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NEAMS Workbench Dakota Application Local and Remote Setup

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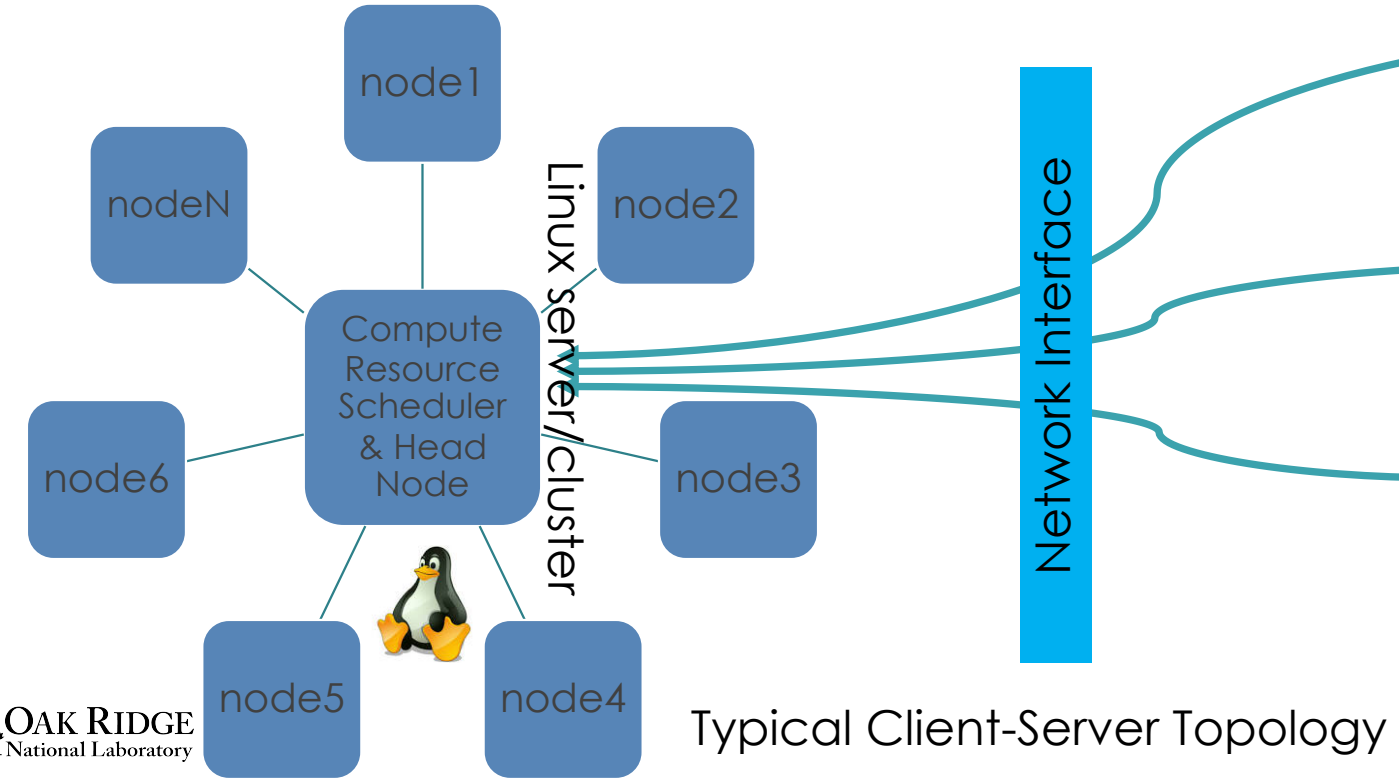
Assumptions

- The following slides assume
  - the NEAMS Workbench has already been installed
    - NEAMS Workbench is freely available from https://code.ornl.gov/neams-workbench/downloads
    - Installation notes are at https://code.ornl.gov/neams-workbench/downloads#install-neams-workbench-beta
  - the Dakota code has been installed
    - Dakota is freely available from https://dakota.sandia.gov/download.html
    - Download and unzip/tar.gz platform install

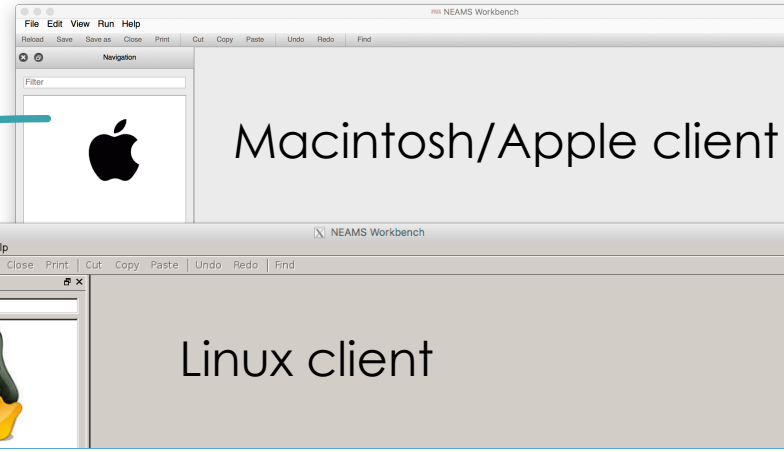
Need assistance? Email nwb-help@ornl.gov

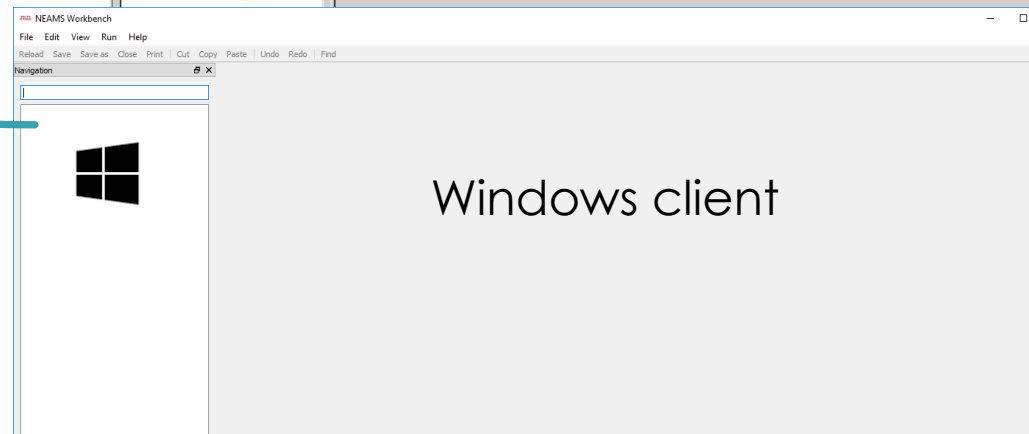
Client vs. Server definition

- 'Server', a.k.a. a 'cluster', is where compute resources are available and jobs can be scheduled
- 'Client', a.k.a. a 'local' machine, is typically a laptop or desktop with limited resource that can be used to locally run small jobs or submit jobs to a remote server



