

Accelrys Discovery Studio Modeling Installation Instructions
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Discovery Studio (DS) is a comprehensive suite of molecular modeling, bioinformatics and simulation applications designed to run on Windows-based computers. The backbone of the DS platform is Discovery Studio Project KM, an Oracle-based infrastructure that captures and stores information generated by discovery studio applications to allow for easy exchange across research teams. More information on Discovery Modeling can be obtained from, <http://www.accelrys.com/products/dstudio> . For technical requirements, please visit <http://www.accelrys.com/products/dstudio/modeling/techreqs.html>

Discovery Studio (DS) Modeling client installation in ABCC has to be done in three stages: i) SVGViewer installation ii) Oracle Client installation, and finally iii) DS Modeling Client installation. Before you start the installation, make sure you have a good internet connection and keep ready the username/password you have received earlier from the ABCC to log into the ABCC-PC software download page (<http://pcsoftware.abcc.ncifcrf.gov>). Also make sure you have already obtained an ABCC user account for using DS Modeling. If you have any questions regarding the DS Modeling software or installation, contact ABCC via our Feedback/Issues web page, http://www.abcc.ncifcrf.gov/issues/issue_frm.php

Note: While preparing this document, Windows XP machine with Internet Explorer as a default browser was used for download and installation. If you use a different OS/Browser combination, the figures shown in the following sections may differ.

I. Adobe SVGViewer Installation

If you have already installed Adobe SVGViewer, you can skip this section.

The very first thing you need to install is Adobe SVG Viewer. Adobe SVGViewer (for Windows) is essential for the DiscoveryStudio/MaterialStudio clients to view and display the contents properly. From the ABCC-Accelrys download page, (<http://pcsoftware.abcc.ncifcrf.gov/Accelrys>) click on "Adobe_SVG_Viewer" link. To install Adobe SVGViewer, left-click on the file "SVGview.exe" to save it to your desktop/lap-top hard-drive (for example, My Documents directory). Upon saving, go to the directory where you had saved the SVGview.exe file (ex., MyDocuments) and double-click on the downloaded "SVGView.exe" and choose "Run" to run and install the Adobe SVG Viewer.

II. Oracle Client Installation:

If you have already installed Oracle client, you can skip this section

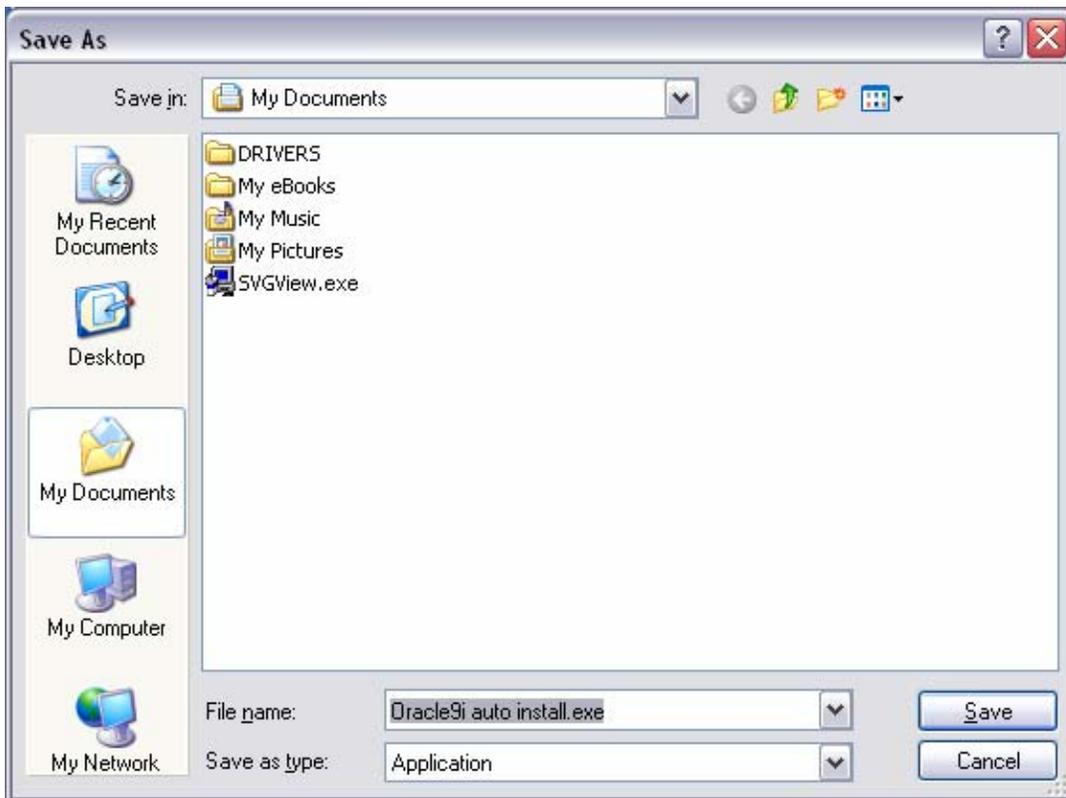
From the ABCC-Accelrys download page (<http://pcsoftware.abcc.ncifcrf.gov/Accelrys>), click on "Oracle_Client" link and then click on "Oracle_Client_Auto_Install" to go into the directory.

