

SYMYX NOTEBOOK BY ACCELRYYS 6.7

# Deployment of Update 2

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# Contents

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## Overview

6.7 Update 2 installation summary:..... 4

## Upgrading from 6.7

Preparation..... 5

Pipeline Pilot Update (required) ..... 5

Notebook/Vault Update ..... 5

## New Installation and Deployment

### Integration with Accelrys Consumable Inventory Management System (CIMS)

Prerequisites..... 8

On Web Core server ..... 8

On the Vault server ..... 9

# Overview

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## 6.7 Update 2 installation summary:

- New Customers
  - Download Accelrys ELN 6.7 Update 2 files and deployment documentation
  - Download Accelrys Vault Server 6.7 SP1 files and documentation
  - **Review the Accelrys ELN 6.7 Update 2 deployment documentation**
  - Install Accelrys Vault Server 6.7 SP1
  - Install the Accelrys ELN 6.7 Update 2 client
- Current Accelrys ELN 6.7 Customers
  - Download Accelrys ELN 6.7 Update 2 files and deployment documentation
  - **Review the Accelrys ELN 6.7 Update 2 deployment documentation**
  - Update to Accelrys ELN 6.7 Update 2 – Client reinstallation is NOT needed
- Current Symyx Notebook 6.6 (or earlier) customers
  - Download Accelrys ELN 6.7 Update 2 files and deployment documentation
  - Download Symyx Notebook 6.7 SP2 from the Previous tab
  - Download Accelrys Vault Server 6.7 SP1 files and documentation
  - **Review the Accelrys ELN 6.7 Update 2 deployment documentation**
  - Upgrade to Accelrys Vault Server 6.7 SP1 using the Vault documentation
  - Install the Accelrys ELN 6.7 Update 2 client
  - Use the ADM Manager to configure the rules to use an Update 2 profile

Determine which Notebook deployment scenario applies to you:

- [Upgrading from 6.7](#)
- [New Installation and Deployment](#)
- Note: The optional Notebook [Integration with Accelrys Consumable Inventory Management System \(CIMS\)](#) assumes you already have an installation of CIMS.

# Upgrading from 6.7

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## Preparation

1. *If you are upgrading from a version prior to 6.7*, from the Accelrys Download Center, install Vault Server version 6.7 SP1. Use the upgrade instructions in the 6.7 SP1 Installation Guide with one exception:  
Whereas the Installation Guide (page 115, Step 2) refers to running the Vault Deployment Utility distributed in the SymyxNotebook6.7\_SP1.zip, you need to run the Vault Deployment Utility distributed in the SymyxNotebook6.7\_SP2.zip. Therefore, on the Download Center, you need to click the **Previous** tab and download the Client for 6.7 SP2.
2. Download the 6.7 Update2 installer, Pipeline Pilot new package zip file and documentation zip file from the Accelrys Electronic Lab Notebook 6.7 Update page in the Accelrys Download Center.

## Pipeline Pilot Update (required)

1. Using the Admin Console, check to be sure that the Vault administrator account can access Vault.
2. Check to be sure that the **Pipeline Pilot – Run Protocol Application Permission** properties have been configured to specify the name and port number for the Pipeline Pilot server in the Configuration - Endpoint entry (Example: <http://cs-be-67vltmp.accelrys.net:9944>).
3. **Important! In the Administration Console, open the Lookup Service Application Permission and make a copy of all the entries.**
4. Locate the files from the original Pipeline Pilot server installation. (Hint: the file `scitegicsetup.exe` will be in the bin folder.)
5. Locate the `scitegic_notebook.pib` file in the Packages subfolder of the Pipeline Pilot installation folder. Rename this file or move it to another location.
6. Replace the original `scitegic_notebook.pib` file with the new version from the Notebook 6.7 Update 2 Pipeline Pilot zip file.
7. Run the `scitegicsetup.exe` installer choosing the [ Add/Remove Packages ] option to replace the Notebook package. Note that the version of the Notebook packaged displayed in the Pipeline Pilot Administrator Portal on the Packages page should be 6.7.3000

## Notebook/Vault Update

1. In the files extracted from the Notebook 6.7 Update 2 zip file locate the `VaultDeploymentUtility` directory. Open a command prompt in this directory.
2. Run the `VaultDeploymentUtility` using the following command:

```
VaultDeploymentUtility server domain\administrator-user password upgrade 6.7
```

where

- `server` represents the fully qualified name of the Vault Server
  - `domain\administrator-user` represents the domain and username of the Vault administrator account
  - `password` represents the password for the Vault administrator account
3. Review the content of the `Debug.log` file created by running the Vault Deployment Utility. Correct any errors.
  4. Use the `VaultADMStoreMananger` from the Notebook 6.7 Update 2 zip file to download and edit the ADM rules to use a new profile. For information on the ADM Store Manager, see the “*Accelrys Deployment Manager for Notebook Administrators*” from the Vault documentation updated in