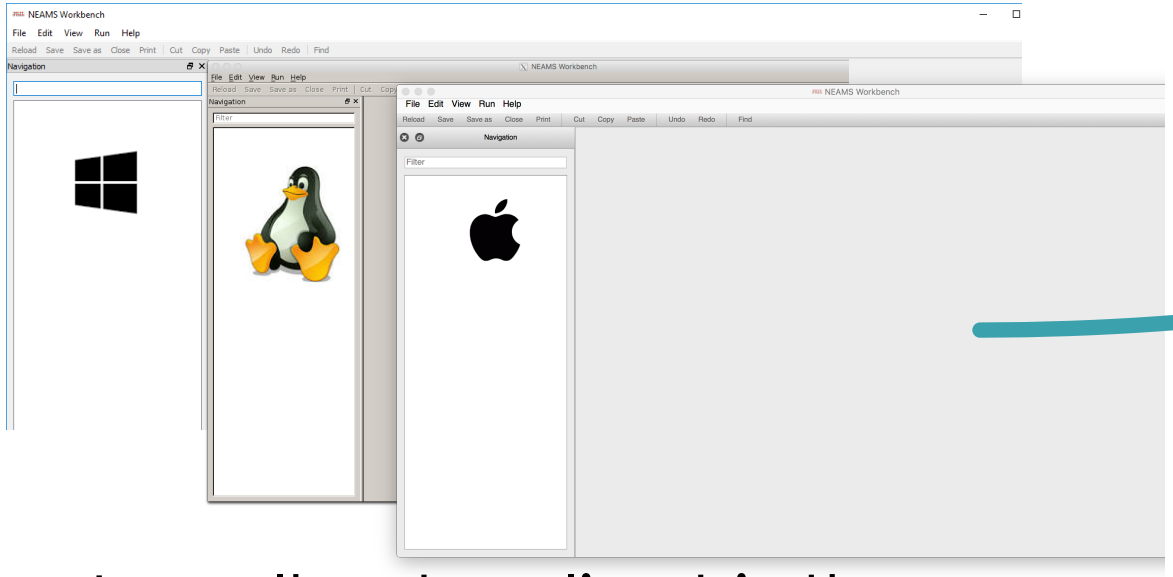
Typical Client-Server Topology

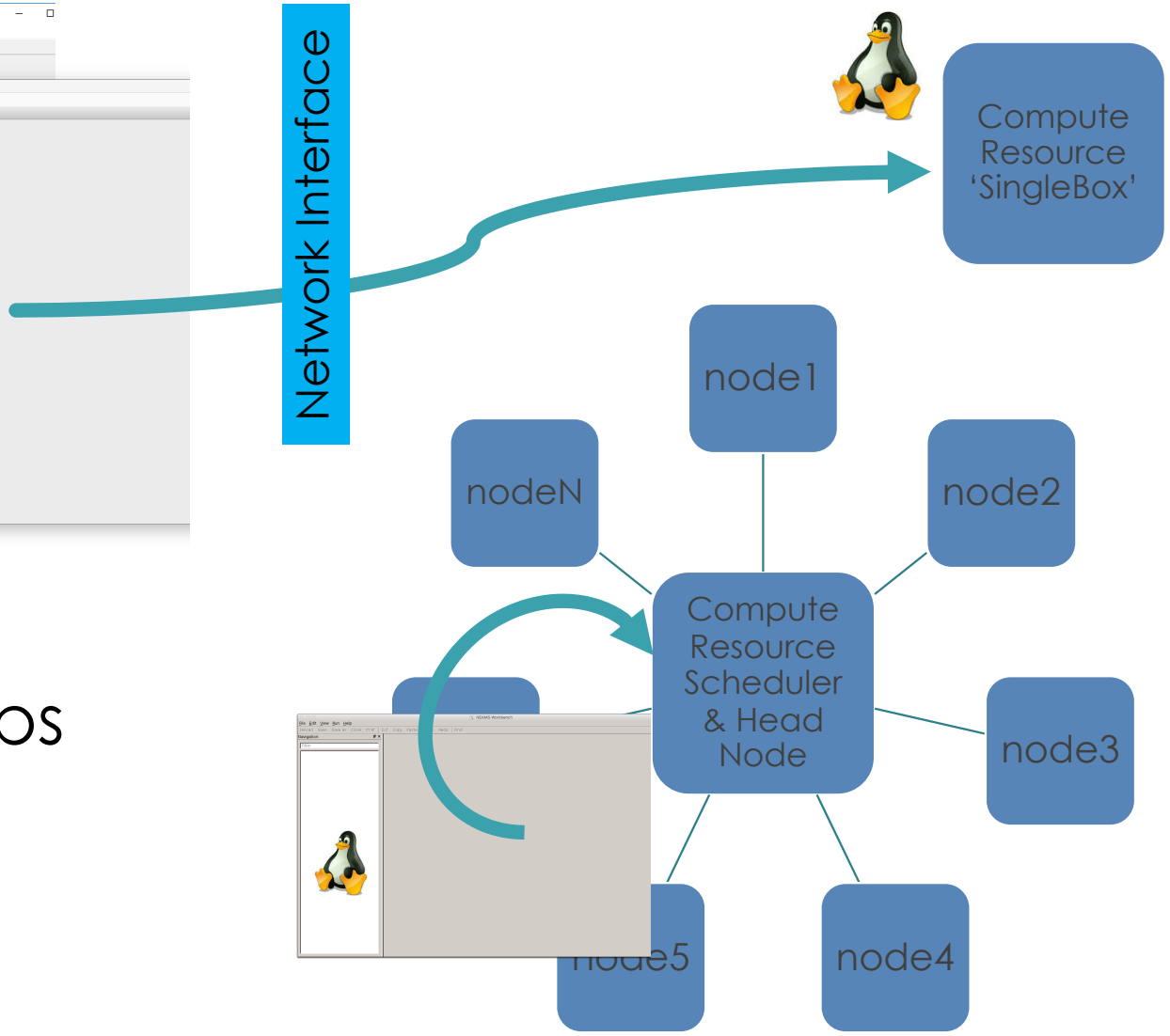




Additional configurations

- Single-box – compute resource without a scheduler where jobs are submitted across the network