- 1) Make sure you are in the Accelrys/Oracle_Client_Auto_Install/ directory

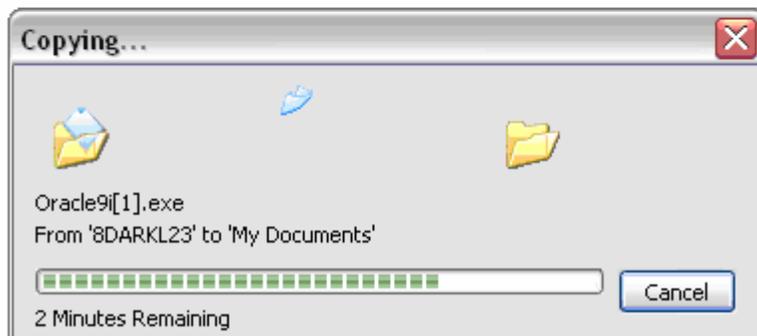
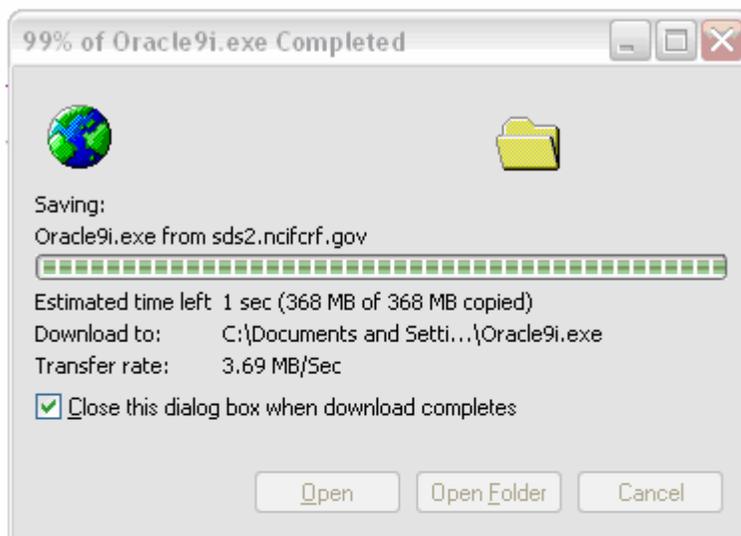
- 2) Left-click on the Oracle9i_auto_install.exe link, the following menu shows up
(NOTE: Depending on the latest Oracle version, the name of the file could be different from the one used in this document. But, the overall procedure remains the same. Also depending on your internet connection, this step may take time)



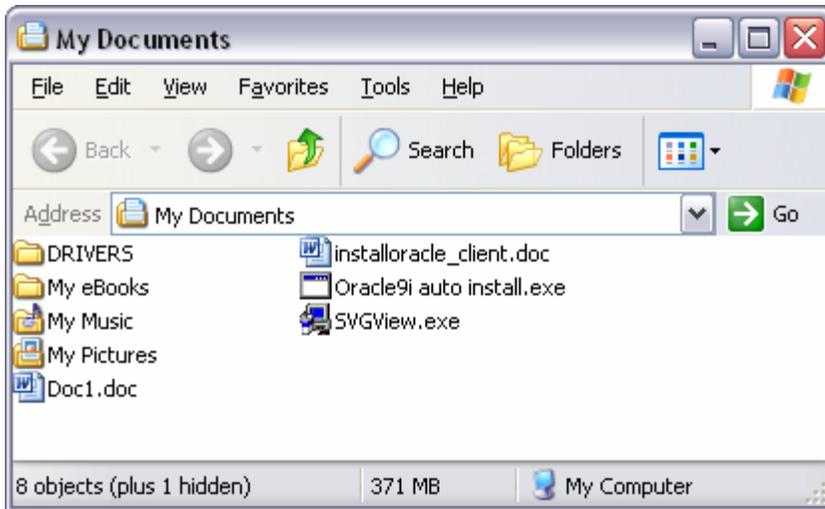
- 3) Click “Save” on the “File Download” window (see above) to see the following “Save As” menu.



- 4) Choose a directory (ex My Documents) and click on “Save”. (NOTE: Oracle9i_auto_install.exe is a 368 MB file. Depending on your internet connection, this step may take time)



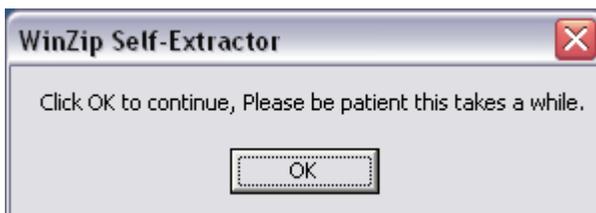
- 5) Go to the directory where you had downloaded and double-click on Oracle9i_auto_install.exe to start the installation. **Note: The listing of files (see the figure below) in your computer may be different.**



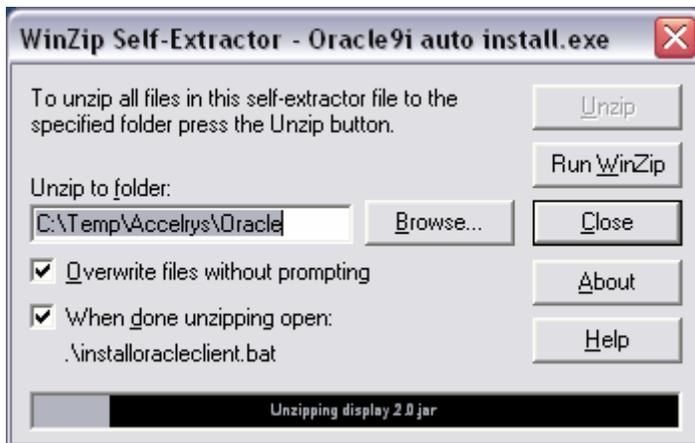
6) Click, Run to start the installation



7) Click OK to continue the installation.



