

Accelrys Discovery Studio Modeling-SBD 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 DS Modeling SBD can be obtained from, http://www.accelrys.com/products/dstudio/modeling/dsmodeling_12.html For technical requirements, please visit <http://www.accelrys.com/products/dstudio/modeling/techreqs.html>

Discovery Studio (DS) Modeling-SBD client installation in ABCC has to be done in three stages: i) SVGViewer installation ii) Oracle Client installation, and finally iii) DS Modeling SBD 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 to use DS Modeling. If you have any questions regarding the DS Modeling software or installation, please 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 desk-top/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, you can skip this section.

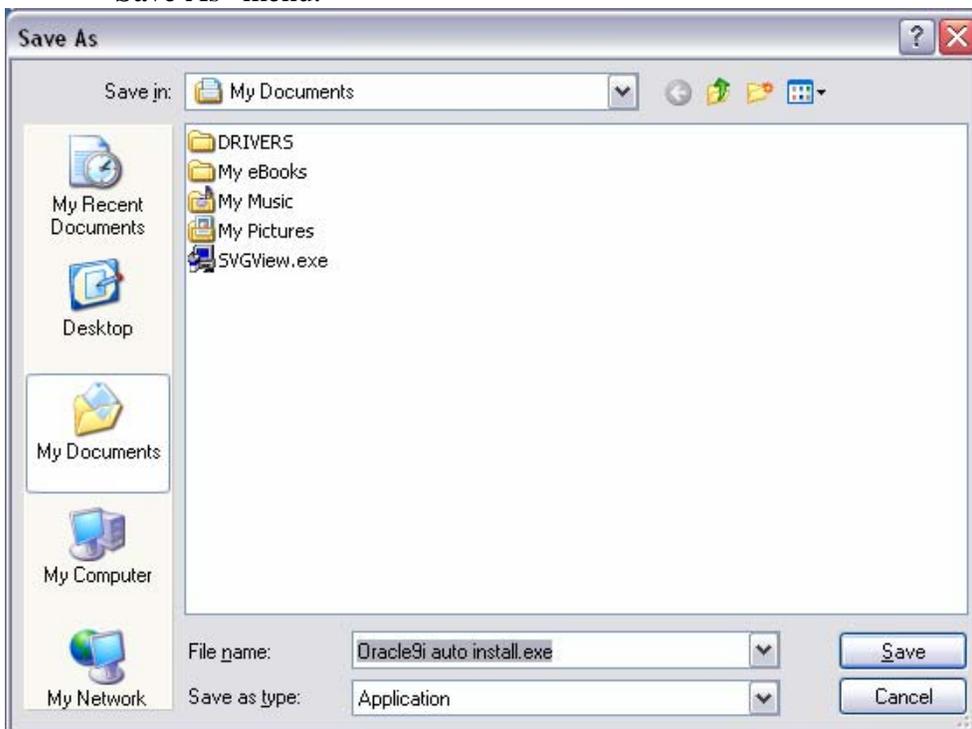
From the ABCC-Accelrys download page (<http://pcsoftware.abcc.ncifcrf.gov/Accelrys>), click on "Oracle_Client" followed by "Oracle_Client_Auto_Install" to go into that directory.

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

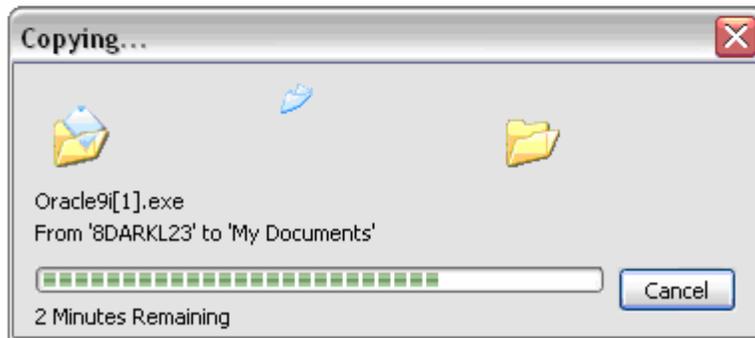
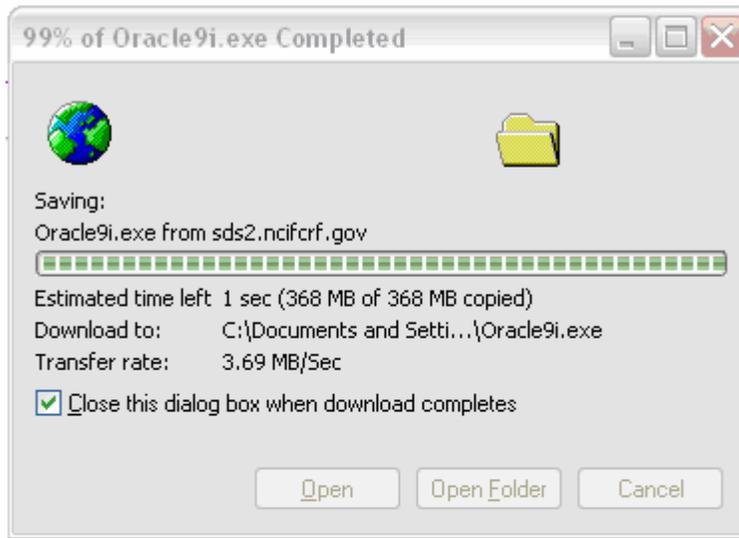
- 2) Left-click on the Oracle9i_auto_install.exe link, the following menu shows up
(NOTE: Depending on the latest Oracle version, the name of the file could be different from the one used in this document. But, the overall procedure remains the same. Also depending on your internet connection, this step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