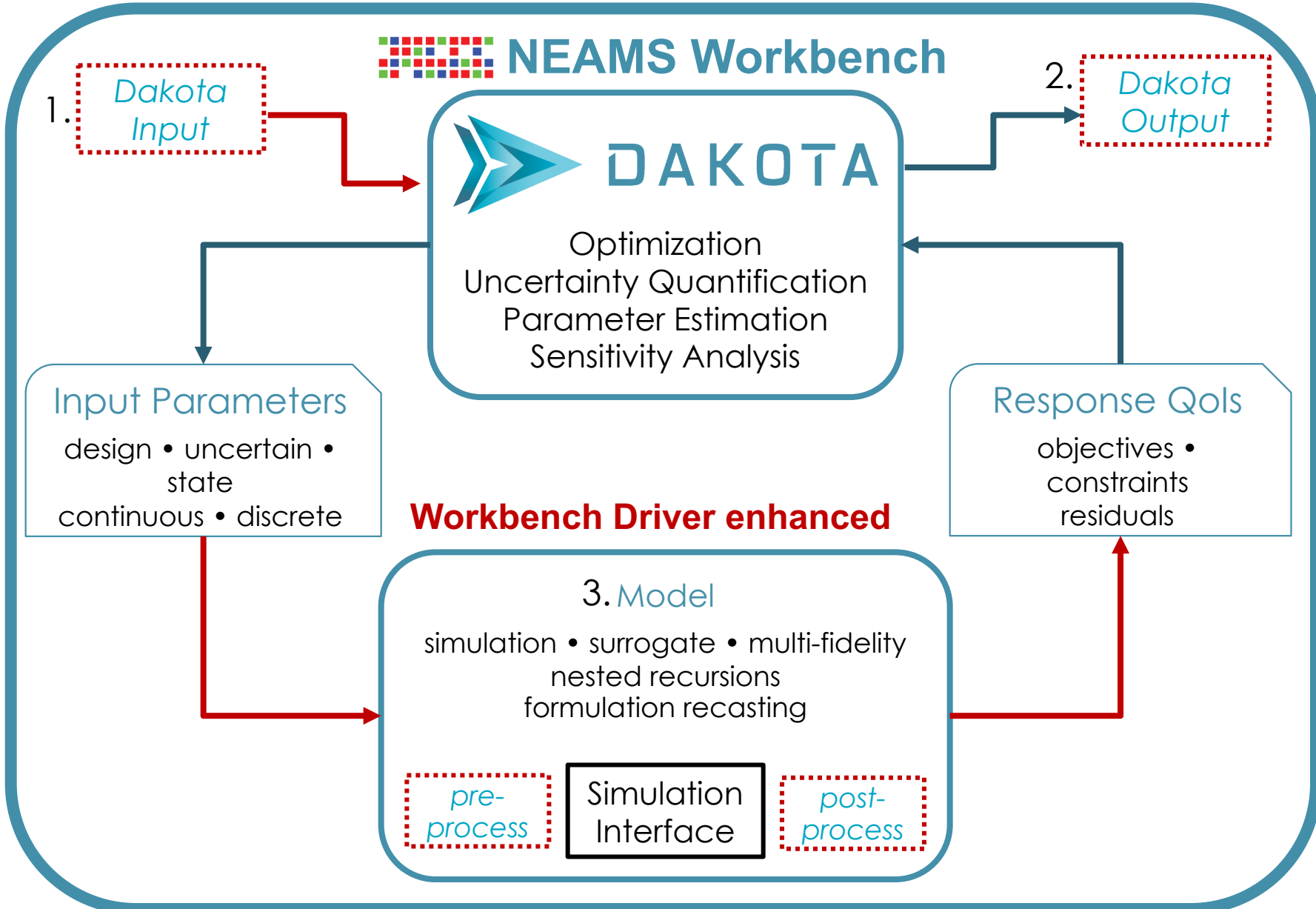




- Localhost – client is the cluster head node with scheduler from which jobs are submitted locally to the scheduler

Dakota within the NEAMS Workbench

1. Dakota Input:
   - Autocompletion
   - verification
2. Dakota Output
   - results plotting
3. Model:
   - Workbench Driver
   - Preprocessing
   - Template editing
   - Postprocessing



NEAMS Workbench Linux Server Installation

1. Download/copy the Workbench-Linux.zip to the server
   - Secure copy from client to server – `scp Workbench-Linux.zip server:`
2. Unzip the deployment – `unzip Workbench-Linux.zip`
3. Untar the archive – `tar -xf Workbench-Linux.tar.gz`
4. Verify installation via the following
   1. Execute **`Workbench-Linux/rte/entry.sh`** which should result in Python terminal with no import errors
   2. Execute **`Workbench-Linux/bin/sonvalidjson`** which should result in a usage message (no library load errors)

Latest Linux distribution is available from https://code.ornl.gov/neams-workbench/downloads

NOTE: be sure to use the same client and server versions. Server installations can be shared between users as long as the administrating user executes the `Workbench-Linux/rte/entry.sh` to configure the necessary Python environment