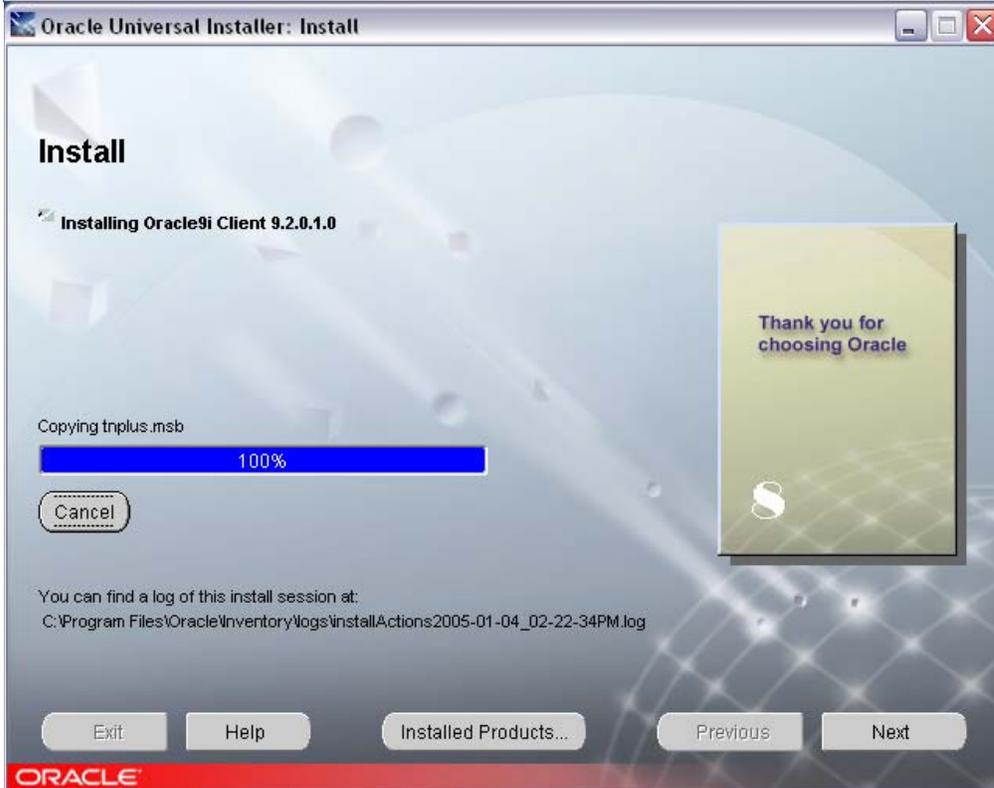
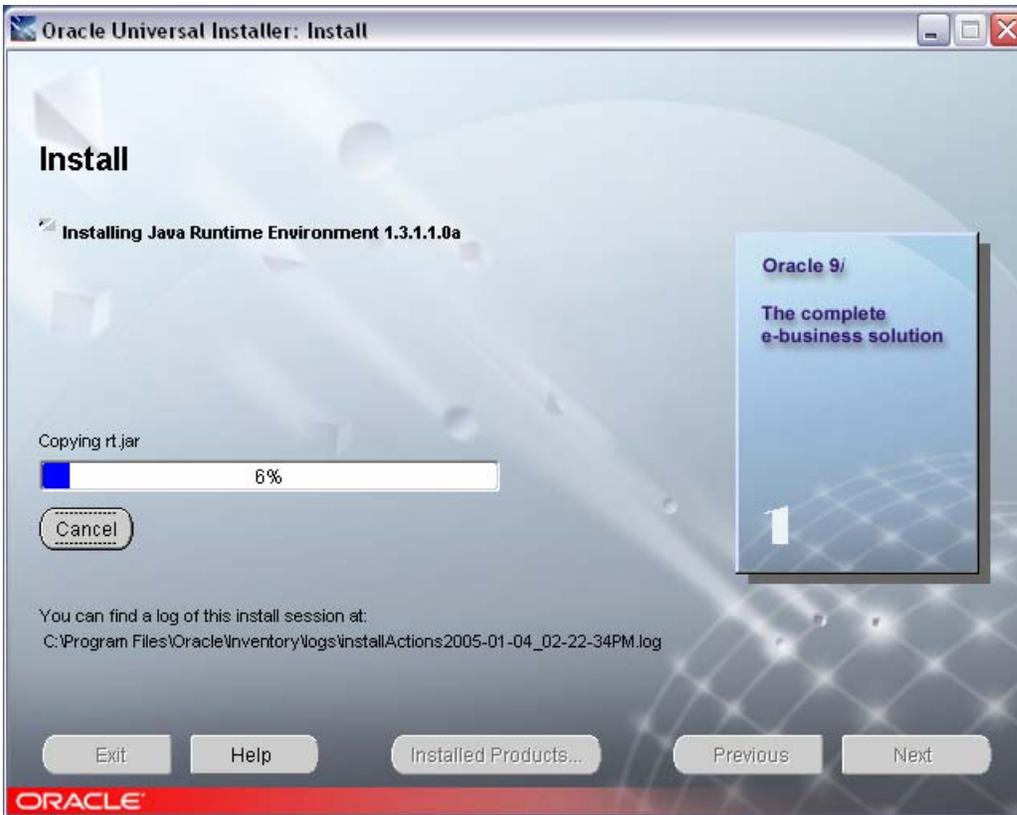
8) Click on “Unzip” to start unzipping the zip file. **Note: This step may take time**