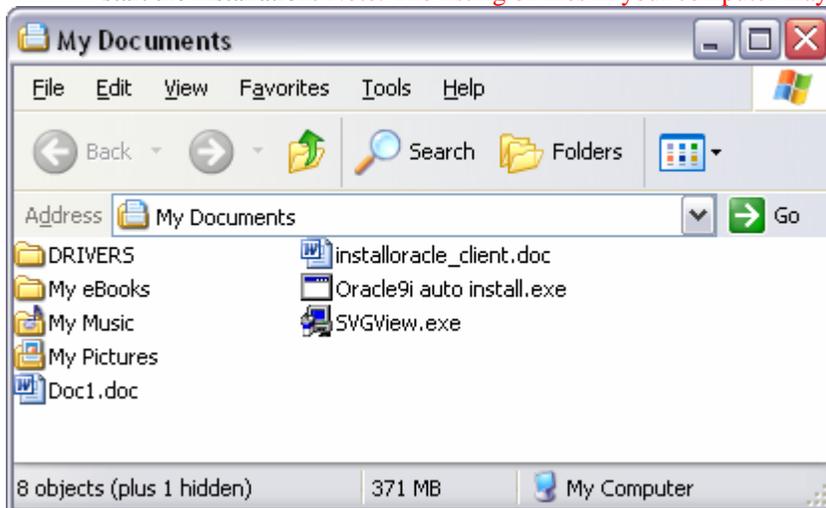
- 3) Click “Save” on the “File Download” window (see above) to see the following “Save As” menu.



- 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)



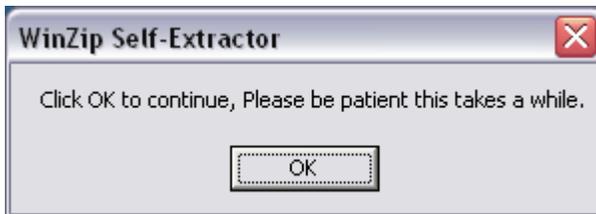
- 5) Go to the directory where you have downloaded and double-click on Oracle9i_auto_install.exe to start the installation. **Note: The listing of files in your computer may be different.**



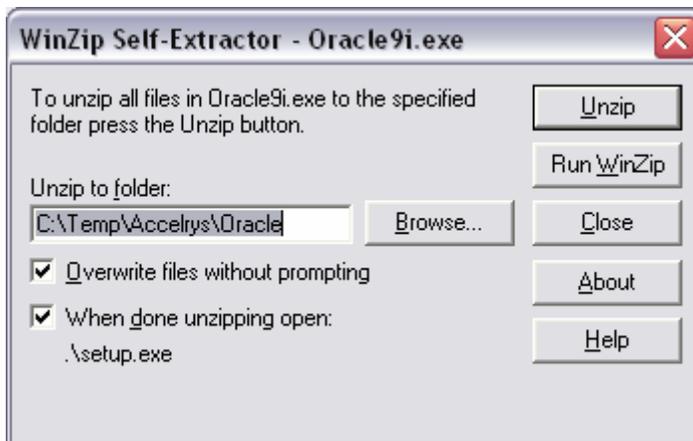
- 6) Click, Run to start the installation

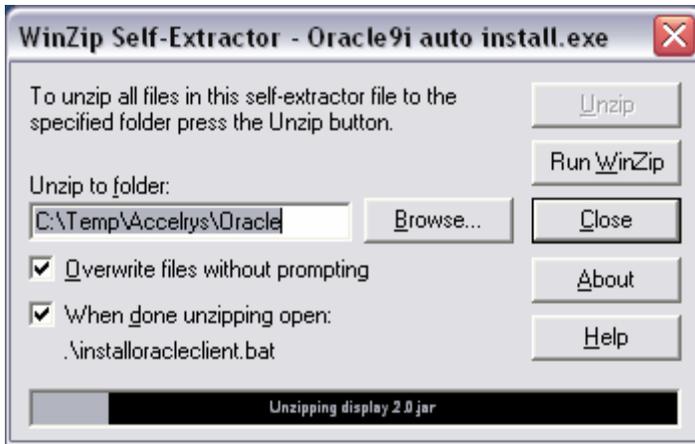


7) Click OK to continue the installation.



