Getting Started With SCALE

Installation and Updates

Robert A Lefebvre

SCALE Users Group Workshop Sept 26-28, ORNL

ORNL is managed by UT-Battelle for the US Department of Energy



Getting Started Overview

- SCALE Release Process
- Distributions
 - Source + executable, executable only
- Prebuilt Binaries
 - Windows, Mac OSX, and Linux
- Data
- Code Compilation
- Installation Verification
- Frequently Asked Questions



SCALE Release Process





SCALE Release Process – Initial Software Request

- Go to https://rsicc.ornl.gov/
- Under Request Software, click Submit Request
- Follow the Request Form steps
- Receive email from RSICC of software license approval.
 - Read each paragraph carefully and understand licensing and export control restrictions.
- Wait for your stack of DVDs to arrive in the mail



SCALE Release Process – Software Updates

Email <u>scalehelp@ornl.gov</u> and request latest SCALE update

- Requires RSICC License
- Download link will be emailed once license is verified
- SCALE 6.2 software updates are cumulative
 - No more missed updates, just request and install the latest
- Data has not changed, only executables
 - Copy or link to existing SCALE 6.2 data
- Follow README instructions



Distributions

Source + Executables

- Includes prebuilt binary executables
- Includes source code from which executables can be recompiled
 - Necessary for parallel MPI executables
- Available to almost everyone*
- Includes Data
- Executable Only
 - Only includes prebuilt binary executables
 - No source can't recompile
 - Cannot compile parallel MPI
 - Includes Data
 - More available to almost everyone*
- * Restricted by export control



Prebuilt Binaries

Prebuilt Serial Executables

- 💑 Linux SCALE-6.2.X.tar.gz
- 🛸 Mac OS X SCALE-6.2.x-setup.dmg
- 🧐 Windows SCALE-6.2.x-setup.exe

Native installers for intuitive installation of executables*

- Linux unzip, untar
- Mac OS X drag-n-drop
- Windows next, next, finish
- * Only executables, not data



Data

- 30 GB requires 9 DVDs
- Exists in *.pak files
- Has not changed for any SCALE 6.2.x release
- Is the reason the installation takes so long



Installation Procedure

Follow the README Instructions

- <u>https://www.ornl.gov/sites/default/files/SCALE%20Code%20System.pdf#page</u> =45
- Step 1 Execute your operating system's native installer
- Step 2 run scale-6.2-data-setup.jar
 - Located on DVD #1
 - Requires Java runtime environment (freely available from Oracle)
- Step 3 follow the *.pak installation prompts
 - This may require substantial time depending on hard disk and DVD reader speeds



Code Compilation

- Specific instructions listed at <u>https://www.ornl.gov/sites/default/files/SCALE%20Code%20System.pdf#p</u> age=71
- Use specific versions:
 - Intel Compiler 14.1 (Linux, Mac), 15.0.0 (Windows)
 - GNU 4.8.x (Linux, Mac)
 - LAPACK/BLAS 3.5
 - CMake 2.8.12.2 (Linux, Mac), 3.3.2 (Windows)
 - OpenMPI 1.8.1 (Linux, Mac)
 - Qt 4.8.x
- Example scripts available under SCALE/script
- Don't overlook configuration instructions
 - Work around for Trilinos Anasazi configuration bug
 - <u>https://www.ornl.gov/sites/default/files/SCALE%20Code%20System.pdf#page=74</u>



Installation Verification

- Useful to determine if installation is functional
- Instructions at <u>https://www.ornl.gov/sites/default/files/SCALE%20Code%20System.p</u> <u>df#page=74</u>
- Can be conducted using Fulcrum or SCALE runtime environment (ScaleRTE)
 - Open Fulcrum and select Run>Run Verification Suite, select directory in which execution will occur*.
 - Go to empty* directory and type path/to/scale/bin/scalerte
 @samples/samples
- Runtime is usually 12 hours, can be longer due to slow disk speed or anti-virus on-access scans
- * Directory will receive all message, output, results files



Frequently Asked Questions

- Google user group community -<u>https://groups.google.com/forum/#!categories/scale-users-group/scale-62</u>
- Data installation issues
- SCALE runtime shortcuts
- Fulcrum input auto-completion issues



Google User Group

- Lots of frequently asked questions already answered
 - Installation questions
 - Technical questions
 - Questions and Answers from prior versions of SCALE

Protected group

must be RSICC licensed for SCALE to be approved



Data Installation Issues

- Location, Location, Location
- When installing, use the SCALE path, not SCALE/data
 - Install at C:\Scale-6.2.2\ Good
 - Installer creates C:\Scale-6.2.2\data
 - Install at C:\Scale-6.2.2\data BAD
 - Installer creates C:\Scale-6.2.2\data\data
- Linking data from prior SCALE 6.2 install is simple:
 - Change into the SCALE directory : cd c:\Scale-6.2.2
 - Windows:mklink /D data c:\SCALE-6.2\data
 - Linux, Mac:ln -s /scale/release/6.2/data data



SCALE Runtime Shortcuts

- Place SCALERTE in the PATH environment variable
 - Must be the absolute path PATH=/scale/release/6.2.2/bin/:\$PATH
 - Allows reference to scalerte
 - Can only be used with single installation of SCALE
- Use aliases on Linux and Mac OS X
 - Allows references to multiple scalerte versions (SCALE 6.1,6.2, etc.)
 - alias scale6.2.2="/scale/release/6.2.2/bin/scalerte"
- Use of doskeys on Windows
 - Allows references to multiple scalerte versions (SCALE 6.1,6.2, etc.)
 - doskey scale6.2.1=c:\scale-6.2.1\bin\scalerte.exe \$*



Fulcrum Auto-completion (CTRL+SPACE) doesn't work

- Fulcrum auto completion feature doesn't work
 - I.e., nothing is generated in your input upon typing enter
- Issue is likely Java runtime environment
 - Is Java installed?
 - No install Java
 - Yes are there multiple versions of Java installed?
 - Is one of them not working?
 - Delete the one that is not working.
 - This is a typical scenario at government offices where 2 Java installations occur, and the operating system (typically Windows) provides the non-functioning Java to Fulcrum





- Read the README or Manual's README section It is useful
 - <u>https://www.ornl.gov/sites/default/files/SCALE%20Code%20System.pdf#page</u> =45
- Have a question?
 - Email <u>scalehelp@ornl.gov</u> or search and use google forum
 - <u>https://groups.google.com/forum/?fromgroups#!forum/scale-users-group</u>