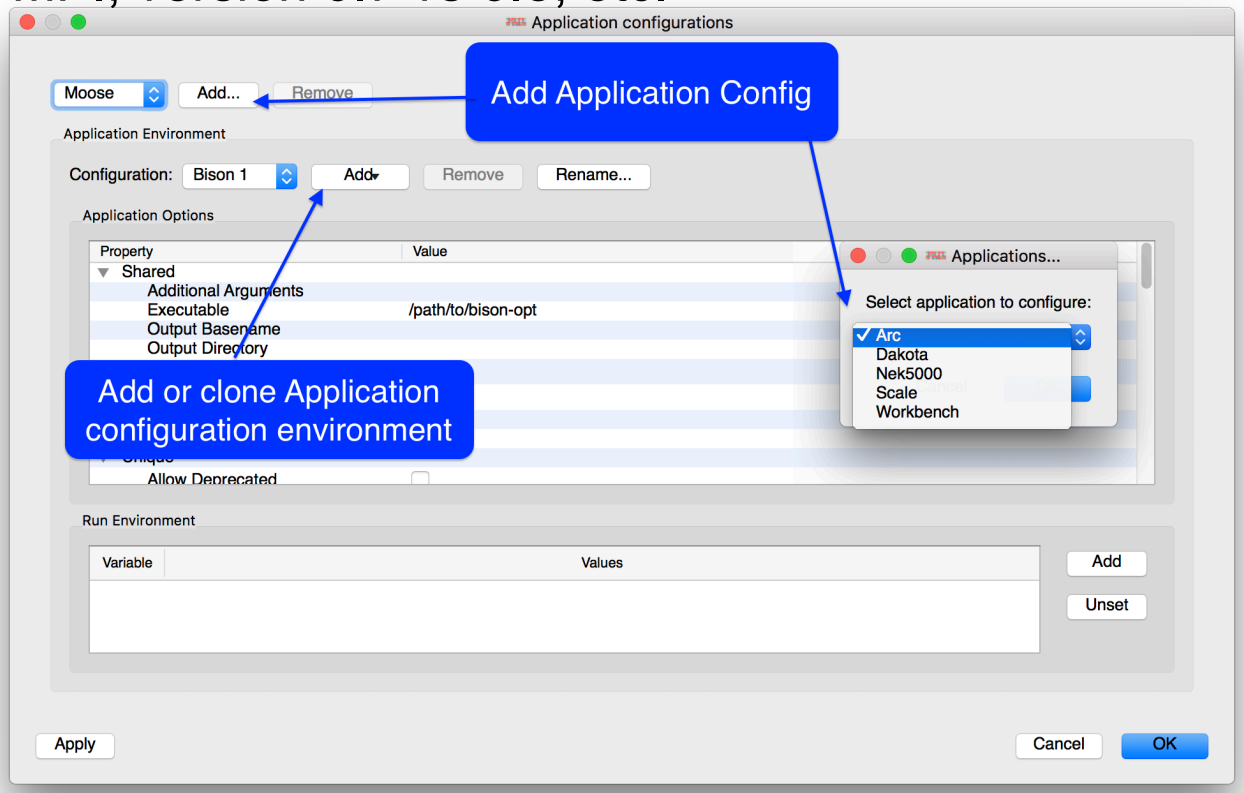
Local and Remote Application Setup Overview

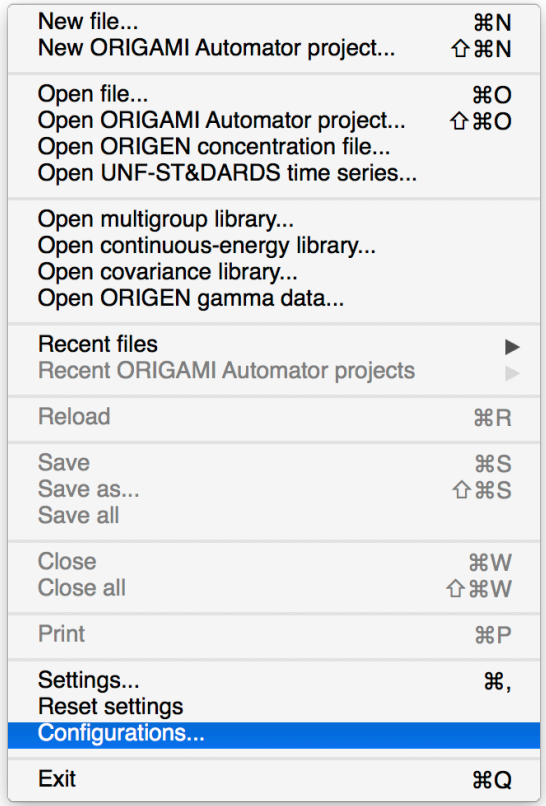
- Local application setup requires installation of the Dakota code on the same machine as is the NEAMS Workbench
- Remote application setup requirements
  - Passwordless SSH* to remote **Linux** machine/cluster
  - PBS-based cluster scheduler
    - Remote application does support scheduler-less single-box
    - Tested with Torque/MAUI, IBM LSF, SLURM
  - Initial setup step using the NEAMS Workbench SetupRemote application*
  - Remote Linux machine installation of the application and the NEAMS Workbench

