NEAMS Workbench Remote Setup of SCALE on ORNL compute resources

Robert A. Lefebvre
Mark L. Baird
L. Paul Miller

Reactor and Nuclear Systems Division

Oak Ridge National Laboratory, USA

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

Presentation Overview

- NEAMS Workbench Installation
- Required ORNL Accounts
- SSH configuration
- NEAMS Workbench SetupRemote configuration of remote SCALE

If any issues arise during these instructions, please contact the NEAMS Workbench help line - nwb-help@ornl.gov - for assistance.

OAK RIDGE National Laboratory

NEAMS Workbench Installation

1. Download the latest version from https://code.ornl.gov/neams-workbench/downloads for your operating system

2. Unzip the software bundle

3. The NEAMS Workbench is now installed
   - An additional Python environment installation will occur upon the first execution of the NEAMS Workbench

OAK RIDGE National Laboratory

Remote Application Setup Requirements

- ORNL UCAMS credentials, login1 and compute resource accounts
- SSH Port forwarding*
  - This will need to be active for all transactions with compute resources
- Passwordless SSH* to remote **Linux** machine/cluster*
- A compute resource installation of the NEAMS Workbench
  - This is ORNL provided, but useful to know if configuring your own install
- A NEAMS Workbench SetupRemote* configuration for remote SCALE on ORNL computer resources

* See later slide instructions

OAK RIDGE National Laboratory

Requires ORNL Accounts

- Work with your ORNL host to obtain:
  - UCAMS account
    - enables ORNL network access
    - You should receive in the mail a **RSA SecurId security token** for network access
  - Login1.ornl.gov account
    - enables SSH via login1 jump server into ORNL network
  - Compute resource account
    - Enables job submission
    - Please review compute resource user guidance and policies

Note: Be sure to take and keep current your ORNL Cyber security training or your accounts will be suspended

SSH Port forwarding

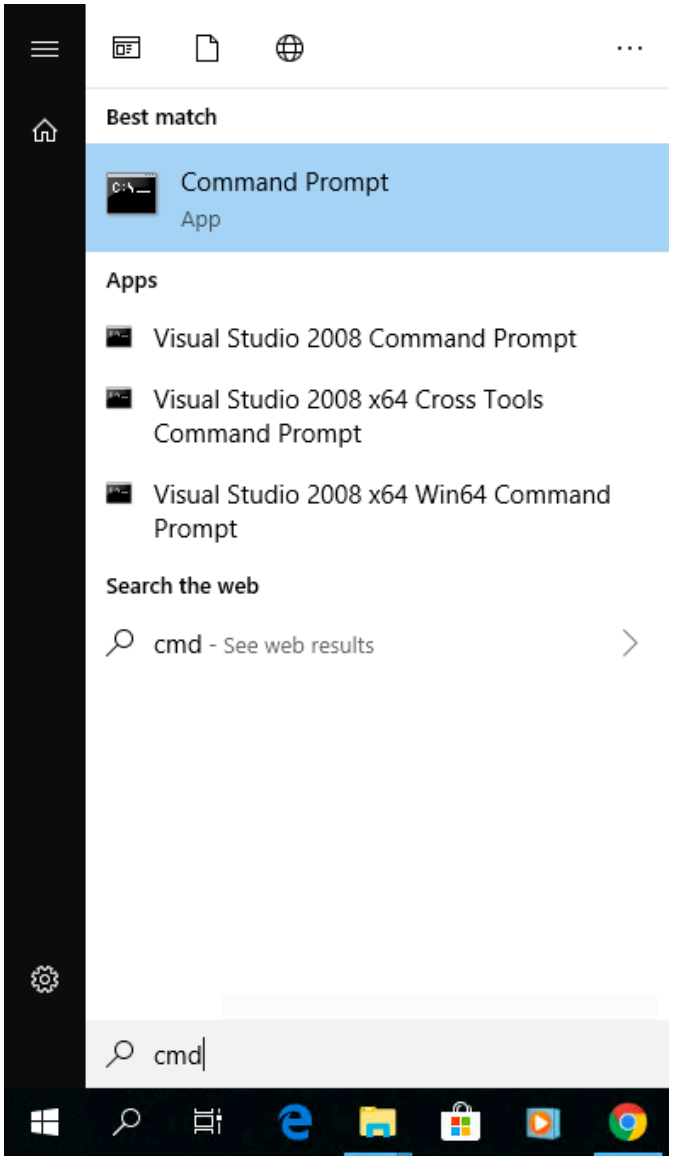
- Requires an SSH client installed
  - Windows can use OpenSSH – included with Windows 10 as of 2018 and later.
- Requires SSH private-public key pair
- Requires SSH port forward configuration

OAK RIDGE National Laboratory

Open CMD

The follow slides and included instructions will use the **CMD** program. Use the Start/Windows search to open the program

1. Press the Windows key or click the Windows icon and type '**CMD**' to search.
2. Press ENTER or left click the **Command Prompt** icon



OAK RIDGE National Laboratory

SSH Client

- Ensure SSH client is available
  - Open CMD program and enter **where ssh**
  - If **SSH** is available, the path to the program will be printed in the console

Command Prompt

```
Microsoft Windows [Version 10.0.17134.885]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Users\raq>where ssh
C:\Windows\System32\OpenSSH\ssh.exe

C:\Users\raq>_
```

If no SSH client is available, please contact nwb-help@ornl.gov

OAK RIDGE National Laboratory

Generate SSH private-public key pairs

- With CMD open, run **ssh-keygen**
- Accept all the defaults (hit enter 3 times)
  - Do not enter a passphrase – this will require additional authentication which will prevent the NEAMS Workbench from operating as expected

Select Command Prompt

```
C:\Users\raq>ssh-keygen
Generating public/private rsa key pair.
Enter file in which to save the key (C:\Users\raq/.ssh/id_rsa):
Created directory 'C:\Users\raq/.ssh'.
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in C:\Users\raq/.ssh/id_rsa.
Your public key has been saved in C:\Users\raq/.ssh/id_rsa.pub.
The key fingerprint is:
SHA256:ftkHFZrobTk2iIWjzcYfpE9PYQIg9vtoxK+D0u2rujo raq@ornl@SCALEPC3
The key's randomart image is:
+---[RSA 2048]----+
|    o ...      .  |
|   . o   o . o .  |
|      . o = = .   |
|     . * B = +    |
|      = S = X     |
|     . * + O +    |
|   . oo + = o .   |
|E . o.o. .   .    |
|.oo+.o+o          |
+----[SHA256]-----+

C:\Users\raq>
```


OAK RIDGE National Laboratory

SSH Port Forwarding - Login1.ornl.gov

SSH tunnel config Steps:

1. Open a new file called 'config' in the HOME/.ssh directory
2. Copy the text from box on right into the 'config' file
3. Update **UCAMS-ID** to be your ORNL-provided user id
4. Update **XXXXX** to be a port number between 10000 and 55555
   - This must be unique across users.
5. Update **YYYYY** to be a port number between 10000 and 55555
   - This must be unique across users.