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

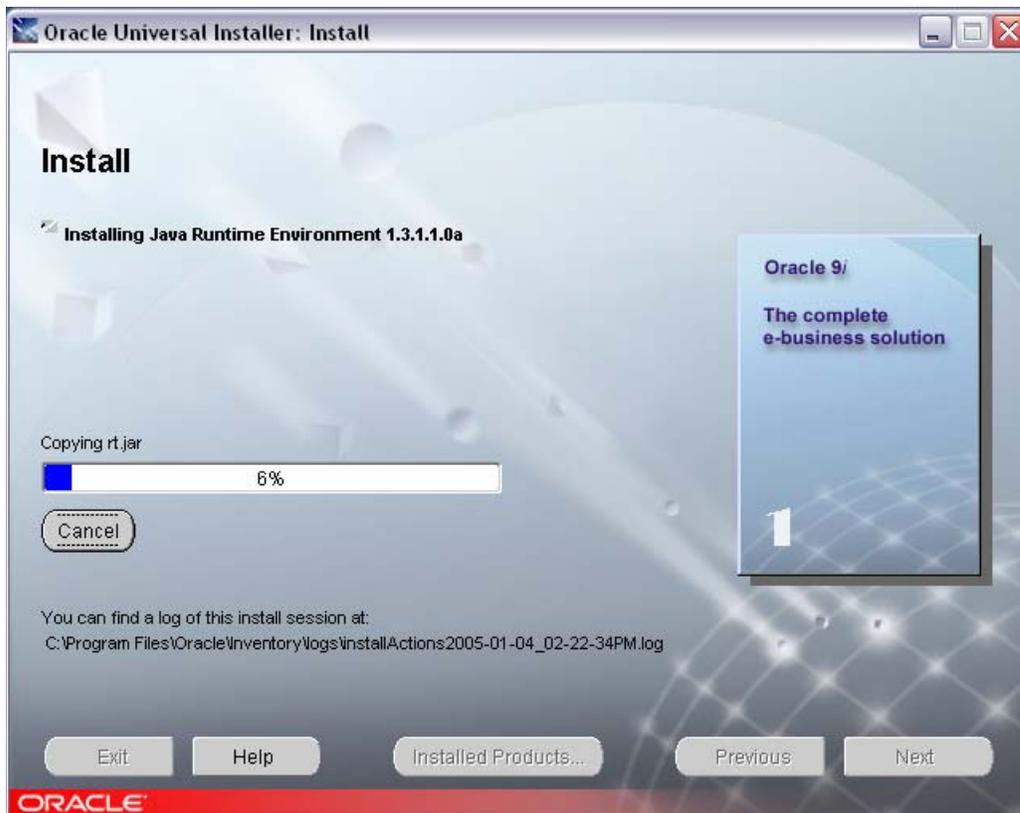


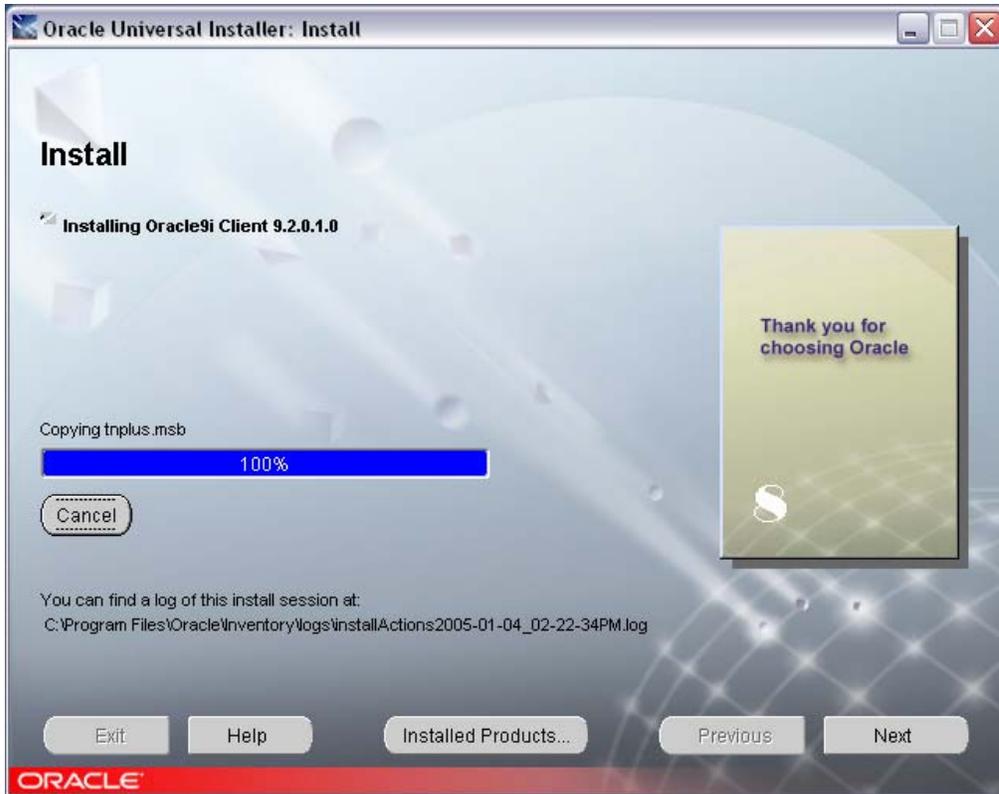


After unzipping, you will see the following menu pop-up. Click OK to continue



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.**





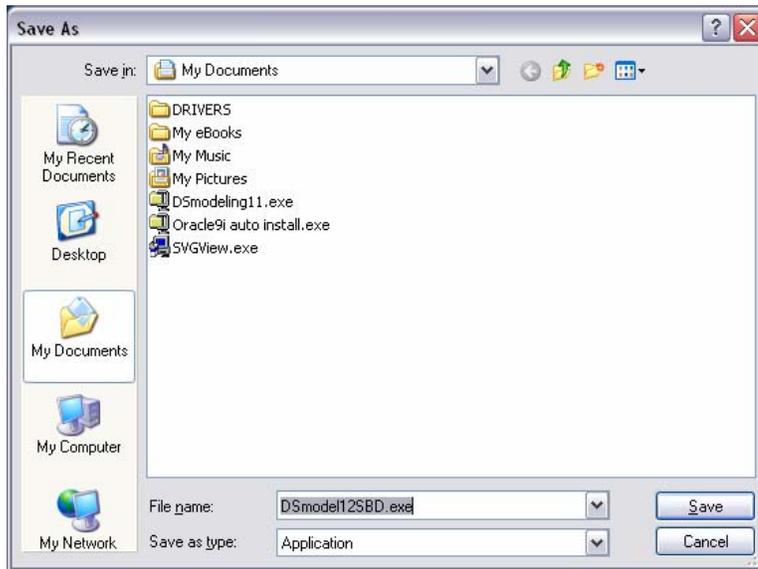
After this step, you should see new entry(ies) for Oracle under Start → All Programs

III. DSModeling SBD Installation:

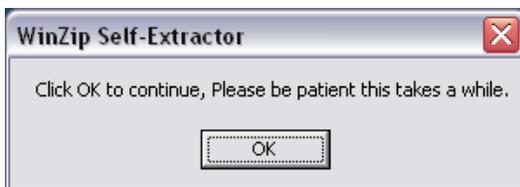
From the ABCC-Accelrys download page, (<http://pcsoftware.abcc.ncifcrf.gov/Accelrys>), left-click on "DS_Modeling_SBD_Client" link to go into the directory, left-Click again on DSmodel12SBD.exe to save the file to your desktop/laptop.