* See later slide instructions

Run Configurations - Overview

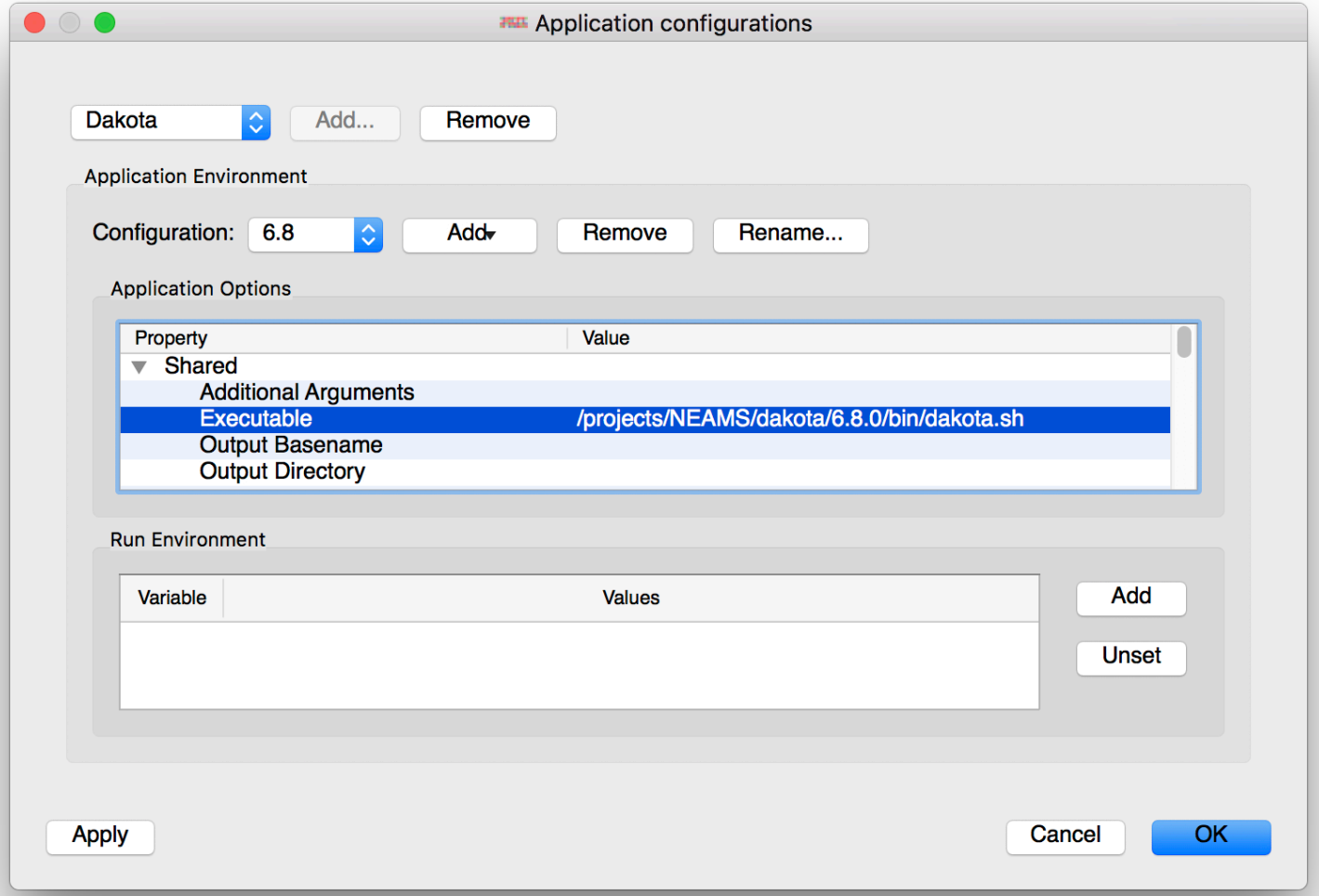
- Application configurations are available under the **File>Configurations…**
- Create application run configuration
  - Connects MOOSE-BISON, Dakota, ARC, etc. to the NEAMS Workbench
- Allows creation of application variants/environments
  - Serial vs MPI, version 6.7 vs 6.8, etc.





Local Configuration of Dakota UQ and Optimization*

- Open the Application Configuration dialog via **File>Configurations**
- Select **Add… Dakota**
- Update the **Executable** property's value to be the absolute path to **dakota.sh** or **dakota.bat**
- A pause can be observed as the NEAMS Workbench requests/generates the Dakota input definition



Remote Run Configuration of Dakota Overview

1. Configure passwordless SSH between the client and the server
2. Using the client install of the NEAMS Workbench, do the following:
   a. Enable the NEAMS Workbench's Setup_Remote application
   b. Create the application-server Setup_Remote input
   c. Run application-server setup remote input to generate the NEAMS Workbench Dakota remote run configuration.
   d. Configure the Dakota_remote
   e. Open any Dakota input and select the Dakota remote run configuration to activate input validation, autocompletion, syntax highlighting and job launch capabilities
   f. Edit input as needed
   g. Use the Dakota remote run configuration to launch the Dakota input from your client to the server
   h. Wait for job to finish
   i. Open files associated with the input file (*.out, etc.)

Passwordless SSH Setup

- Required for remote run configurations
- Appends client machine's authorized public key to the user's list of authorized keys residing on the server. The following statement is sufficient to do so on **Linux** or **Mac** clients:

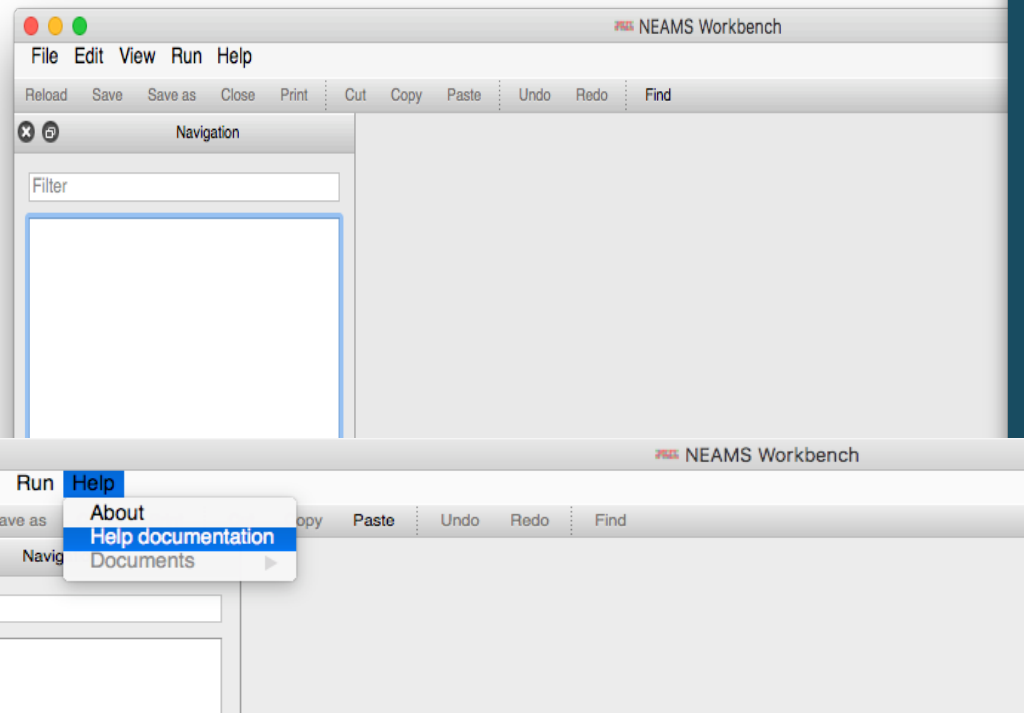
```
ssh server 'cat >> .ssh/authorized_keys && chmod 644 .ssh/authorized_keys' < ~/.ssh/id_rsa.pub
```