After unzipping, you will see the following menu pop-up. Click OK to continue



After this step, you will see the command prompt window pop up and vanish. Give some time for the Oracle Universal Installer window to come up. **From this point till the end, no intervention is needed. The Oracle Universal Installer will finish copying and finally go away. Don't click/choose any option in the Installer. PLEASE WAIT PATIENTLY.**

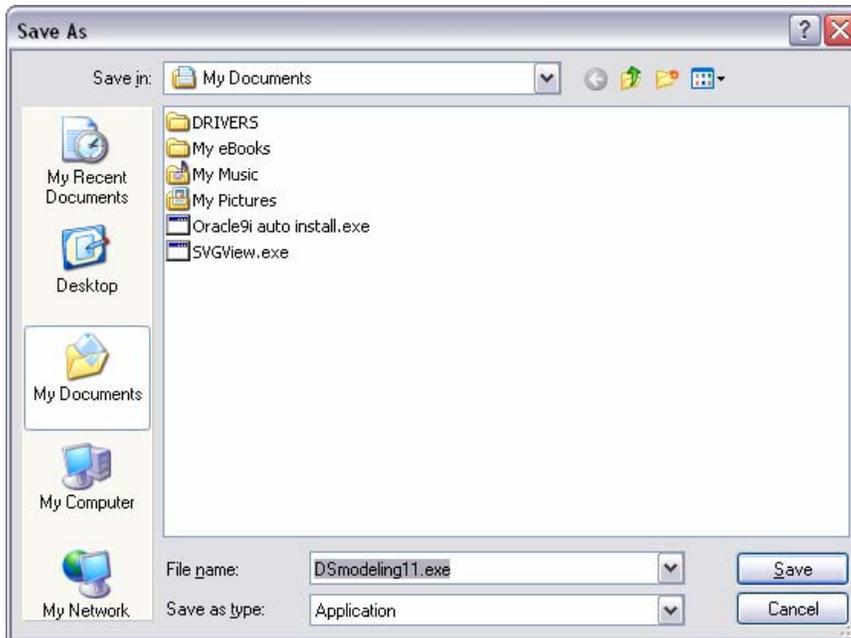


After this step, you should see new entry(ies) for Oracle under Start → All Programs

III. DSModeling Installation:

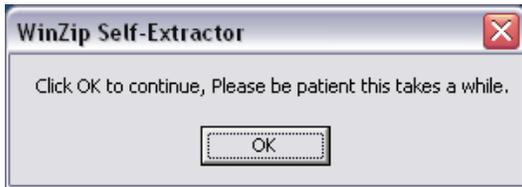
From the ABCC-Accelrys download page, (<http://pcsoftware.abcc.ncifcrf.gov/Accelrys>), left-click on "DS_Modeling_Client" link followed by one more left-Click on DSmodeling11.exe to save the file to your desktop/laptop.

(NOTE: Depending on the latest DSModeling version, the name of the file could be different from the one shown in this document. But, the overall procedure remains the same. DSmodeling11.exe is a 156 MB file, and depending on your internet connection, this process may take time. Please be patient!)

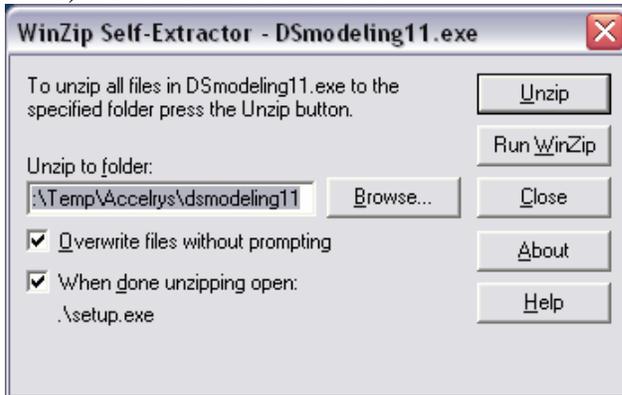


- 1) Go to the directory (Desktop/lap-top) where you had saved the file, and double-click and choose "Run" to start the installation. **Note: DSmodeling1.1.exe is a 168 MB file. Depending on your internet connection, this step may take time.**

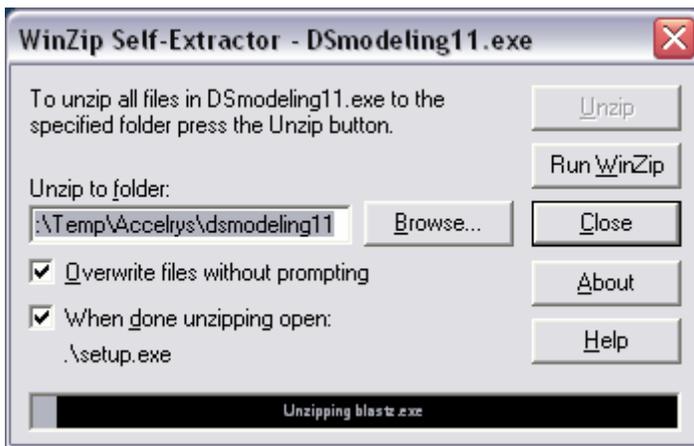
- 2) There will be a time lag before the WinZip Self-Extractor (see below) menu shows up.



- 3) Click OK to continue.