(NOTE: Depending on the latest DSModeling-SBD version, the name of the file could be different from the one shown in this document. But, the overall procedure remains the same. Also depending on your internet connection, this step may take time.)

- 1) Left-Click on DSmodel12SBD.exe and save the file to your desktop. Note: DSmodel12SBD.exe is a 77 MB file, and depending on your internet connection, this process may take time. Please be patient.



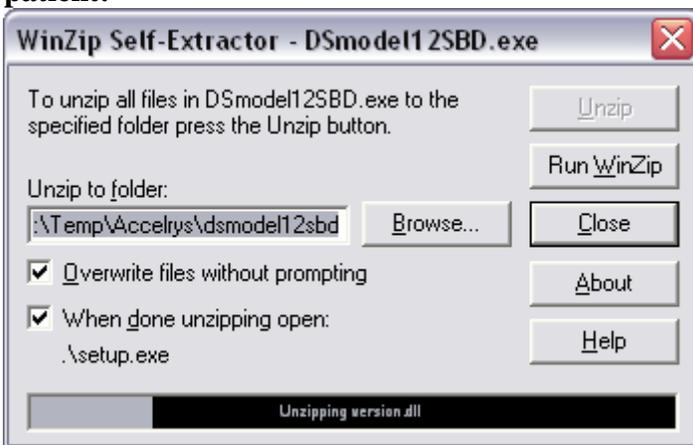
- 2) Go to the directory where you had saved the file (DSmodel12SBD.exe), and double-click and choose "Run" to start the installation. **Note:** DSmodel12SBD.exe is a 73 MB file. Depending on your internet connection, this step may take time.
- 3) There will be a time lag before the WinZip Self-Extractor menu shows up. **Please be patient!**



Click OK to continue.