TEXT TO COPY INTO CONFIG FILE

```
host tunnelinit
Hostname login1.ornl.gov
User UCAMS-ID
LocalForward XXXXX remus.ornl.gov:22
LocalForward YYYYY romulus.ornl.gov:22

Host remus_via_tunnel
HostKeyAlias remus.ornl.gov
Hostname localhost
Port XXXXX
User UCAMS-ID

Host romulus_via_tunnel
HostKeyAlias romulus.ornl.gov
Hostname localhost
Port YYYYY
User UCAMS-ID
```


OAK RIDGE National Laboratory

SSH Port Forward check

- Ensure **HOME\.ssh\config** file exists
  - e.g., did you create **HOME\.ssh\config.txt** by accident? Move/rename it to **HOME\.ssh\config**
- HOME\.ssh\config should look like:
  - BE SURE TO USE DIFFERENT **USER** and **PORT NUMBERS**

EXAMPLE HOME\.ssh\config

```
host tunnelinit
Hostname login1.ornl.gov
User raq
LocalForward 12345 remus.ornl.gov:22
LocalForward 54321 romulus.ornl.gov:22

Host remus_via_tunnel
HostKeyAlias remus.ornl.gov
Hostname localhost
Port 12345
User raq

Host romulus_via_tunnel
HostKeyAlias romulus.ornl.gov
Hostname localhost
Port 54321
User raq
```


OAK RIDGE National Laboratory

Initialize SSH tunnel

1. Open a CMD windows
2. Activate the tunnel by performing '`ssh tunnelinit`'
3. If the 'authenticity of host login1.ornl.gov' can't be established, response '**yes**' to proceed
4. Enter your ORNL **pin** and the **RSA SecurID token number**
5. Observe the login1.ornl.gov user notice and active prompt indicating success

Select raq@login1:~

```
C:\Users\raq>ssh tunnelinit
The authenticity of host 'login1.ornl.gov (160.91.5.101)' can't be established.
ECDSA key fingerprint is SHA256:4lDrTsnT+/8DjqFKbgqWRBVzXrbviRT4ng3zy0lvjkI.
Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added 'login1.ornl.gov,160.91.5.101' (ECDSA) to the list of known hosts.
Enter PASSCODE:
Last login: Wed Jul 31 06:37:18 2019 from dyn010159202189.dz.ornl.gov

                          NOTICE TO USERS

This is a Federal computer system and is the property of the United States
Government.  It is for authorized use only.  Users (authorized or
unauthorized) have no explicit or implicit expectation of privacy.

Any or all uses of this system and all files on this system may be
intercepted, monitored, recorded, copied, audited, inspected, and disclosed
to authorized site, Department of Energy, and law enforcement personnel, as
well as authorized officials of other agencies, both domestic and foreign.
By using this system, the user consents to such interception, monitoring,
recording, copying, auditing, inspection, and disclosure at the discretion
of authorized site or Department of Energy personnel.

Unauthorized or improper use of this system may result in administrative
disciplinary action and civil and criminal penalties.  By continuing to use
this system you indicate your awareness of and consent to these terms and
conditions of use.  LOG OFF IMMEDIATELY if you do not agree to the
conditions stated in this warning.
--------
Authorized users who need help can see /usr/local/etc/login-server.policy .


[raq@login1 ~]$
```


OAK RIDGE National Laboratory

Compute Resource Access via login1

1. From a new CMD windows enter **ssh remus_via_tunnel**
2. If the 'authenticity of host remus.ornl.gov' can't be established, response '**yes**' to proceed
3. Enter your **UCAMS password** when prompted
4. Observe the user notice and remus prompt indicating success

Note: the ssh tunnel must be initialized prior to this or future compute resource transactions

Select raq@remus:~

```
C:\Users\raq>ssh remus_via_tunnel
The authenticity of host 'remus.ornl.gov ([::1]:21435)' can't be established.
RSA key fingerprint is SHA256:jCTk/LL/JoCqBv49Da+J0CLNNMi2RDO4r7/nPAPDo4Y.
Are you sure you want to continue connecting (yes/no)? yes
Warning: Permanently added 'remus.ornl.gov' (RSA) to the list of known hosts.
raq@remus.ornl.gov's password:
Last login: Thu Aug  1 08:22:23 2019 from dyn010159195140.dz.ornl.gov

                          NOTICE TO USERS

This is a Federal computer system and is the property of the United States
Government.  It is for authorized use only.  Users (authorized or
unauthorized) have no explicit or implicit expectation of privacy.

Any or all uses of this system and all files on this system may be
intercepted, monitored, recorded, copied, audited, inspected, and disclosed
to authorized site, Department of Energy, and law enforcement personnel, as
well as authorized officials of other agencies, both domestic and foreign.
By using this system, the user consents to such interception, monitoring,
recording, copying, auditing, inspection, and disclosure at the discretion
of authorized site or Department of Energy personnel.

Unauthorized or improper use of this system may result in administrative
disciplinary action and civil and criminal penalties.  By continuing to use
this system you indicate your awareness of and consent to these terms and
conditions of use.  LOG OFF IMMEDIATELY if you do not agree to the
conditions stated in this warning.

[raq@remus ~]$
```


OAK RIDGE National Laboratory

Activate Port Forwarding

1. Open a Terminal
   - Windows provides **CMD** as a terminal
2. Activate the tunnel by performing '`ssh tunnelinit`'
3. Enter ORNL pin and the RSA token number

OAK RIDGE National Laboratory

Perform SSH to remote resource through tunnel

- Open a new terminal
  - Make sure the tunnel is active from previous slide's instructions
  - Windows provides CMD as a terminal
- SSH to remus_via_tunnel
  - `ssh remus_via_tunnel`
  - Enter UCAMS password
- Observe you are logged into the remote resource (remus.ornl.gov) from outside the ORNL network via the active tunnel.
  - Remember, the tunnel must be active for any SSH to remote resource to function.

OAK RIDGE National Laboratory

Passwordless SSH Setup

- Required for remote SCALE configurations to operate
- Appends client machine's public key to the user's list of authorized keys residing on the server.

For **Windows** clients the following statement executed in your **home directory** from a **CMD** terminal is sufficient to configure passwordless ssh to the computer resource:

```
type .ssh\id_rsa.pub | ssh remus_via_tunnel "cat >> .ssh/authorized_keys && chmod 644 .ssh/authorized_keys"
```

Note: The SSH tunnel must be active for these commands to function.

OAK RIDGE National Laboratory

Passwordless SSH Setup Check

1. Conduct the command to append your public SSH key to your server account's list of authorized keys
2. When prompted enter your **UCAMS password**
3. Test the passwordless SSH by running **ssh remus_via_tunnel**
4. Observe no password is requested, the user notice and the remus prompt indicating success