September/October 2012. If you have not already downloaded the updated Vault documentation, download the `Accelrys Vault Server 6.7 SP1 Documentation (Updated)` file from the `Accelrys Download Center` page for `ELN - Symyx Notebook by Accelrys > Vault > 6.7 SP1`

5. Using an account with an updated profile, import the new templates from the `ExperimentTemplates` folder from within the `Notebook 6.7 Update 2` zip file.
6. Update your user templates.
7. Test the updated user templates.

# New Installation and Deployment

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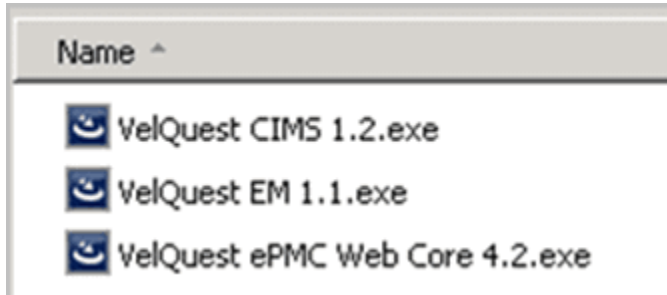
1. Download Accelrys Vault Server 6.7 SP1 and Accelrys Electronic Lab Notebook (Accelrys ELN) 6.7 Update 2 and the associated documentation.
2. Unzip onto the Vault Server the rar and zip files, including Pipeline Pilot PP85CU2\_NB67\_win64.rar.
3. Replace the original `scitegic_notebook.pib` file in the Pipeline Pilot “packages” subfolder with the new version from the Notebook 6.7 Update 2 Pipeline Pilot zip file.
4. Install Accelrys Vault Server 6.7 SP1 by following the Vault 6.7 SP1 installation documentation EXCEPT the following:
  - Run the Vault Deployment Utility from Symyx Notebook 6.7 Update 2 instead of the one mentioned in the Installation Guide (page 78).
5. Continue with the rest of the Accelrys Vault Server 6.7 SP1 installation as specified in the documentation.

# Integration with Accelrys Consumable Inventory Management System (CIMS)

The integration with Accelrys Consumable Inventory Management System (CIMS) is optional.

## Prerequisites

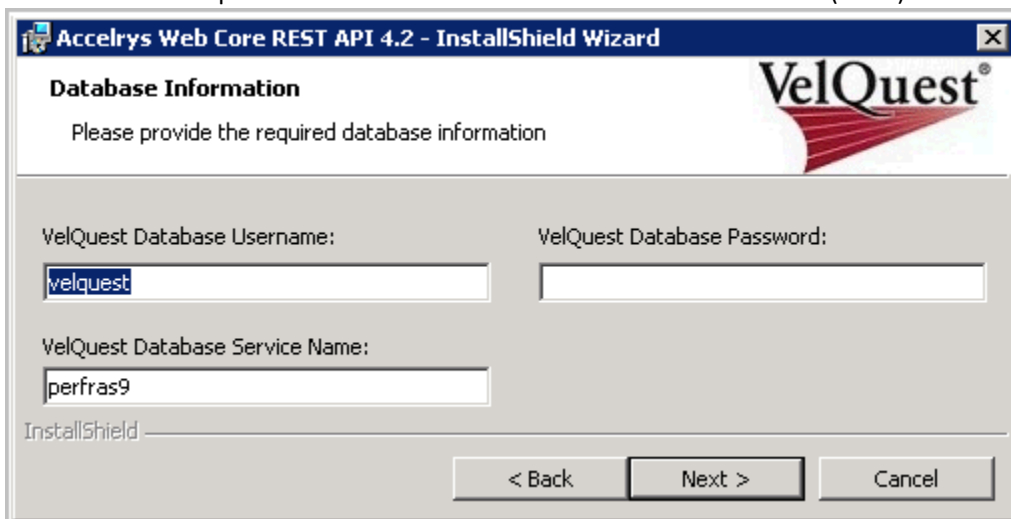
- A fully functional Web Core Server 4.2 with CIMS 1.2. In the Windows Control Panel, the installed programs must indicate the following names and version numbers.