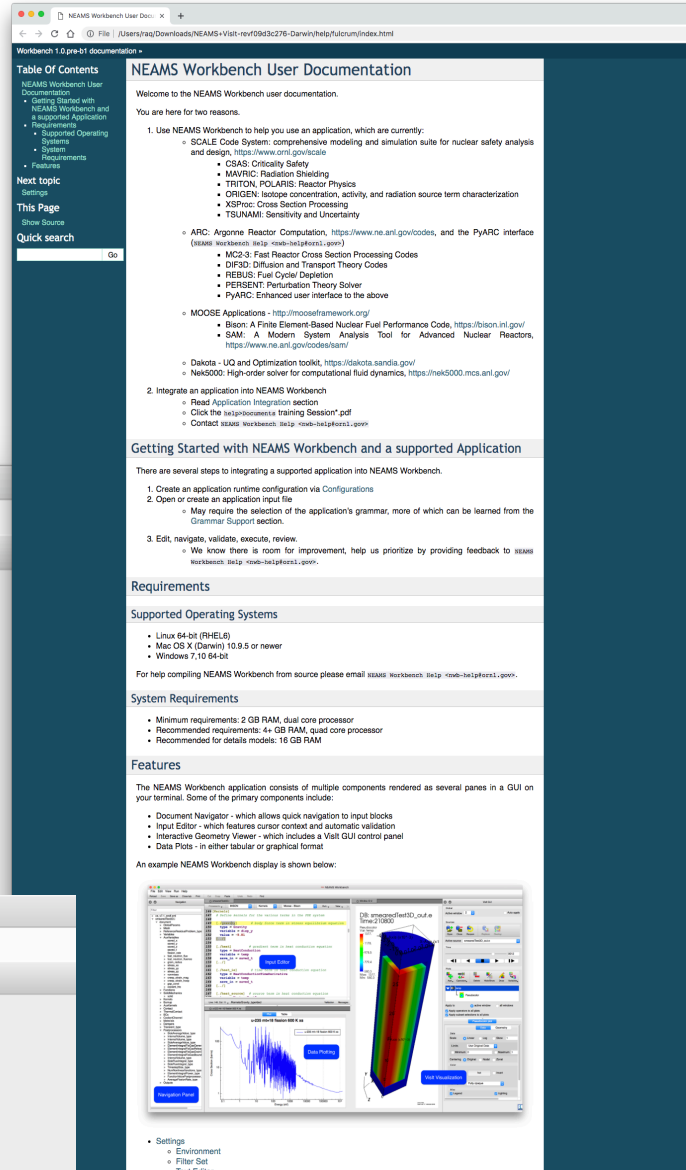
- Replace 'server' with the name of target server. Test the passwordless ssh by attempting to ssh to the server. You should no longer observe the need to specify a password.
- Assumes server:**.ssh** directory exists. If this does not exist, run **ssh-keygen** on the server to generate the SSH directory.
- On **Windows** clients use the **CMD** console program to execute

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

Start the client install of the NEAMS Workbench

- Execute **Workbench-<OS>/bin/Workbench**
- Help documentation will display during the first startup
- Help documentation is accessible via **Help>Help Documentation**