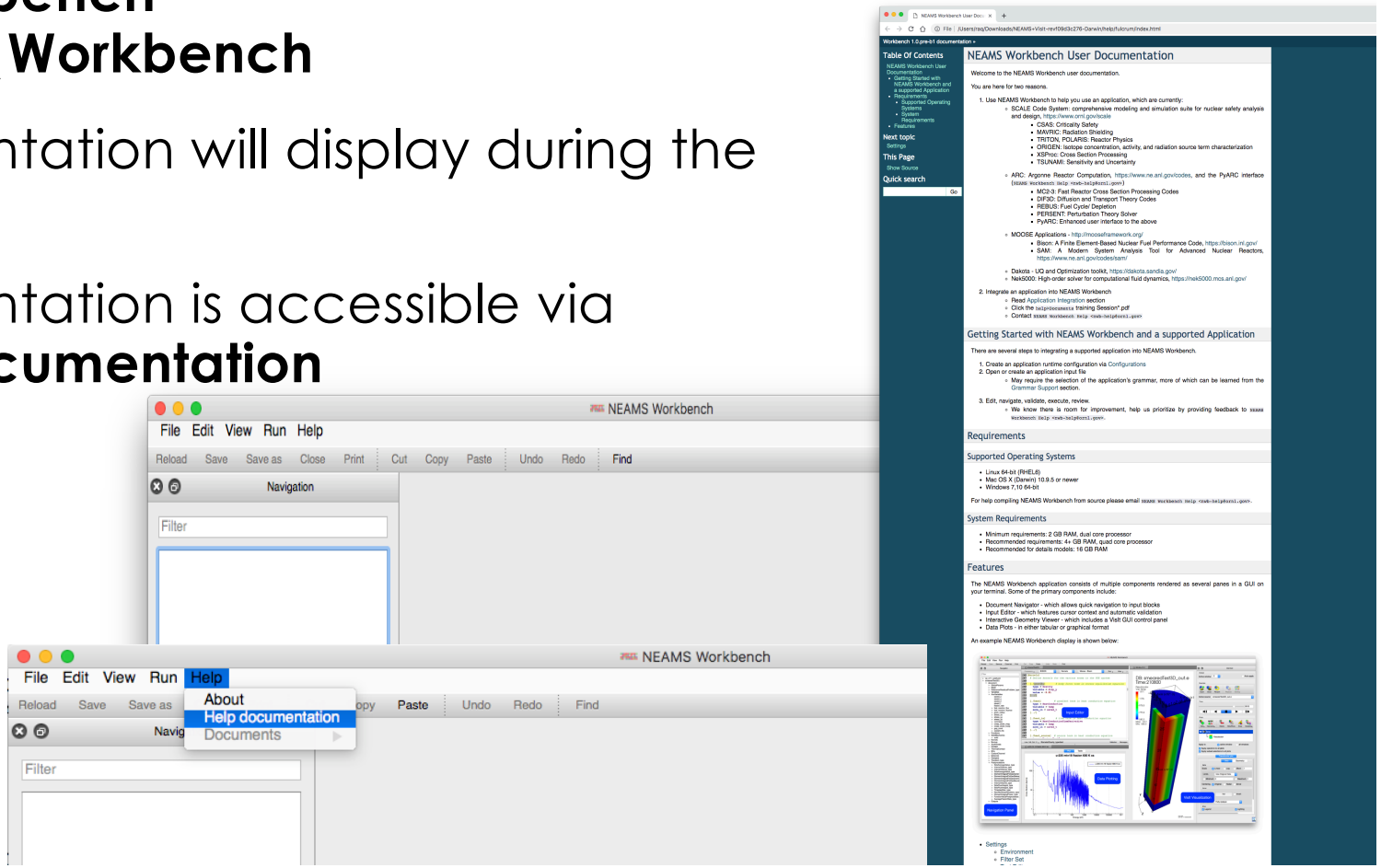
Select raq@remus:~

```
C:\Users\raq>type .ssh\id_rsa.pub | ssh remus_via_tunnel "cat >> .ssh/authorized_keys && chmod 644 .ssh/authorized_keys"
raq@remus.ornl.gov's password:

C:\Users\raq>ssh remus_via_tunnel
Last login: Wed Aug  7 09:03:46 2019 from login1.ornl.gov

                         NOTICE TO USERS

This is a Federal computer system and is the property of the United States
Government.  It is for authorized use only.  Users (authorized or
unauthorized) have no explicit or implicit expectation of privacy.

Any or all uses of this system and all files on this system may be
intercepted, monitored, recorded, copied, audited, inspected, and disclosed
to authorized site, Department of Energy, and law enforcement personnel, as
well as authorized officials of other agencies, both domestic and foreign.
By using this system, the user consents to such interception, monitoring,
recording, copying, auditing, inspection, and disclosure at the discretion
of authorized site or Department of Energy personnel.

Unauthorized or improper use of this system may result in administrative
disciplinary action and civil and criminal penalties.  By continuing to use
this system you indicate your awareness of and consent to these terms and
conditions of use.  LOG OFF IMMEDIATELY if you do not agree to the
conditions stated in this warning.

[raq@remus ~]$
```


OAK RIDGE National Laboratory

Start the client install of the NEAMS Workbench

- Execute **Workbench-Windows\bin\Workbench**
- Help documentation will display during the first startup
- Help documentation is accessible via **Help>Help Documentation**