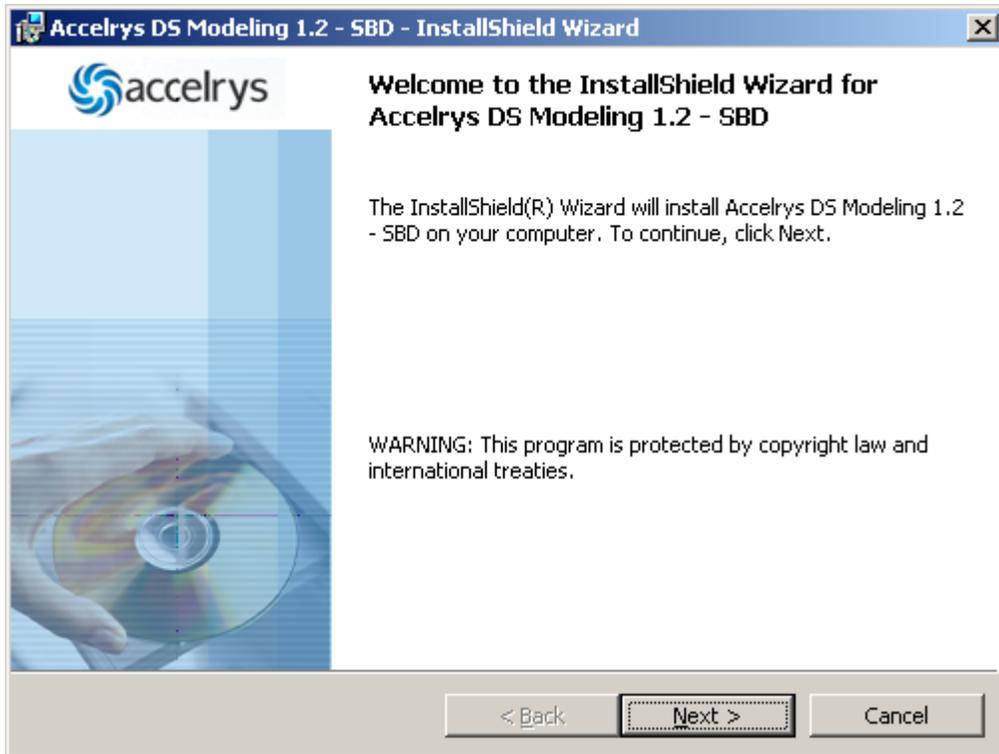
Click “Unzip” with the default options. The following radio-box will appear detailing the unzipping information. Unzipping can be time consuming. Please be patient!



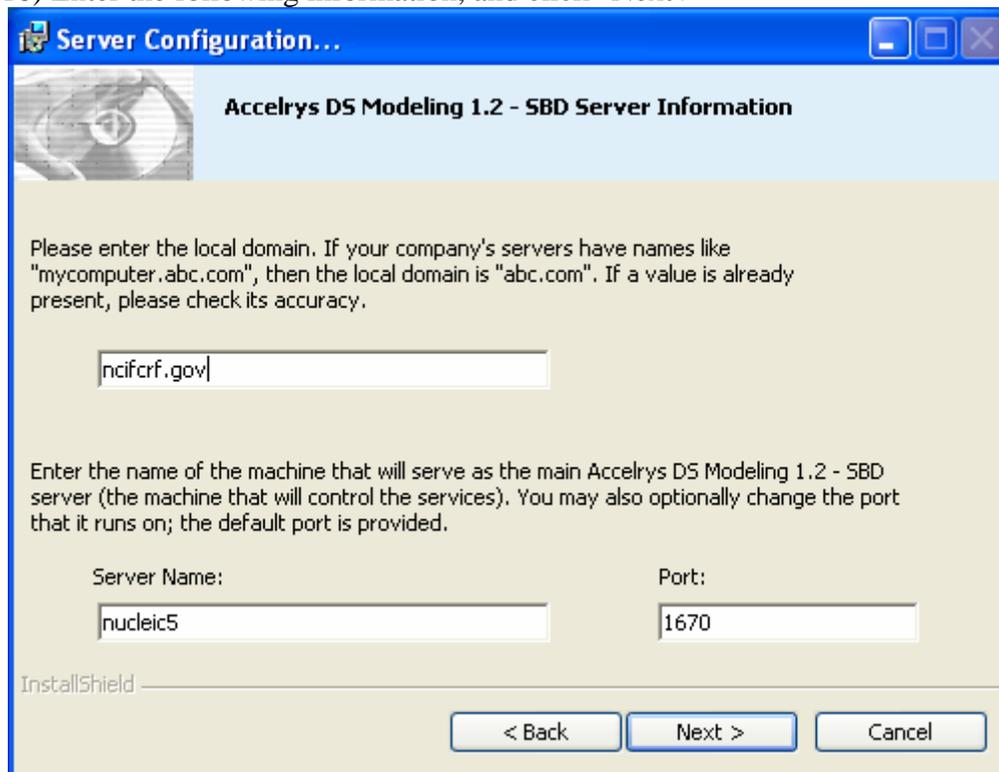
After unzipping, the following menu will show up. Click OK to continue.