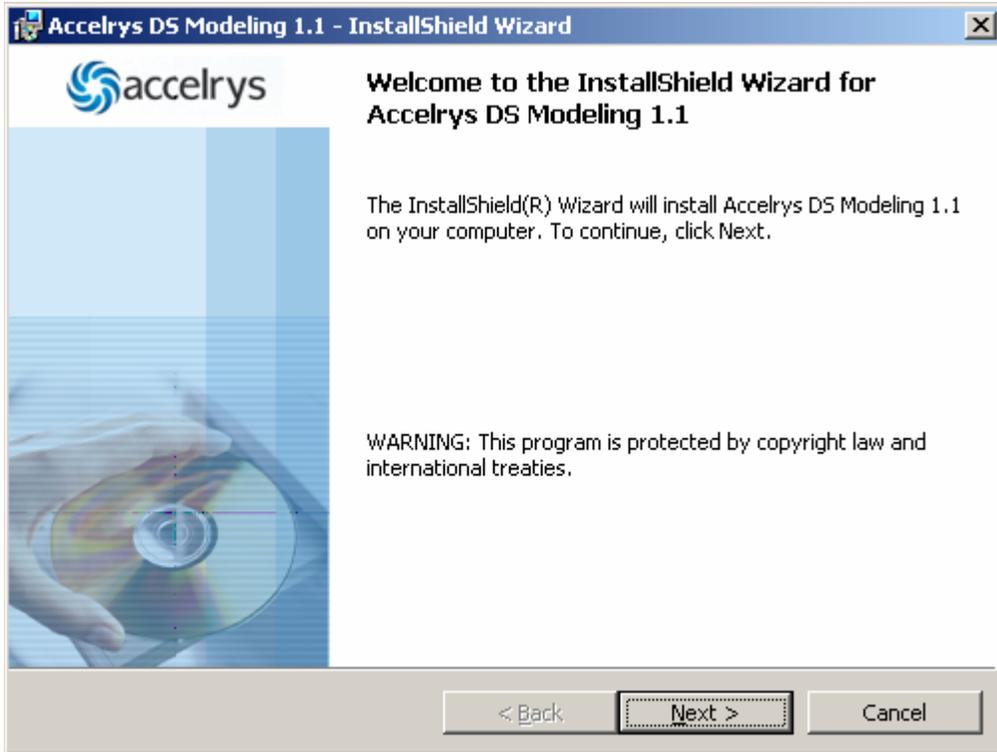
- 4) Click Unzip with the default options. The following radio-box will appear detailing the unzipping information. **Unzipping can be time consuming. Please be patient!**



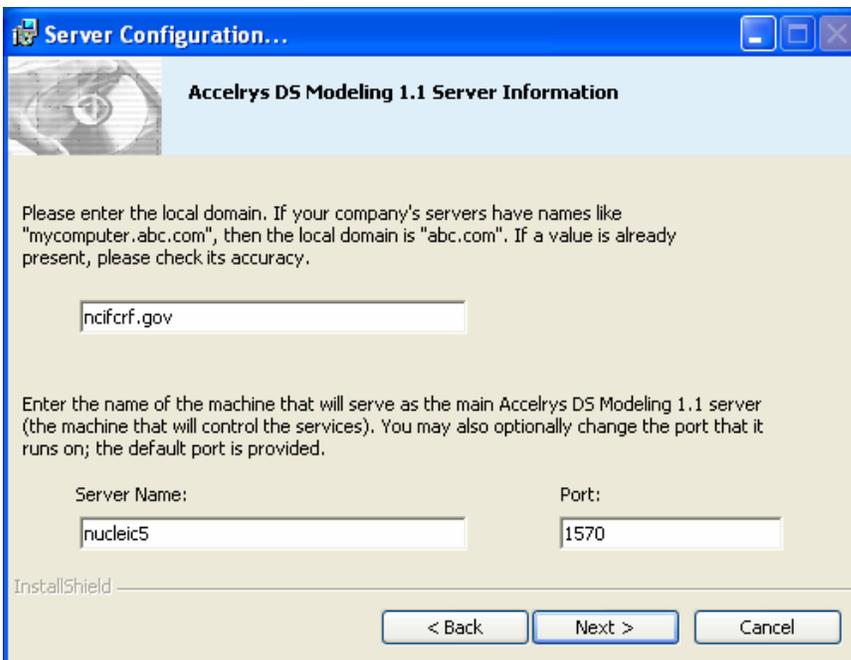
- 5) After unzipping, the following menu will show up. Click **OK** to continue.



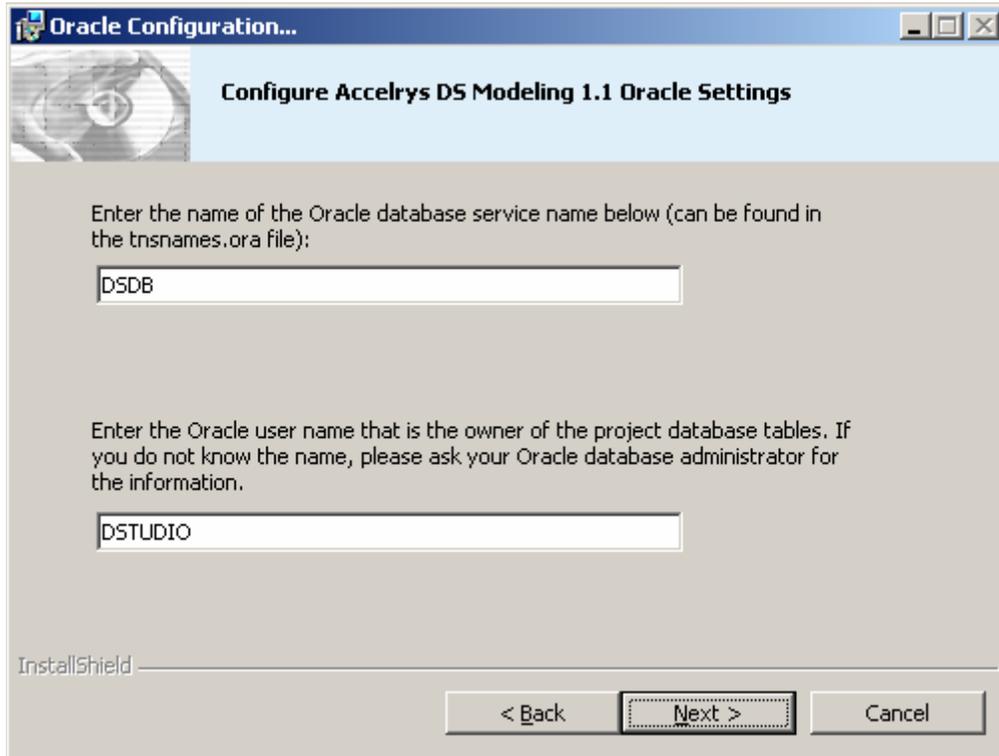
- 6) **After unzipping, the installation starts automatically.** You should see the following menu. Click “Next >” to continue