OAK RIDGE National Laboratory

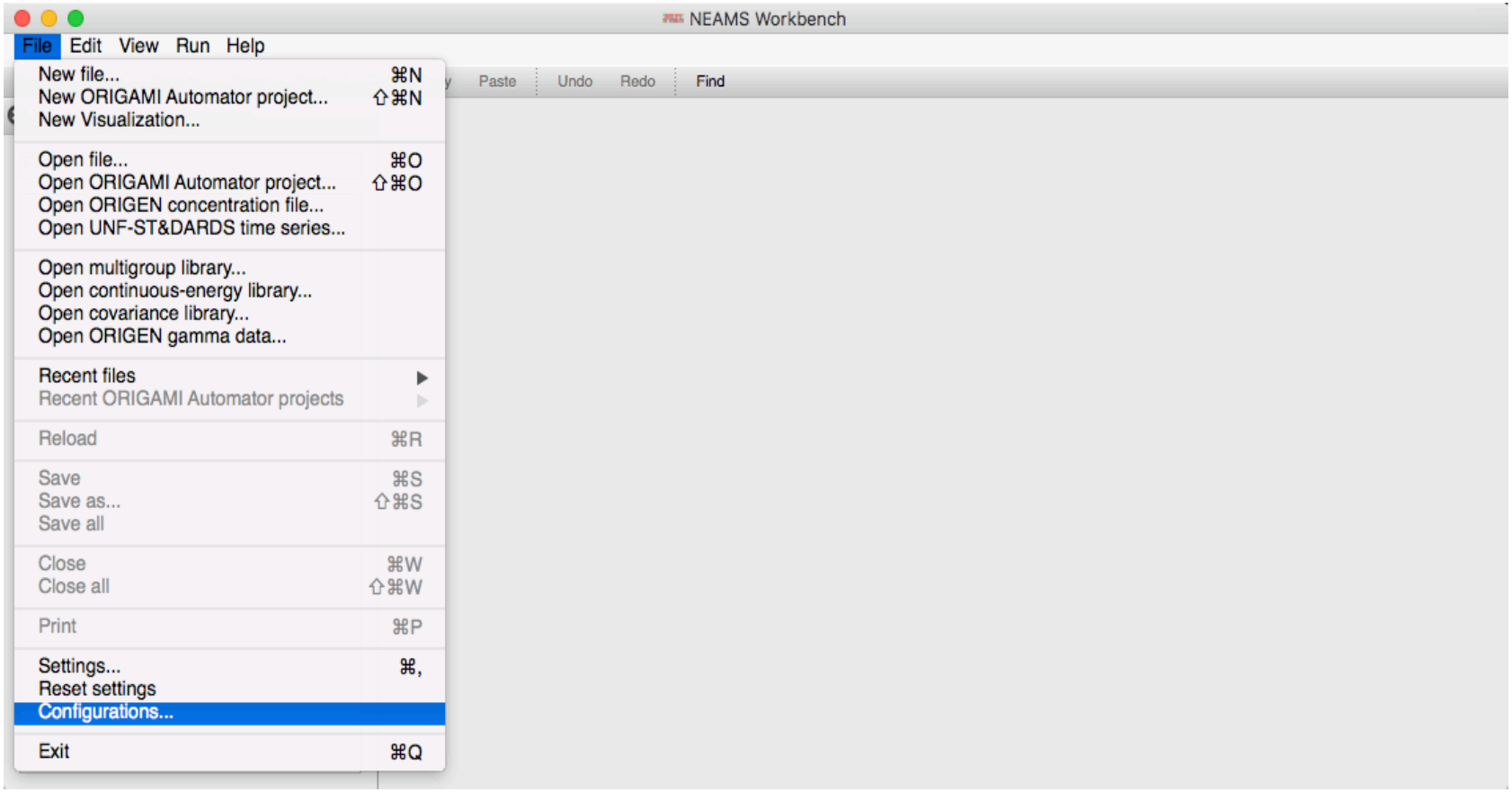
Remote Run Configuration Overview

1. Enable the NEAMS Workbench's Setup_Remote application
2. Create the application-server Setup_Remote input
3. Run application-server SCALE remote input to generate the NEAMS Workbench SCALE remote run configuration.
4. Configure the SCALE remote
5. Open any SCALE input and select the SCALE remote run configuration to activate input validation, autocompletion, syntax highlighting and job launch capabilities
6. Edit input as needed
7. Use the SCALE remote run configuration to launch the SCALE input from your client to the server
8. Wait for job to finish
9. Open files associated with the input file (*.out, *.msg, *.3dmap, etc.)