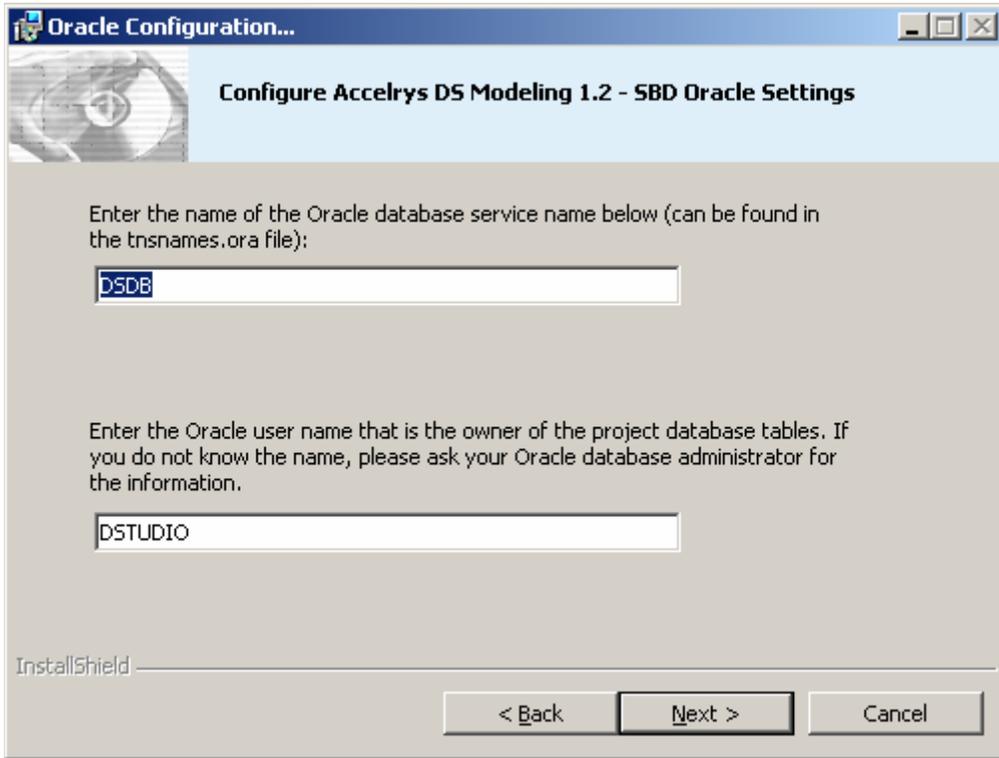
9) After unzipping, the installation starts automatically. (This step may take some time, please be patient!) Once the setup is complete, you should see the following menu. Click “Next >” to continue



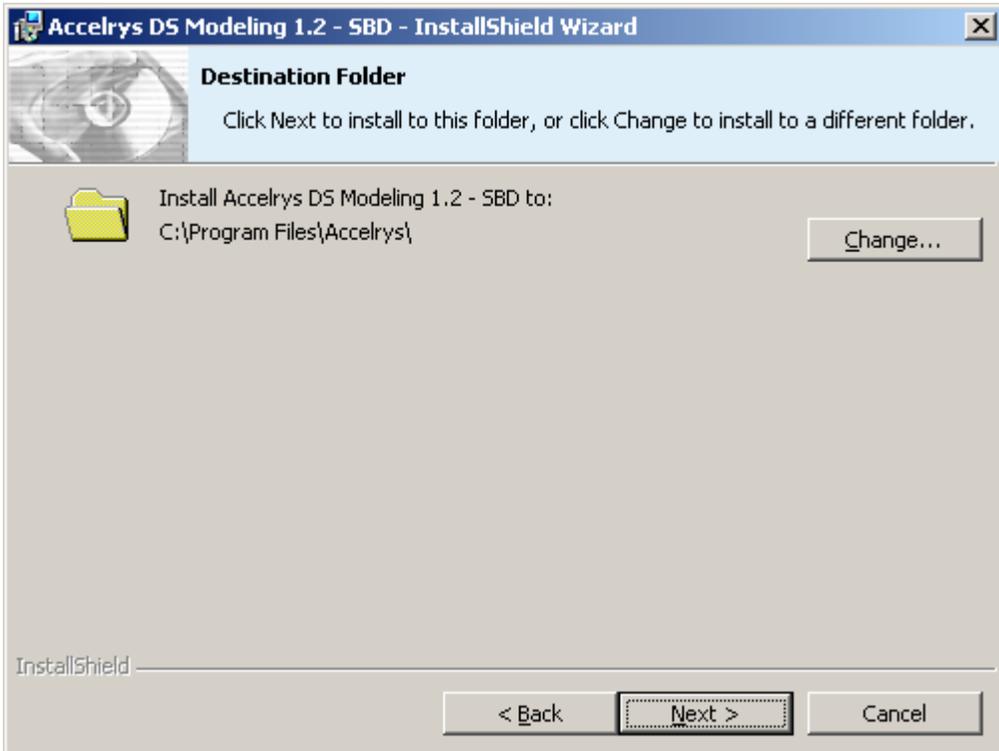
10) Enter the following information, and click “Next >”