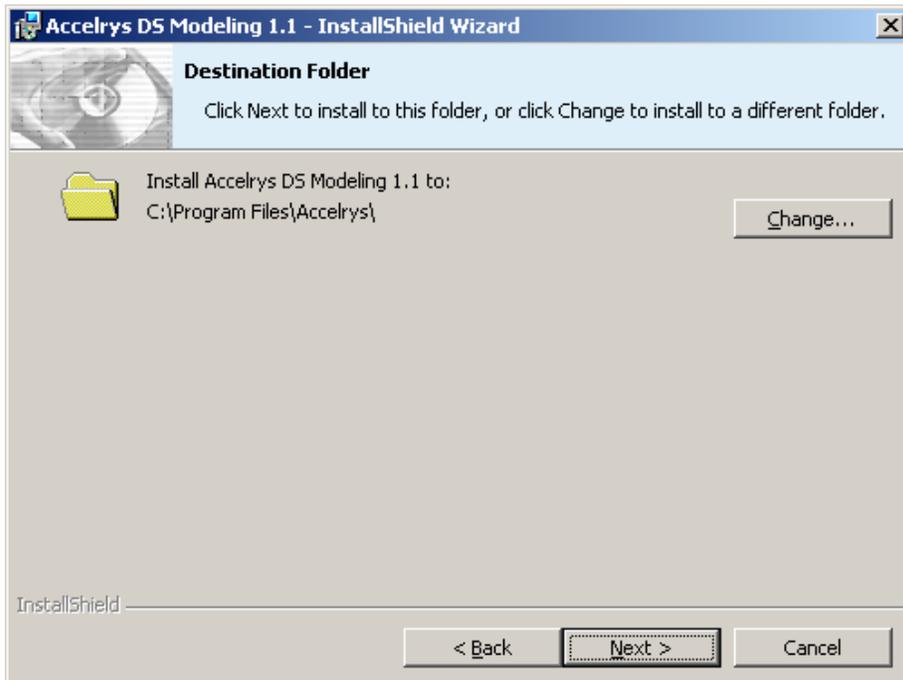
- 7) Enter the server information (see below) and click “Next >” to continue