OAK RIDGE National Laboratory

Configure the Setup Remote Application

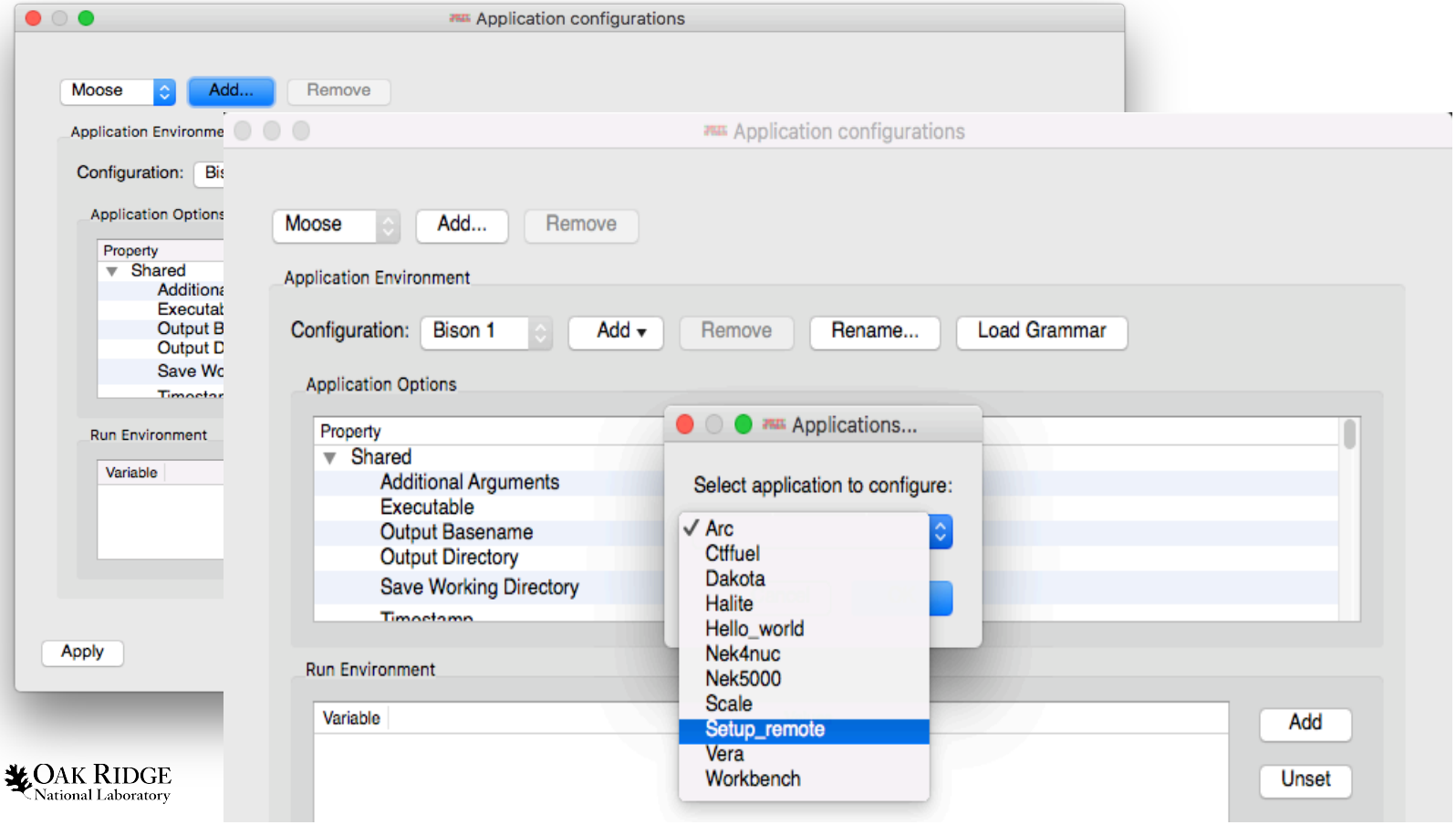
- Click **File>Configurations…**



OAK RIDGE National Laboratory

Configure the Setup Remote Application

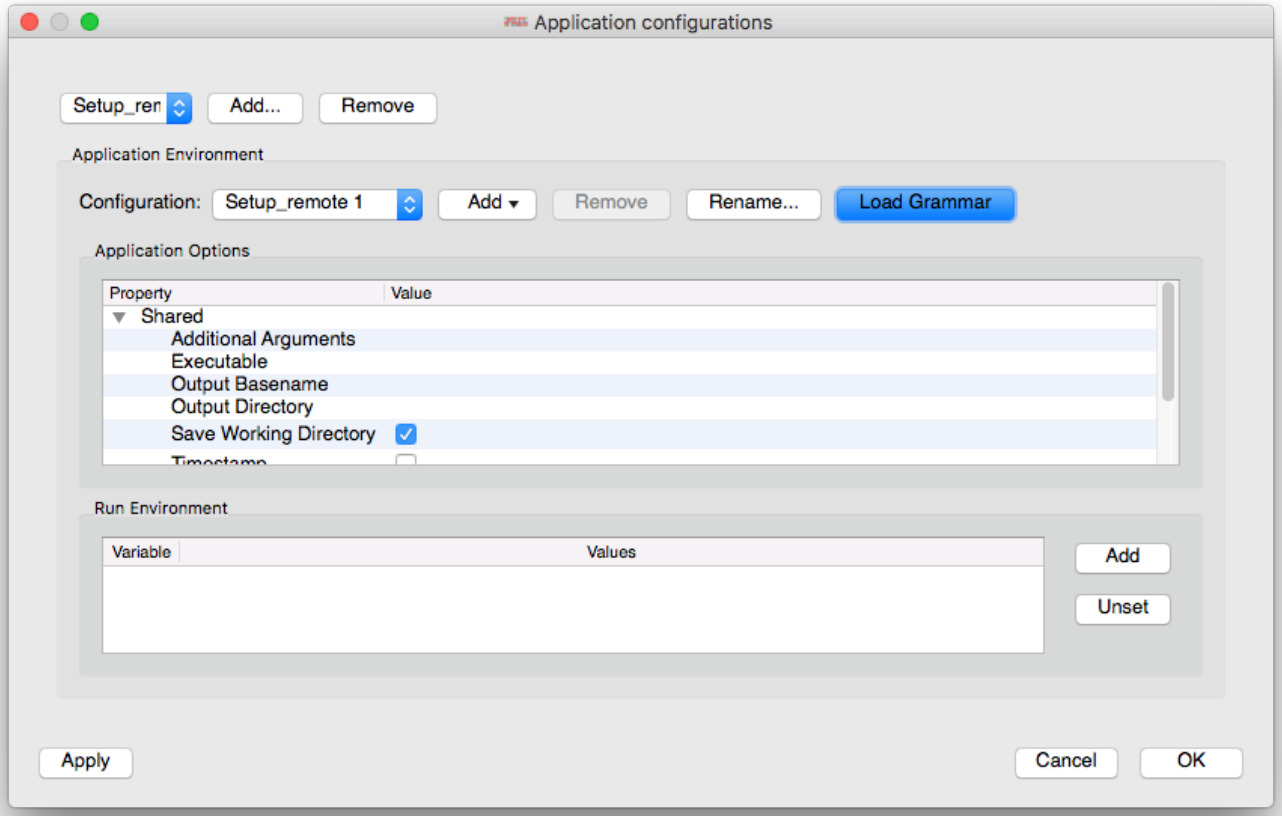
- Click **Add…** and select **Setup_remote** and click **OK**



OAK RIDGE National Laboratory

Configure the Setup Remote Application

- Click **Load Grammar**, **Apply**, and **OK.** This enables SetupRemote input creation.

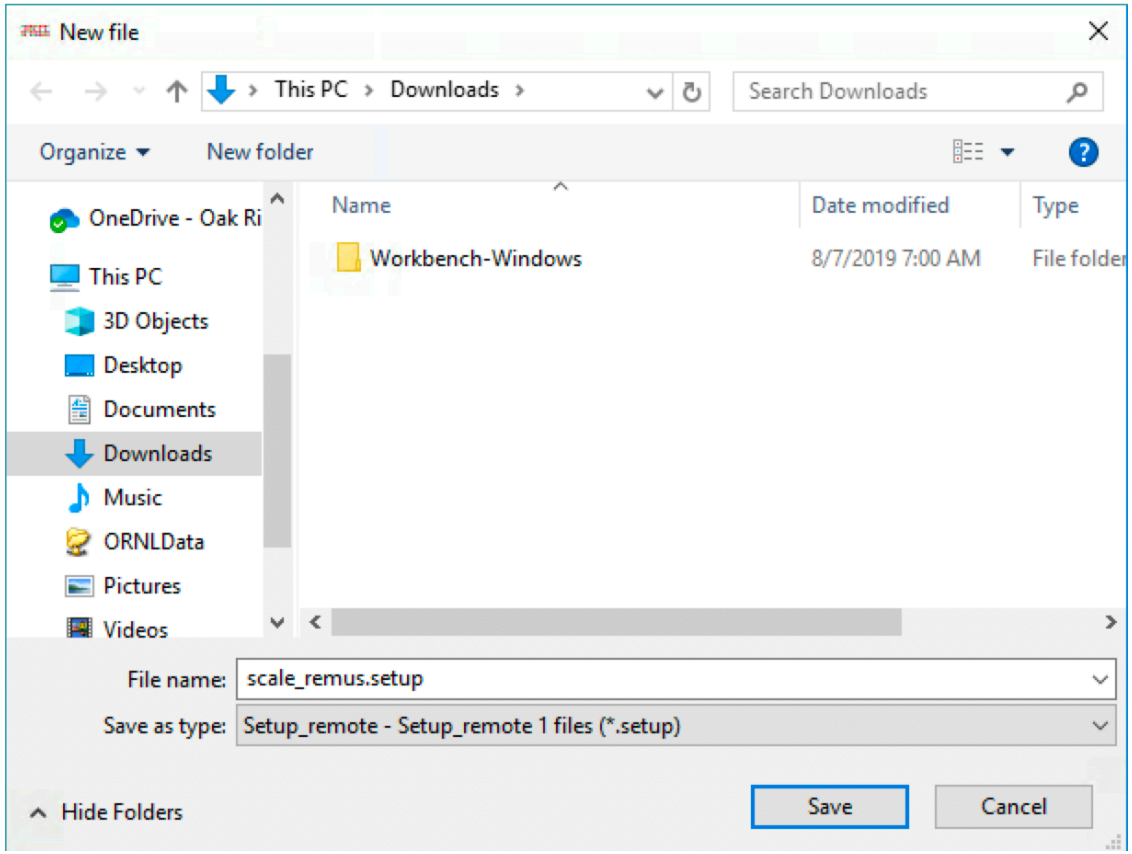


OAK RIDGE National Laboratory

Create the remote SCALE Setup file

- This connects the local NEAMS Workbench to the remote NEAMS Workbench and application installation

1. Click **File>New file…**
2. Provide file name of **scale_remus.setup** and select **Setup_remote** as the file type.
3. Click **Save**



OAK RIDGE National Laboratory

Create the remote SCALE Setup file

Enter the following content and replace **UID** with your UCAMS id.

```
setup_properties {

    runtime_command = "/home/raq/workbench/rte/entry.sh /home/raq/workbench/rte/scale.py"
    application_path = "/scale/scale_dev/mpi/bin/scalerte"
    hostname = "remus_via_tunnel"
    username = "UID"
    remote_execution_home = "/home/UID"
    application_name = "scale_remus_n16"
    upload_patterns = []
    download_patterns = ["${BASENAME}.*"]
    follow_pattern = "${BASENAME}.msg"

    version_number = "1.0.0"

    scheduler_type = pbs
    scheduler_specs {
        submit_path  = "/usr/local/bin/qsub"
        status_path  = "/usr/local/bin/qstat"
        delete_path  = "/usr/local/bin/qdel"
        hold_path    = "/usr/local/bin/qhold"
        release_path = "/usr/local/bin/qrls"
    }

    scheduler_header [
        "#PBS -l nodes=1:ppn=16"
        "module load toolchain/gcc/4.8.3"
    ]
    communication_type = ssh
}
```