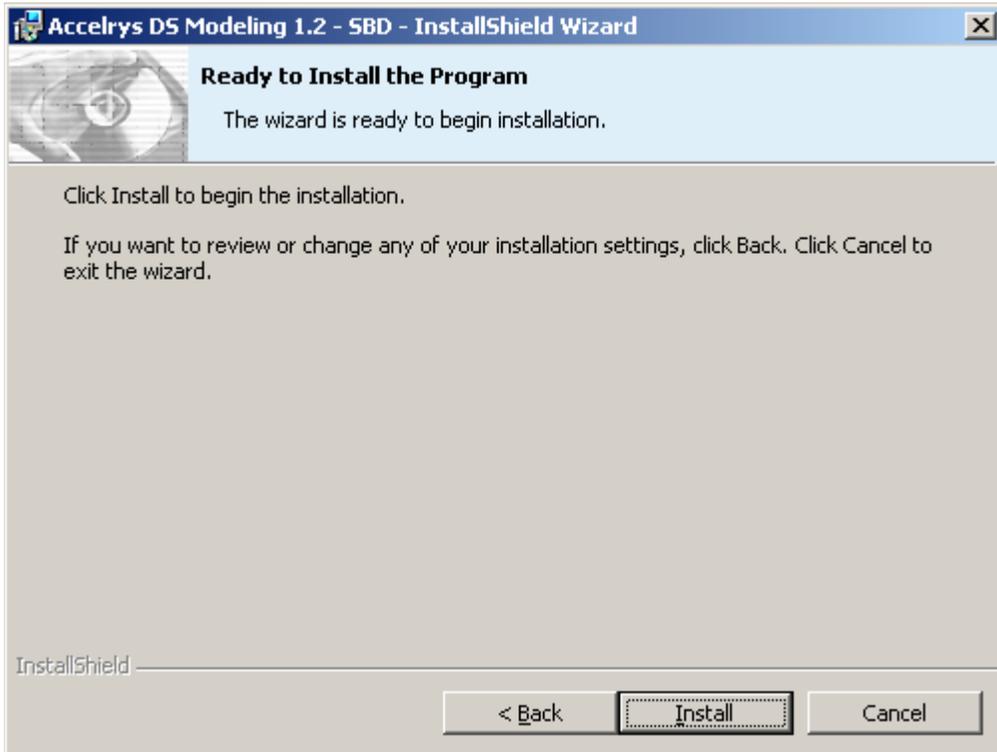
11) Enter the Oracle configuration as shown below, and click “Next>”



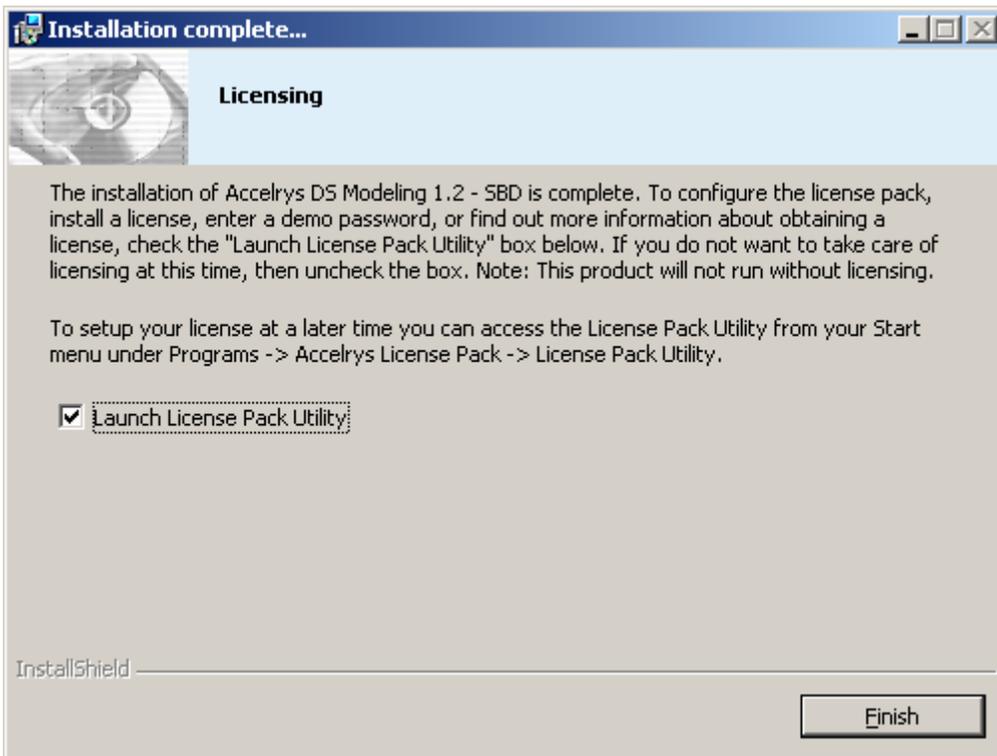
12) Keep the default Destination folder and click “Next>” to continue