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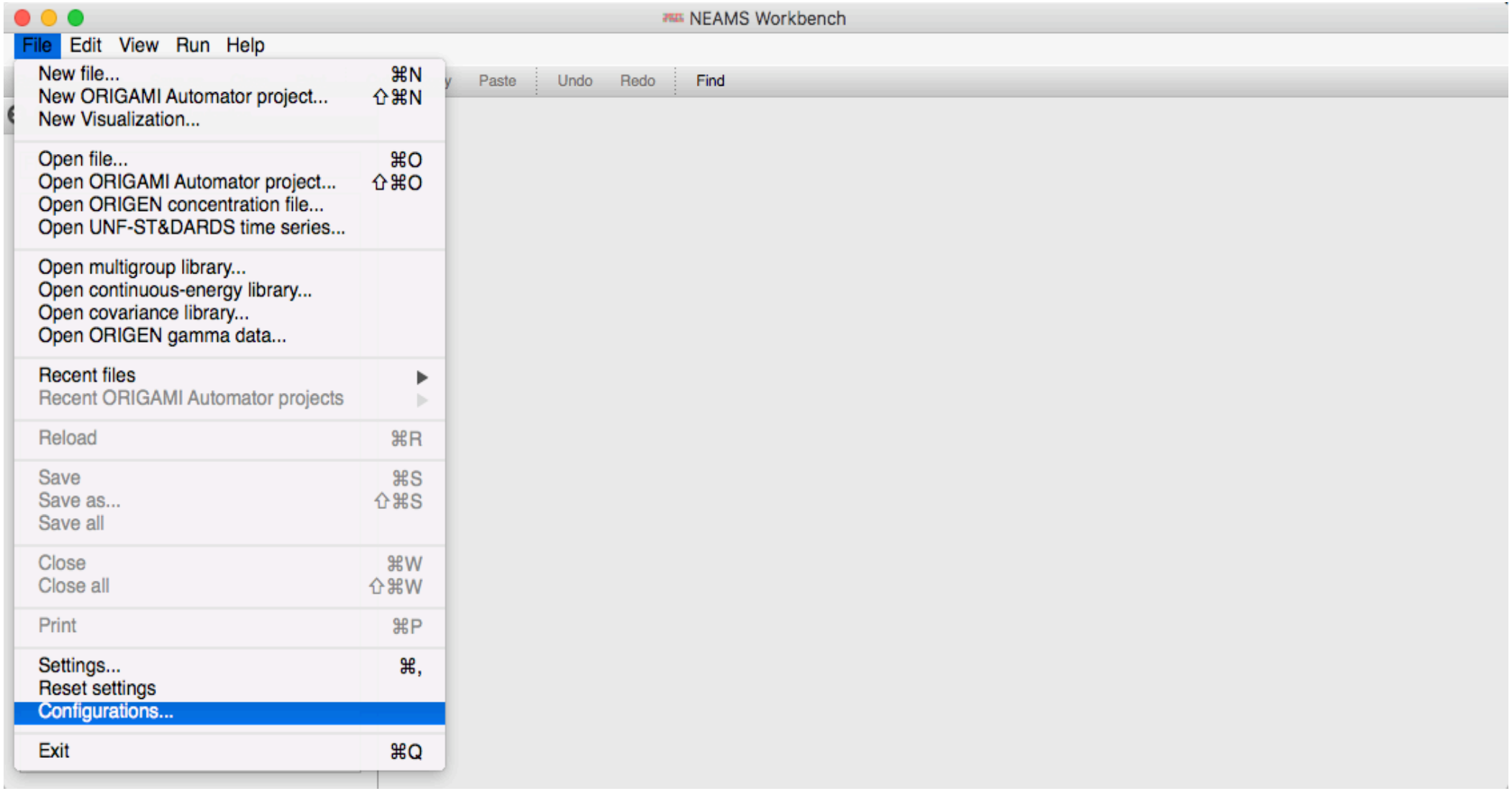
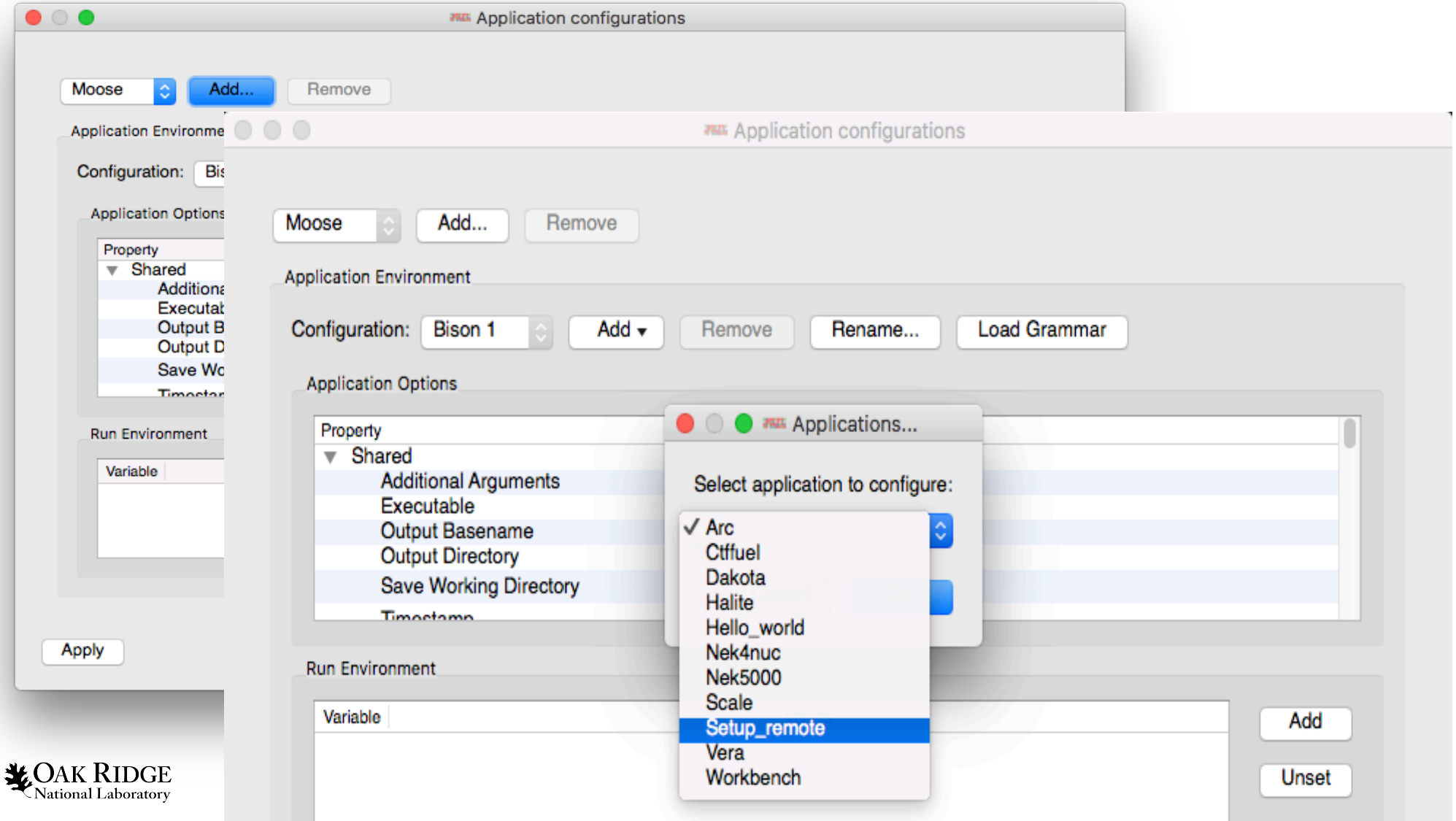
Configure the Setup Remote Application