OAK RIDGE National Laboratory

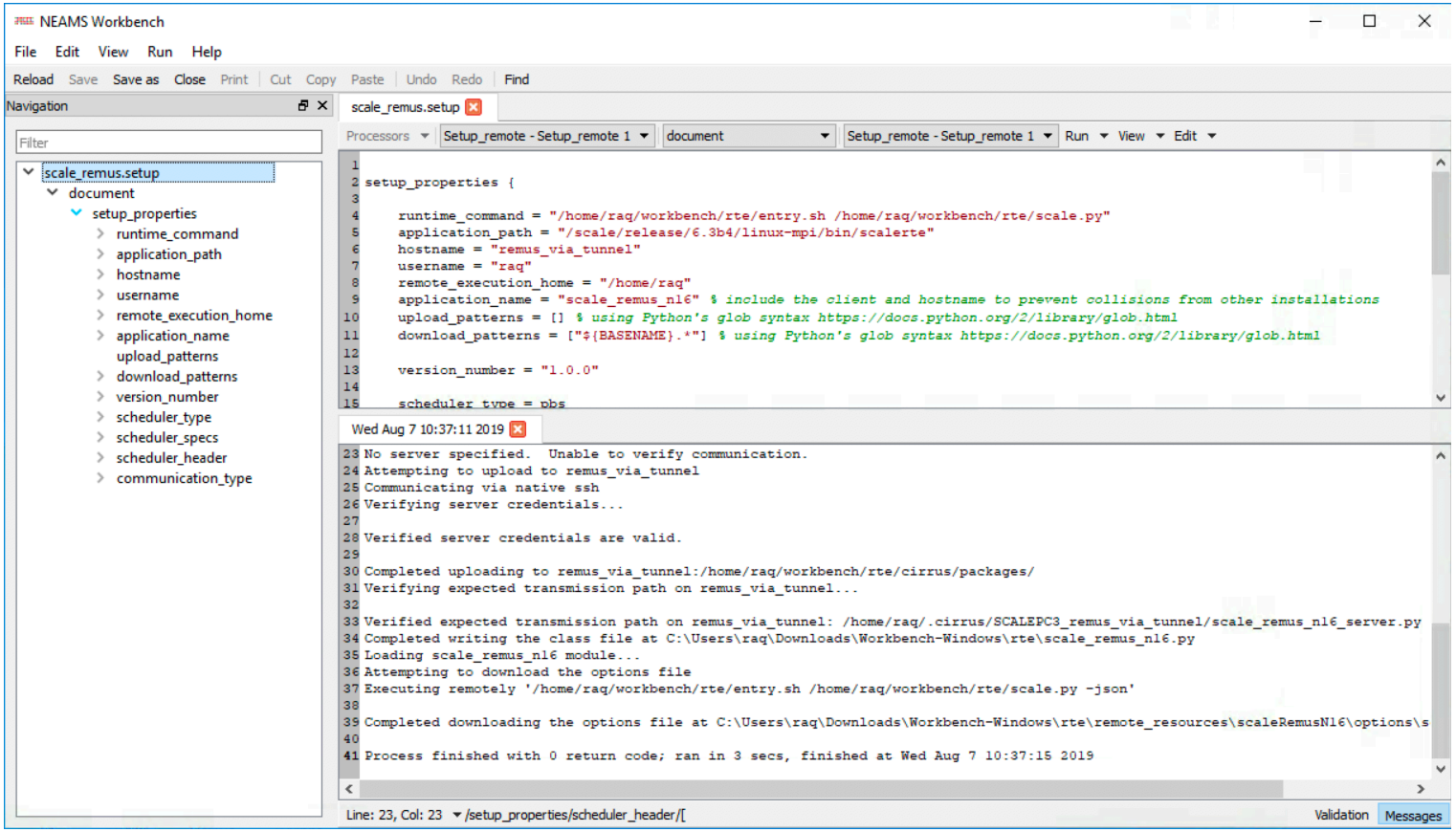
Remote SCALE Setup parameter review

1. **application_path –** the server's SCALE installation location –
   1. Beta installs - **/scale/release/6.3b#/linux/bin/scalerte**, **/scale/release/6.3b#/linux-mpi/bin/scalerte**
   2. Production installs - **/scale/release/6.2.#/linux/INSTALL/bin/scalerte**, **/scale/release/6.2.#/linux-mpi/INSTALL/bin/scalerte**
   3. Latest development - **/scale/scale_dev/serial/bin/scalerte**, **/scale/scale_dev/mpi/bin/scalerte**
2. **Hostname –** the compute resource that will host the compute job. E.g., remus_via_tunnel, romulus_via_tunnel
3. **application_name** – the name of the generated remote configuration. Best practice dictates this be a combination of application, hostname, and parallelism – e.g., **scale_remus_n16**
4. **scheduler_specs -** Important for indicating scheduler queues, job runtime, parallelism and memory, and compiler modules
   1. **#PBS -l nodes=1:ppn=16** # PBS scheduler instructions to run the job on 1 node using 16 **p**rocessors **p**er **n**ode
   2. **module load toolchain/gcc/4.8.3**

OAK RIDGE National Laboratory

Run the remote SCALE Setup file

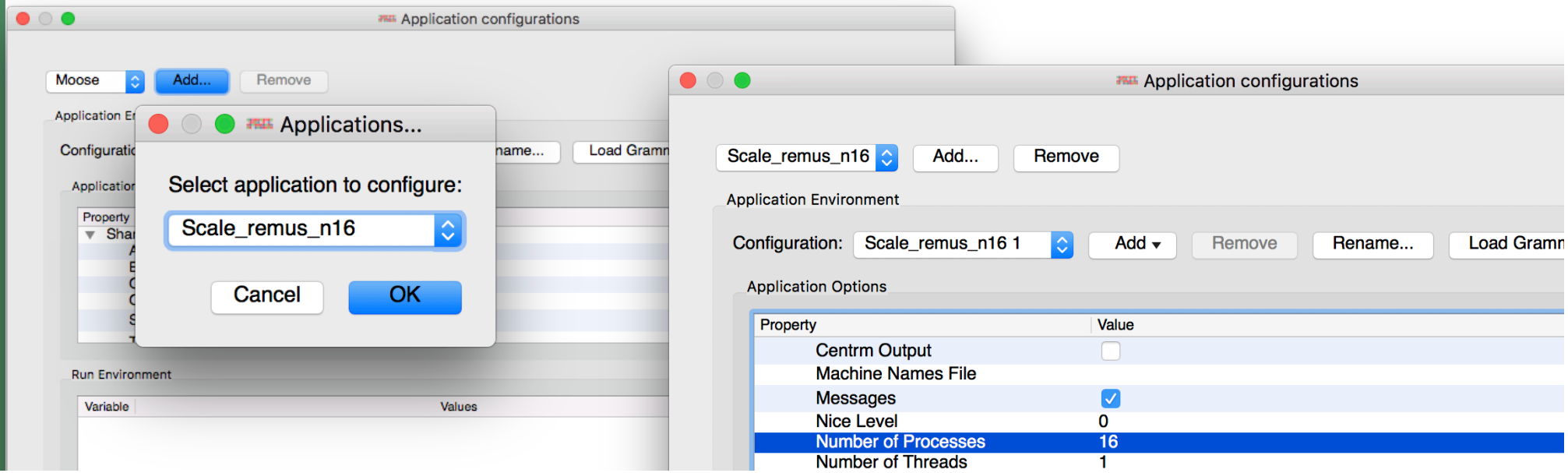
- Click the **run** button to execute the SCALE setup file
  - Ensure the **setup_remote** run configuration is selected, adjacent to the **run** button