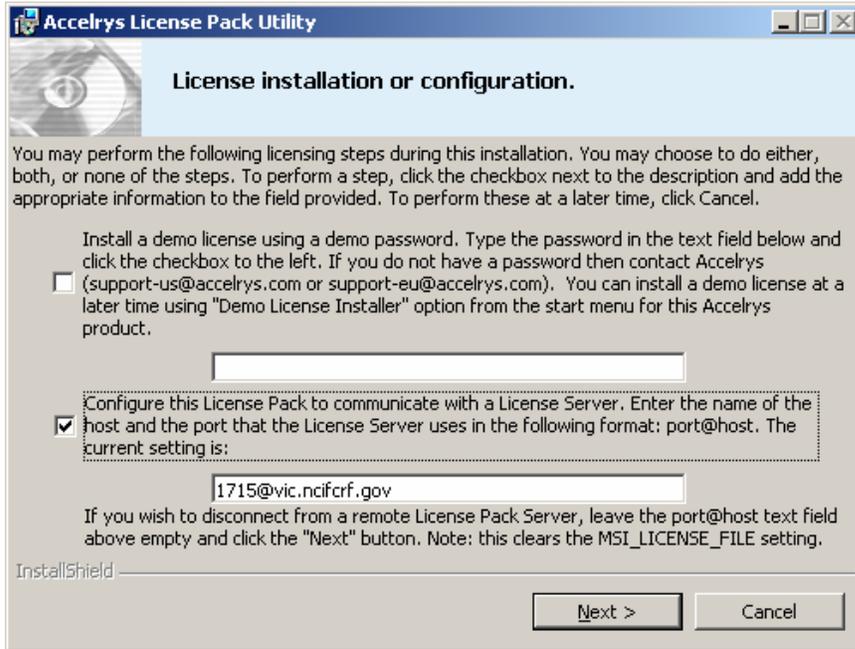
13) Click “Install” to start the installation (Note: This step may be time consuming, please be patient!)



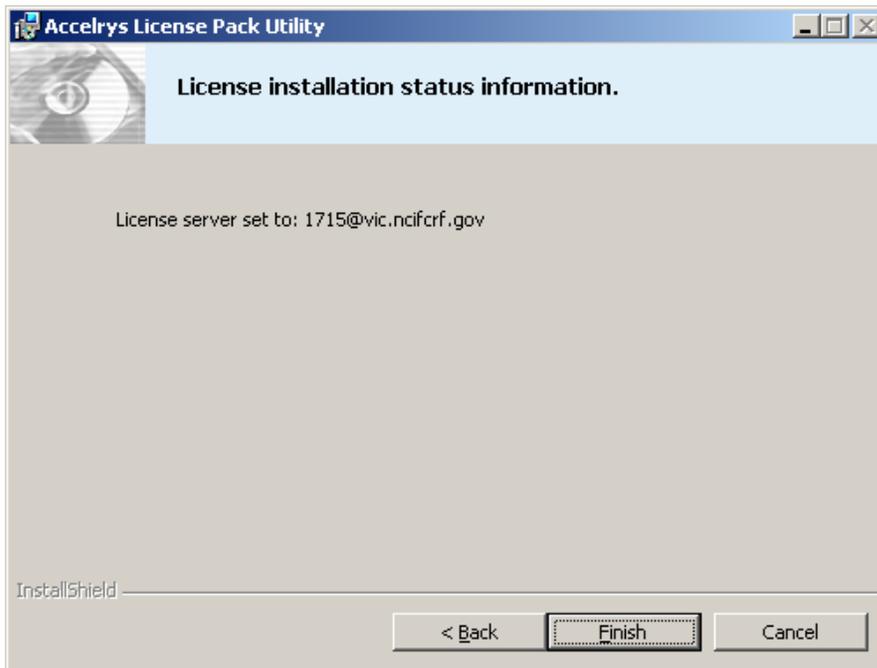
14) Click “Finish” to finish up the Licensing setup



15) Enter the license server setup, and click “Next >”



Finally finish up the license installation by clicking “Finish”



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 1.2 - SBD\config, and edit the file DSModeling12.cfg and make sure you have the following line:
DS_NAMESERVICE_HOST nucleic5.ncifcrf.gov

Please note that, C:\Program Files\Accelrys\DS Modeling 1.2 - SBD\config, correspond to the version number '1.2'. If you are installing version '3.5', then you need to go to C:\Program Files\Accelrys\DS Modeling 3.5 - SBD\config

After DS ModelingSBD installation, you will see, DS Modeling-SBD icon on your desktop, and new entries for “Accelrys DS Modeling-SBD” 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 have downloaded the exe files (ex. MSmodeling31.exe or 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 **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 1.2-SBD installation.

DS-Modeling SBD Quick-start:

Double-click on DS-Modeling-SBD icon on the desktop. Once the DS Modeling window shows up, enter the DS Modeling username/password to login.

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