- Make a list of the CIMS properties that your end-users need to see in the CIMS Notebook table section. This will help you be prepared for the “mapping” process described in the step on page 10 named “Map the configured properties”.

## On Web Core server

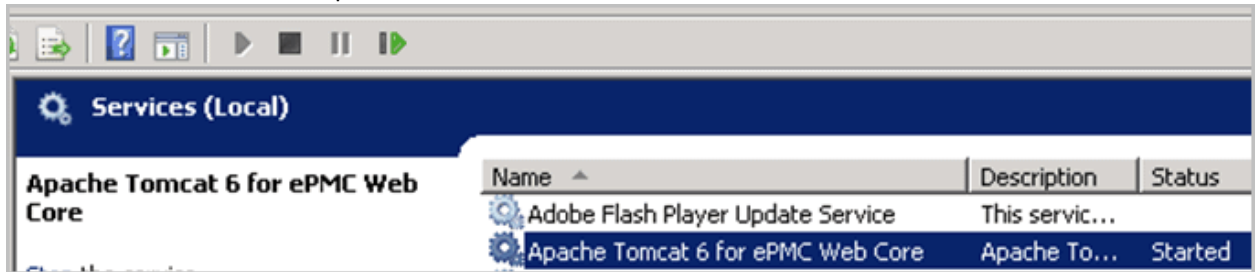
1. Download `Accelrys Web Core REST API 4.2.exe` from the Accelrys Download Center under Process Management and Compliance > WebCore > Web Core API.
2. Install the integration running `Accelrys Web Core REST API 4.2.exe`.
3. During the installation, in the **Velquest Database Service Name** field, if Web Core is correctly installed, the correct value displays. The **VelQuest Database Username** and the **VelQuest Database Password** are the username and password for the Oracle schema where the Web Core (CIMS) data is stored.



(Otherwise, enter the Oracle TNS alias, which might or might not be the same as the Oracle SID.)



- Copy the Symyx notebook server certificate (PFX file) from the Vault server to the Web Core server and install it to 'Trusted Root' | Local Computer.
- Restart the service named "Apache Tomcat 6 for ePMC Web Core".



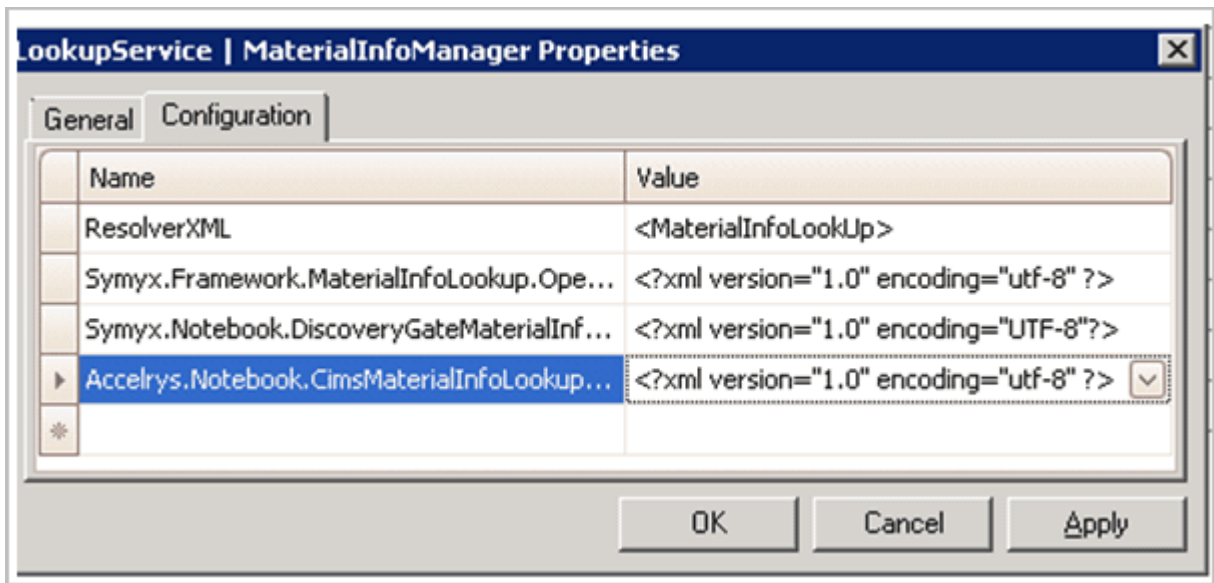
- Run the installed shortcut to stop and start the **World Wide Web Publishing Service**. This ensures that the first request to the site (which is what initializes the web application) is to the root address. This step is especially important for load balancing configurations where it may not be possible to otherwise control how the application is initialized on every single web server. Note that this shortcut should be used any time the web site restarts.