8) Enter the Oracle settings (see below) and click “Next >” to continue



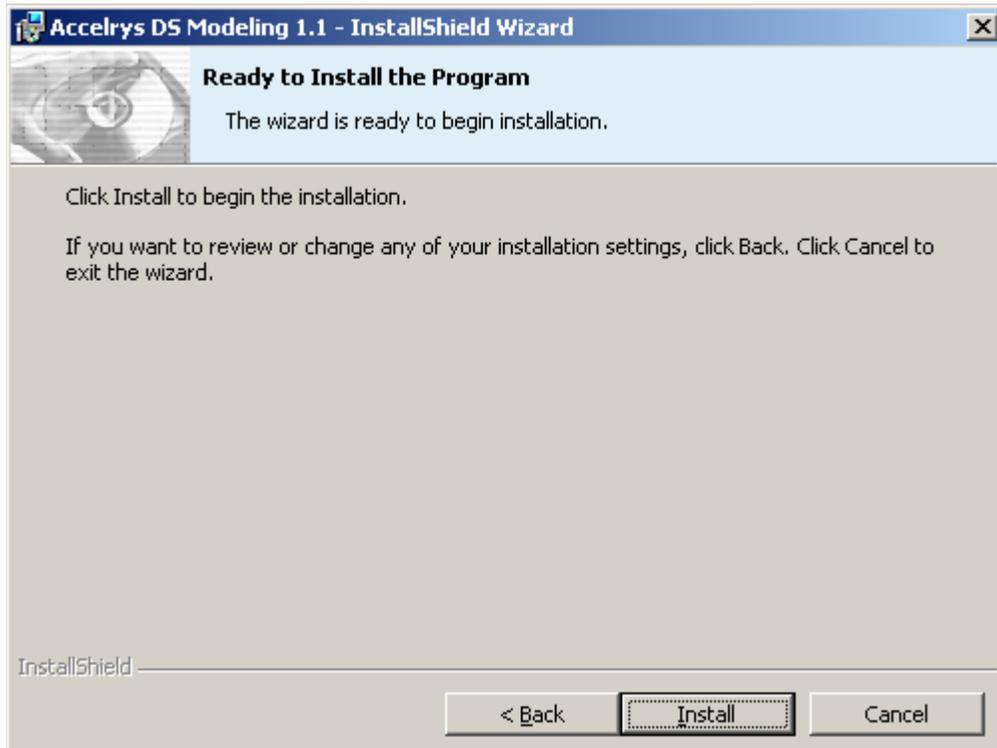
9) Click “Next >” to continue



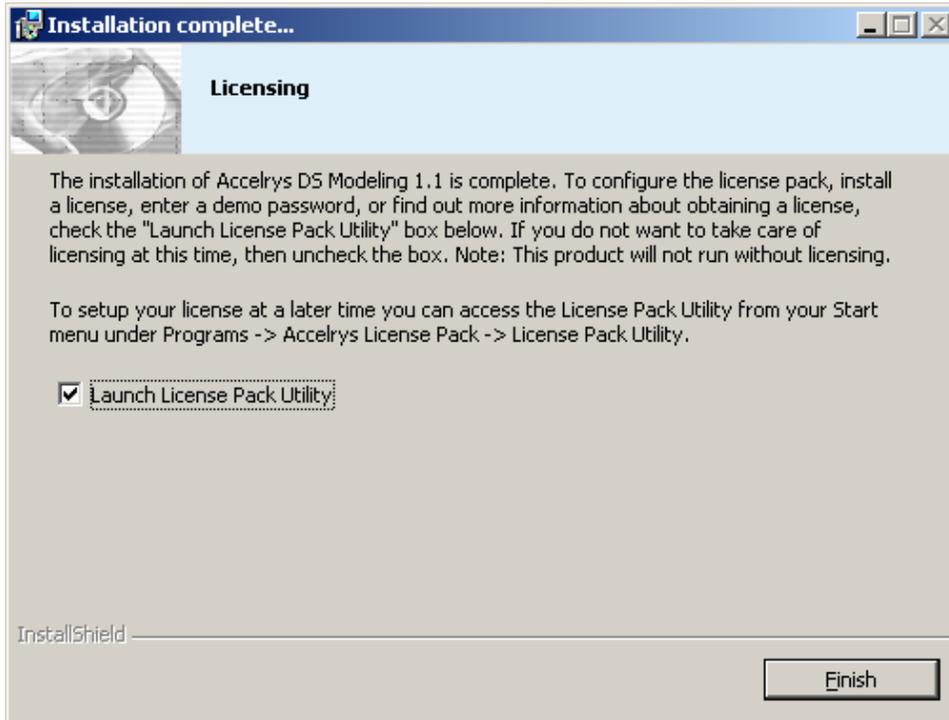
10) Choose the setup type (see below) and click “Next >” to continue



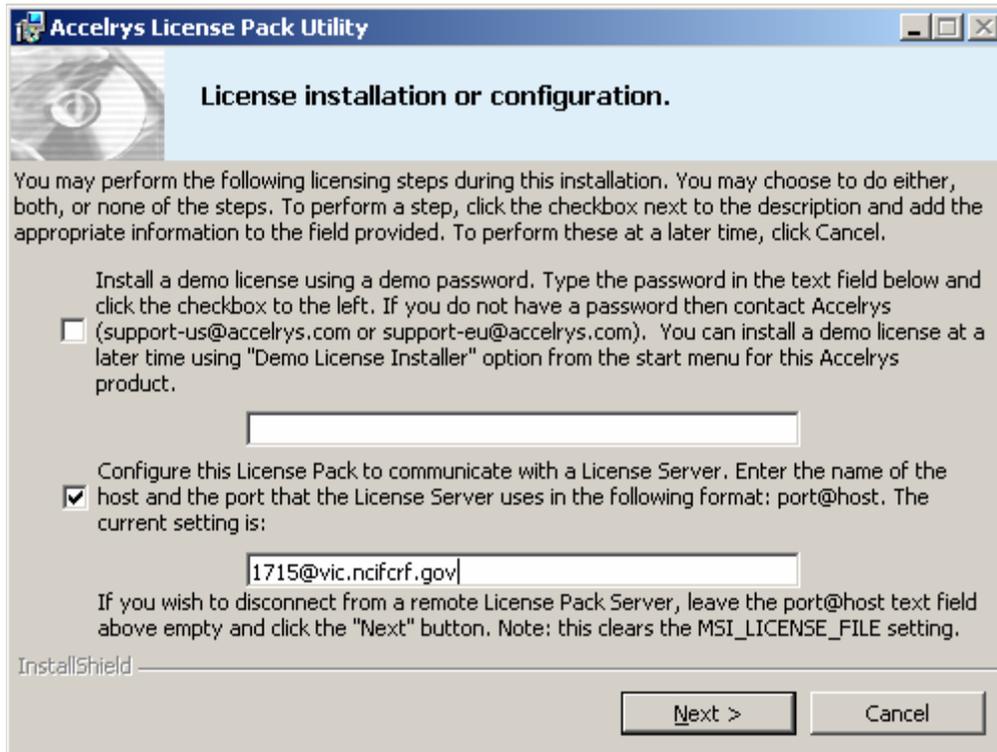
11) Click “Install” to begin the installation. **Note: Time consuming step. WARNING: At this step you may see a pop-up window from VIRUS-Scan, if you happen to see that, please ignore it. If you have any other problems at this stage, contact ABCC support desk.**