OAK RIDGE National Laboratory

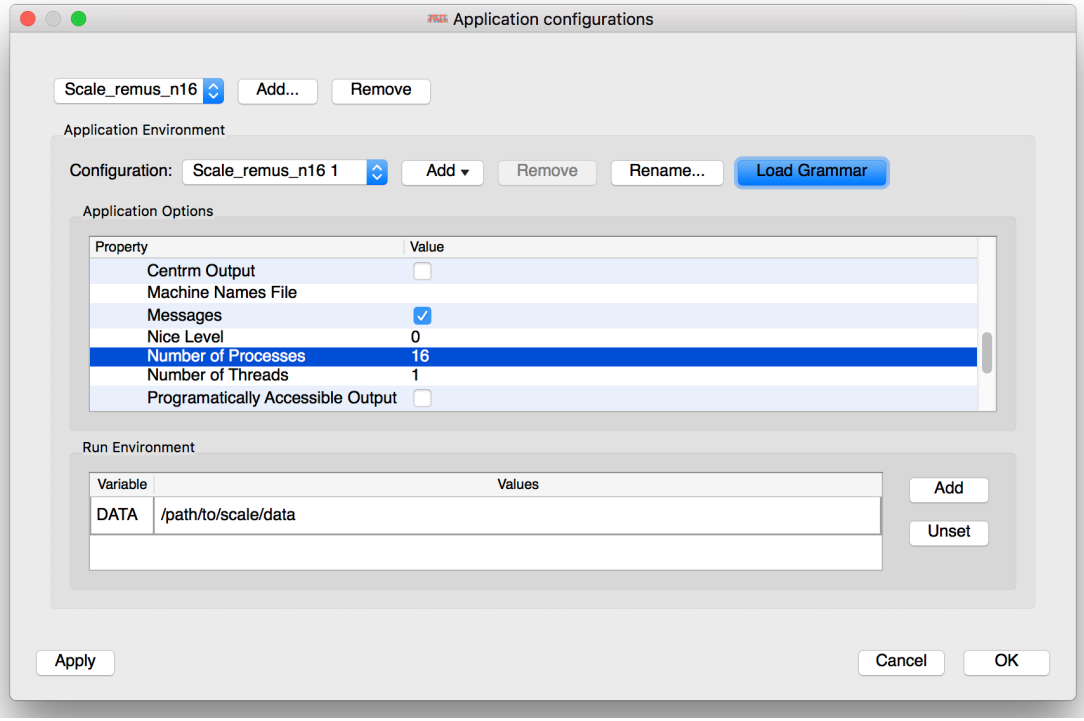
Configure the SCALE remote application

- Click **File>Configurations…**
- Click **Add…** and select **scale_remus_n16** and click **OK**
- In the Application Options panel update the **Number of Processes value** to 16



Configure the SCALE remote application

- Click **Load Grammar**, **Apply**, and **OK.** This enables SCALE input creation.
- Runtime Environment allows assign of alternate DATA, TMPDIR
  - Remove if not desired
- Note: Load grammar may pause for a moment while Workbench retrieves the grammar files from the server.



OAK RIDGE National Laboratory

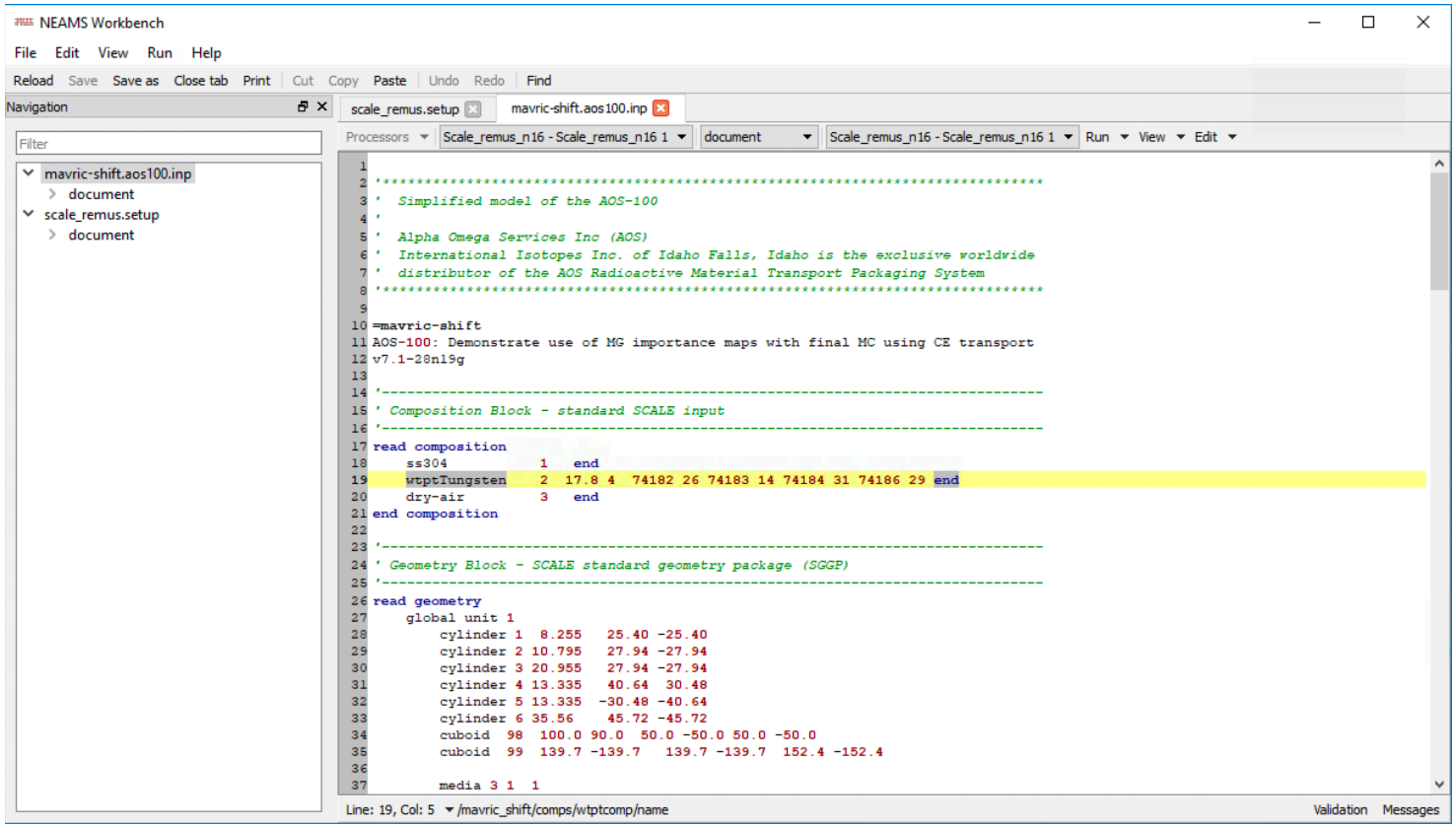
Run Configurations

- The Run Configuration is what communicates SCALE's grammar to the NEAMS Workbench
  - The grammar is the definition of how to interpret the input syntax, data, color and verify input.
- Note: If you open an application input and there is no grammar available (no input navigation tree), check that your application's run configuration is setup.

