitegic/service/sync/Web%20Services/Examples/Generic/Plot%20Data

Services:
- PlotData
  - PlotDataPortType

Operations:
- DeleteJob
- Execute
- ListMethods
- Login

1 service(s) found at address
'http://ace:9944/scitegic/service/sync/Web%20Services/Examples/Generic/Plot%20Data?wsdl'.

Namespace:
PipelinePilot
static void Main(string[] args)
{
    PipelinePilot.ExecuteRequest job = new PipelinePilot.ExecuteRequest();
    job.

    Equals
    GetHashCode
    GetType
    sessionID
    settings
    Source
    ToString
    XProperty
    YProperty

    bool object.Equals(object obj)
    Determines whether the specified System.Object is equal to the current System.Object.

    Description
    File
    Line
    Column
    Project
    Only assignment, call, increment, decrement, and new object expressions can be used as a statement
    Program.cs
    13
    13
    13
    SOADemo
    ; expected
    Program.cs
    13
    17
    17
    SOADemo
    Identifier expected
    Program.cs
    13
    17
    17
    SOADemo
Robust Developer Support

Developer Support:
- Visual Studio/.NET Framework
- Java/Eclipse
- Web Services Description Language

Benefits:
- Robust Developer Support
- Structure Team Development for Applications
- Deployment and Change Management Controls
Scalability - Platform

Server
- Single Server
- Windows or Linux

Cluster
- Multi-Server
- Linux

Grid
- Sun Grid Engine
- HP MPI
- Linux
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Thank You

- Accelrys will be holding additional IT focused webinars. Please check back often and register at
  - http://accelrys.com/events/webinars/

- Please visit our Pipeline Pilot Enterprise Page at:

- Pfizer / Microsoft SharePoint / Accelrys Customer Story:

- For additional information, we encourage you to contact us at:
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  - Conrad Agramont: cagramont@accelrys.com