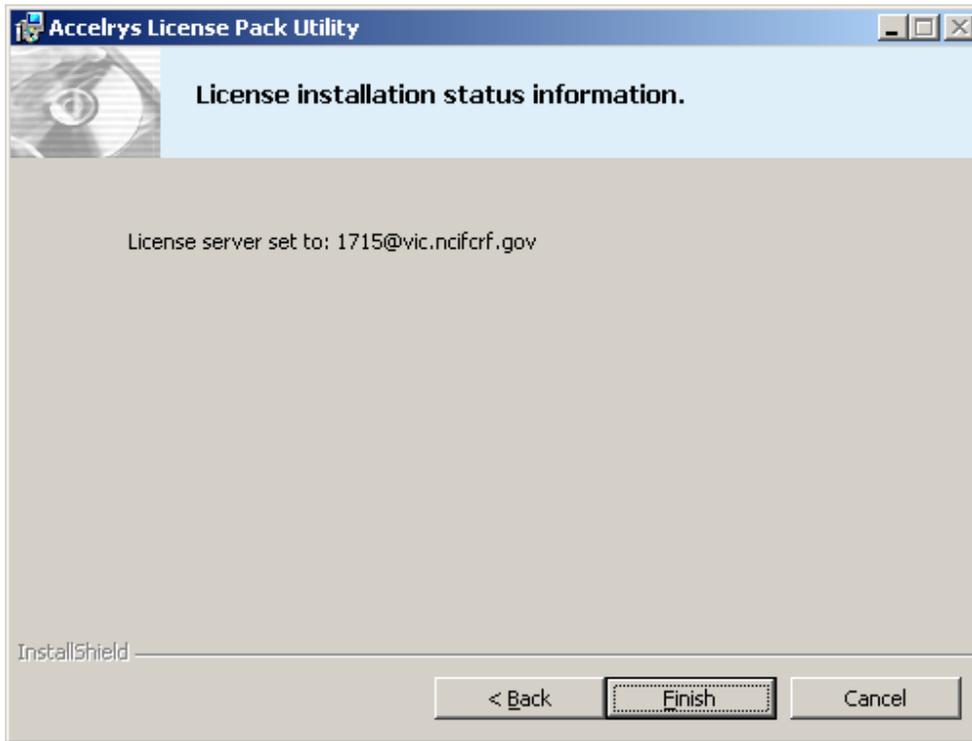
12) Make sure you check the Launch License Pack Utility, and click “Finish”



13) Enter the license server information and click “Next >”



14) Click on “Finish” to finish the License Pack Utility setup



IMPORTANT FINAL STEPS:

- 1) Go to C:\oracle\ora92\network\admin directory. Edit (open with WORDPAD) the file, tnsnames.ORA and make sure you have the following entry for HOST, (HOST = ncip595.ncifcrf.gov)**
- 2) Also go to C:\Program Files\Accelrys\DS Modeling 1.1\config, and edit the file DSModeling1.1.cfg and make sure you have the following line:
DS_NAMESERVICE_HOST nucleic5.ncifcrf.gov**

Please note that, C:\Program Files\Accelrys\DS Modeling 1.1\config, correspond to the version number '1.1'. If you are installing version '3.5', then you need to go to C:\Program Files\Accelrys\DS Modeling 3.5\config

After DS Modeling installation, you should see, DS Modeling icon on your desktop, and new entries for “Accelrys DS Modeling 1.1” and “Accelrys License Pack 6.1” in your Start → All Programs

Note: License Pack version could be different from the one shown here

Clean-up Instructions: These final steps will help you clean-up the temporary files created during the installation and download:

1. In your desk-top, go to the directory (My Documents etc.), where you had downloaded the exe files (ex.Oracle9i_auto_install.exe) and delete them.
2. All the intermediate installation files following the download are unzipped under a newly created temporary directory called c:\temp\Accelrys. Go to c:\temp directory and delete everything under the **Accelrys** directory.

Uninstalling DS/MS/Oracle products

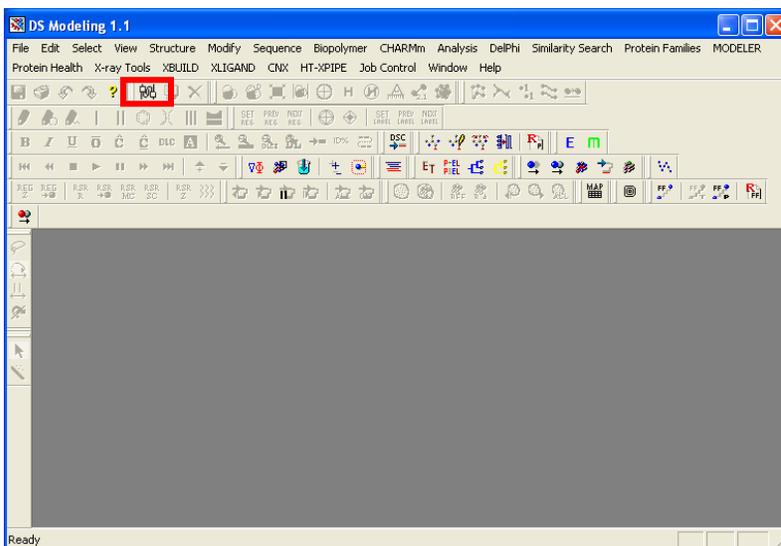
If you want to uninstall DS/MS products, go to, Start → Control Panel → Add or Remove Programs, and select the appropriate products for removal.

To uninstall/remove oracle, Start→ Programs → Oracle Installation Products → Universal Installer, and click on “Deinstall Products” option and select oracle and click on remove.

This completes the DS Modeling 1.1 installation.

DS-Modeling Quick-start:

Double-click on DS-Modeling icon on the desktop. Once the DS Modeling window shows up, click on New-Connection button (shown in red box) and enter the DS Modeling username/password given to you by ABCC.



If you have any questions, comments, suggestions about this document, contact me at sravi@ncifcrf.gov

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