OAK RIDGE National Laboratory

Test the remote configuration – open the sample problem

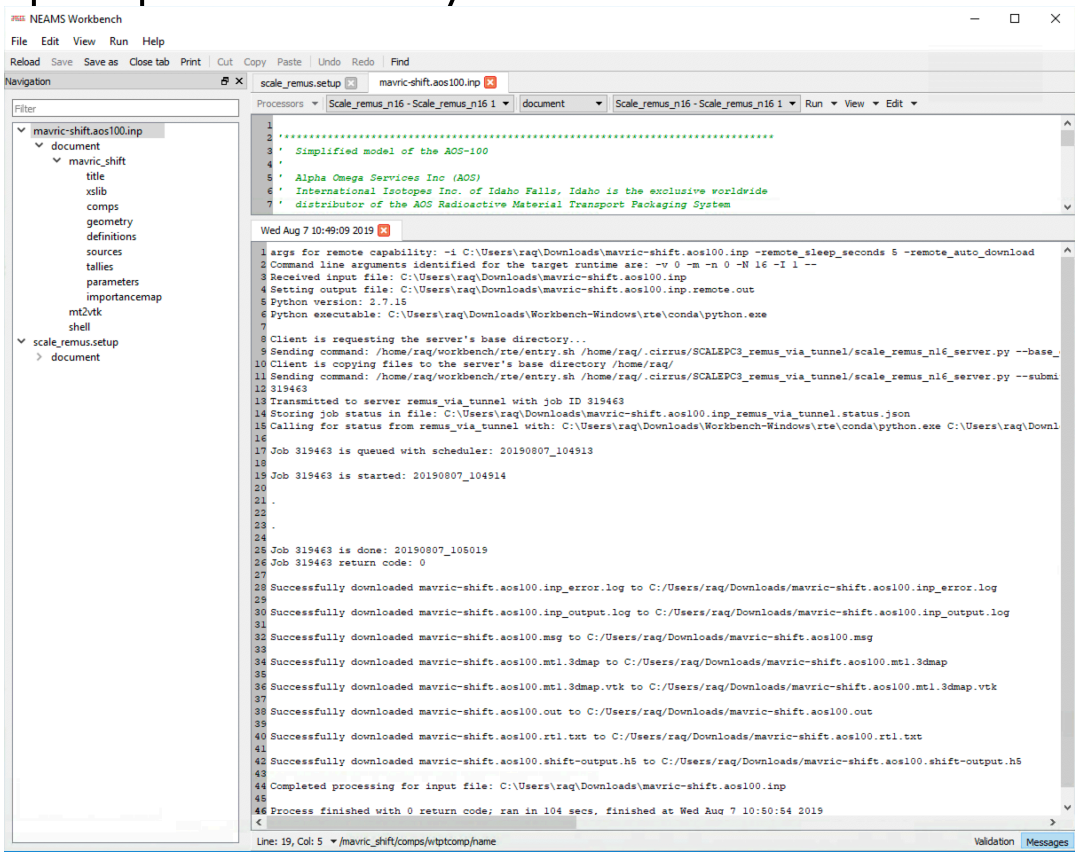
- Open the provided **mavric-shift.aos100.inp** sample problem
  - Note the SCALE grammar is automatically selected



OAK RIDGE National Laboratory

Test the remote configuration – run the sample problem

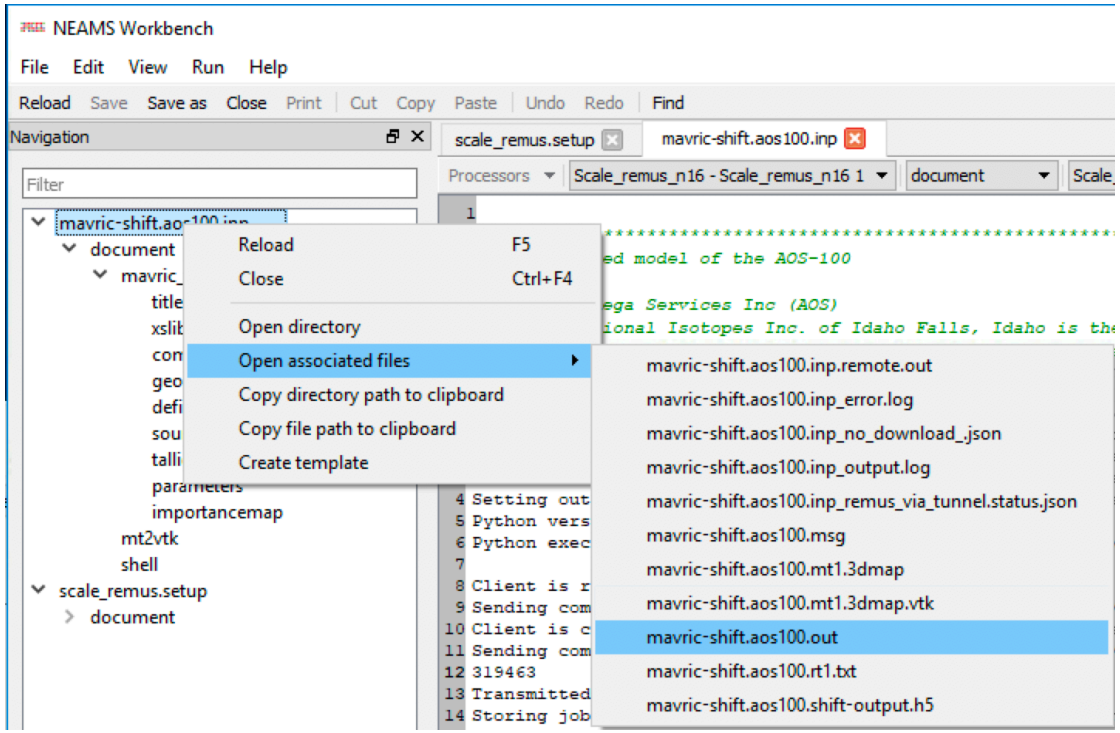
- With the **scale_remus_n16** run configuration selected, adjacent to the run button, run the sample problem by click the **run** button
- Notice the **Messages** panel button (lower right corner) highlight in red. Select this to display the execution log.
- Notice the log shows the Job transmits, queues, starts, statuses, completes, and results are downloaded to your machine



OAK RIDGE National Laboratory

Test the remote configuration – examine results

- To examine associated files, right click the input file and select **Open associated files**
- Select **mavric-shift.aos100.out**



Summary

- You have performed the following:
  1. Configured SSH Tunnel into the ORNL Network using your UCAMS credentials
  2. Configured Passwordless SSH into ORNL compute resources
  3. Configured the NEAMS Workbench to execute parallel (16 processes) SCALE jobs on ORNL compute resources
     - For serial execution repeat slides 24 (Create the remote SCALE Setup file) through 28 (Configure the SCALE remote application) with the following substitutions
       1. Slide 25 - Update '`scale_remus_n16'` to be `'scale_remus'` and delete `"#PBS -l nodes=1:ppn=16"` from the `scheduler_header`
       2. Slides 25-28 use/select '`scale_remus`' instead of '`scale_remus_n16`'
       3. Slide 27 – do not specify the Number of Processes (leave as default of 1)

       Note : Some input parameters are only available during parallel execution (Mavric-Shift x/yblocks). These will need to be removed/commented out when executed in serial.

OAK RIDGE National Laboratory

Questions

- Please email nwb-help@ornl.gov with questions, issues, concerns

OAK RIDGE National Laboratory