To initialize the Web Service:

- Click the **Start** menu and browse to: Programs/Accelrys/SmartLab/Initialize ePMC Web Core.
- Right-click **Initialize ePMC Web Core** and select Run as administrator. This is required to start and stop the service successfully. The World Wide Web Publishing Service stops, restarts, and then launches a web browser to the site.

## On the Vault server

- Make sure that Vault 6.7 SP2 Update2 is installed and that the Vault Deployment Utility has run.
- Start the Notebook Administration console.
- Grant users/group permission to the LookUpService.
- For each of your end-users, make sure that the CIMS and Notebook user name are the same.
- Select Application Permissions | LookUpService and then select the Configuration tab.
- Open the Configuration for `Accelrys.Notebook.CimsMaterialInfoLookup.CimsMaterialInfoResolver`



7. Edit the xml to replace localhost with your WebCore server name and port number.

```
<Configuration>
  <Property name="URL">http://localhost:1000/cimsapi</Property>
  <Property name="ReplaceExistingPropertyValues">True</Property>
  <Property name="MaxNumberOfResults">50</Property>
  <Property name="SearchGridColumnOrder">Container.Barcode,Material.Name,Inventory_SYS.IsExpired,AnalyticalMaterial.ExpiryDate,Material.InitialAmount</Property>
  <Property name="AutoCalculateAmount">True</Property>
</Configuration>
```

8. Note that some CIMS properties are pre-mapped by the integration with Notebook: Barcode, InventoryId, ParentId, TemplateId, SiteId, Site, FullLocation, QuantityWhenCreated, IsExpired, WorkflowStage.
9. Map the configured properties.

Properties that are not pre-mapped are user-configured and need mapping. Using the Notebook property set editor, create a property set for each *configured* property so that the property set maps between CIMS and Notebook the names of each *configured* property. You must map each name, even if the names are spelled identically. Note that name mapping is case-sensitive. The example below maps the BoilingPoint Notebook property to the CIMS name represented by the key 'Boiling Point' as well as MeltingPoint, IsAvailable, Recycle\_Date and Color.

```
<PropertySet name="Cims_custom">
  <Property name="BoilingPoint">
    <xpath path="ParentDef[@key='Properties']/ParentDef[@key='Boiling Point']/FieldDef[@key='Value']" />
  </Property>
  <Property name="MeltingPoint">
    <xpath path="ParentDef[@key='Properties']/ParentDef[@key='Melting Point']/FieldDef[@key='Value']" />
  </Property>
  <Property name="IsAvailable">
    <xpath path="ParentDef[@key='Properties']/ParentDef[@key='Is Available']/FieldDef[@key='Value']" />
  </Property>
  <Property name="Recycle_Date">
```

```

    <xpath
    path="ParentDef[@key='Properties']/ParentDef[@key='Recycle_date']/Field
    Def[@key='Value']" />
  </Property>
  <Property name="Color">
    <xpath
    path="ParentDef[@key='Properties']/ParentDef[@key='Color']/FieldDef[@ke
    y='Value']" />
  </Property>
</PropertySet>

```

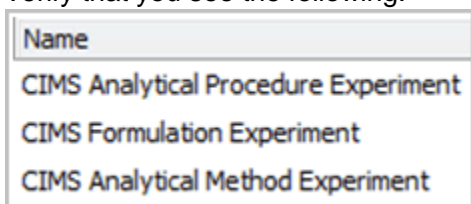
TIP: Before pasting your XML into the Notebook property set editor, make sure the XML is well formed.

10. Insert the property set definition(s) into your CIMS-related experiment templates.
11. Use the following table to learn which CIMS property type “maps” to which Notebook data type:

NOTEBOOK	CIMS
String	Text
Integer	Numeric
Decimal	
Date	Date

CIMS	NOTEBOOK
Boolean	String
Text	
Numeric	Integer
	Decimal
Date	Date

12. Note that the following CIMS Property Types do NOT map to Notebook:
  - NFPA Label
  - Relationship Property
  - Components
13. Log in to Notebook as administrator.
14. Import the Experiment Templates located within `VaultDeploymentUtility\ExperimentTemplates` that are specific to CIMS by importing the `CIMSTemplates.voexp` to whatever location you want.
15. Verify that you see the following:



16. Make sure the appropriate Accelrys Deployment Manager (ADM) package is installed and users assigned to the appropriate profile.