- Click **File>Configurations…**



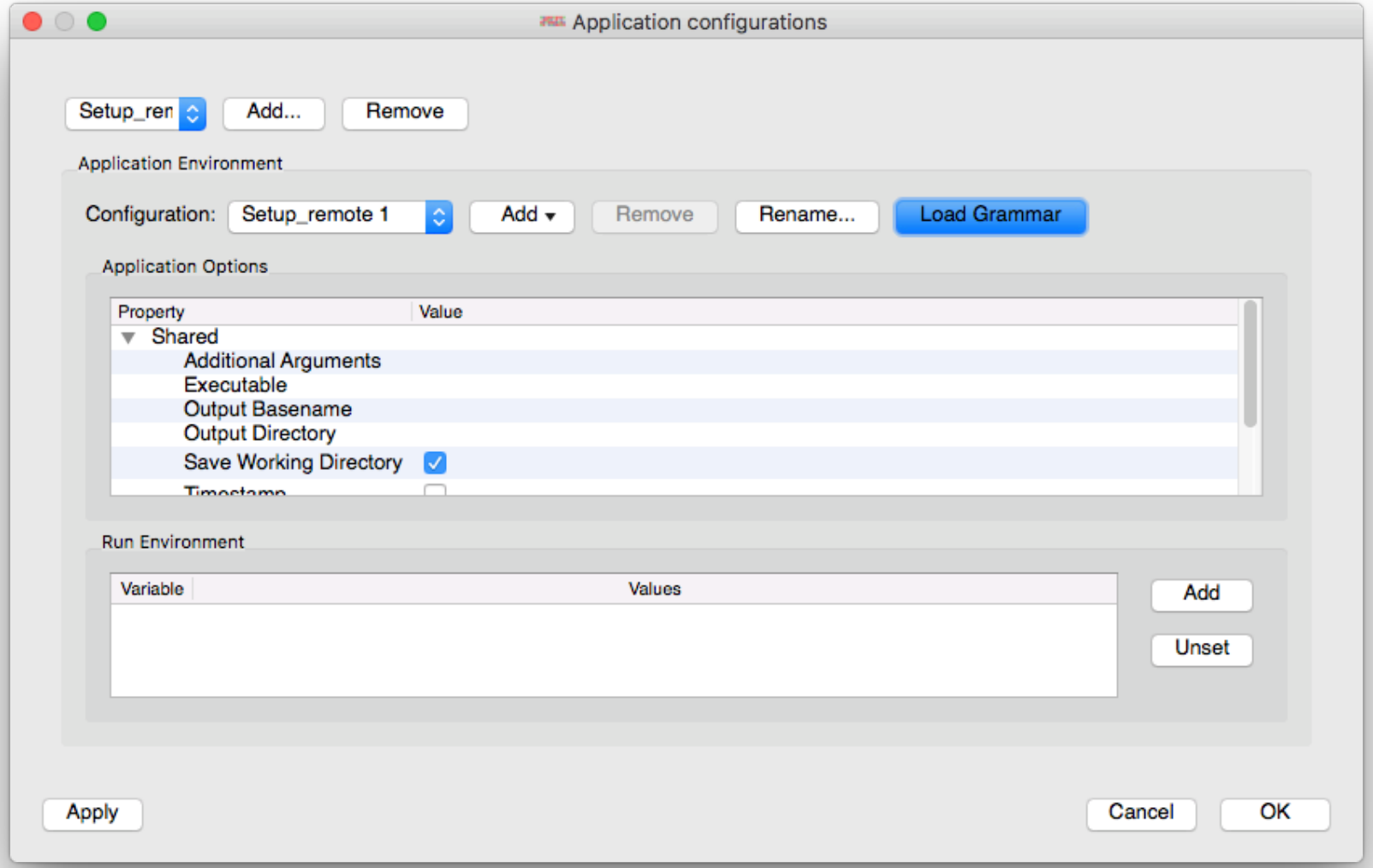
Configure the Setup Remote Application

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



Configure the Setup Remote Application

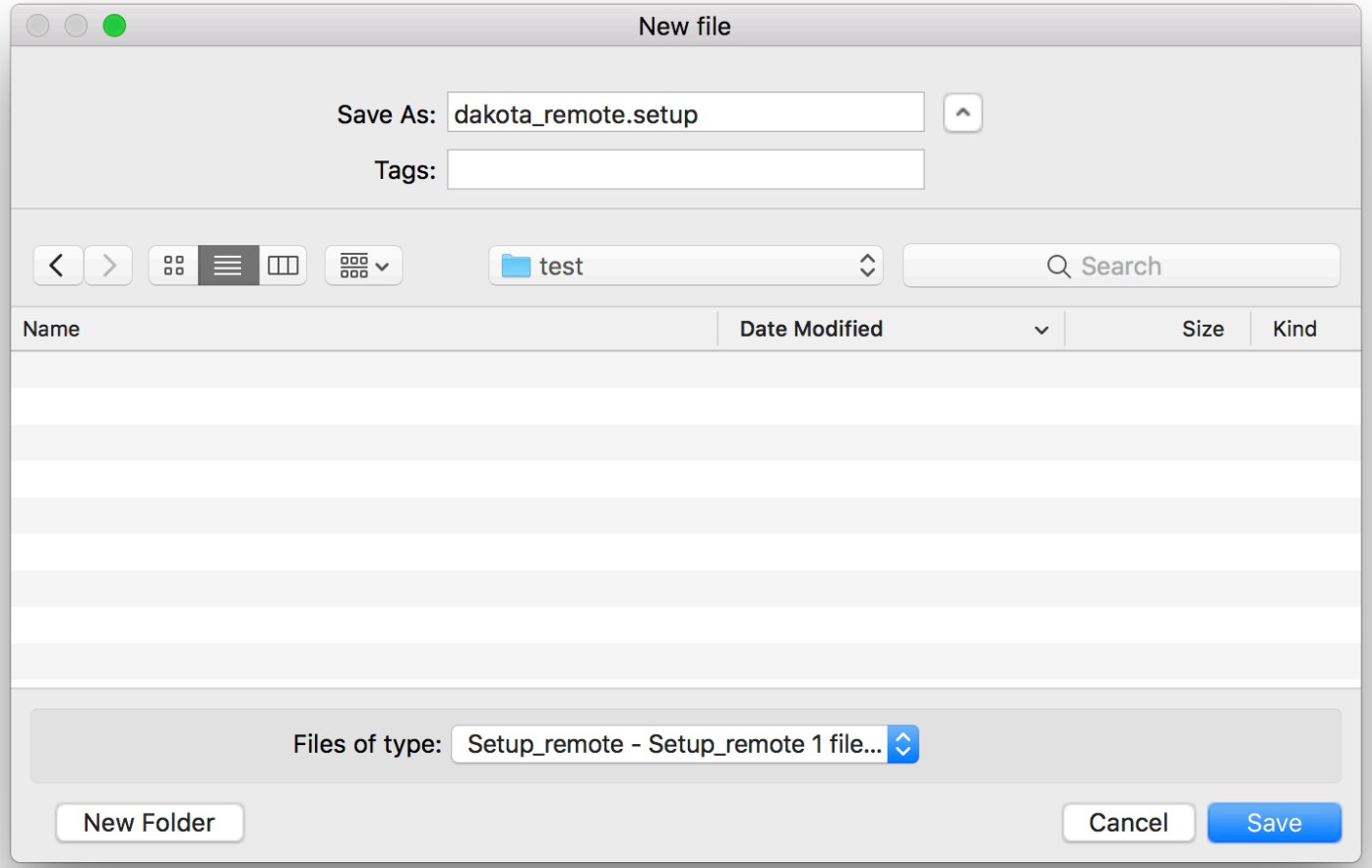
- Click **Load Grammar**, **Apply**, and **OK.** This enables SetupRemote input creation.



Create the remote Dakota Setup file

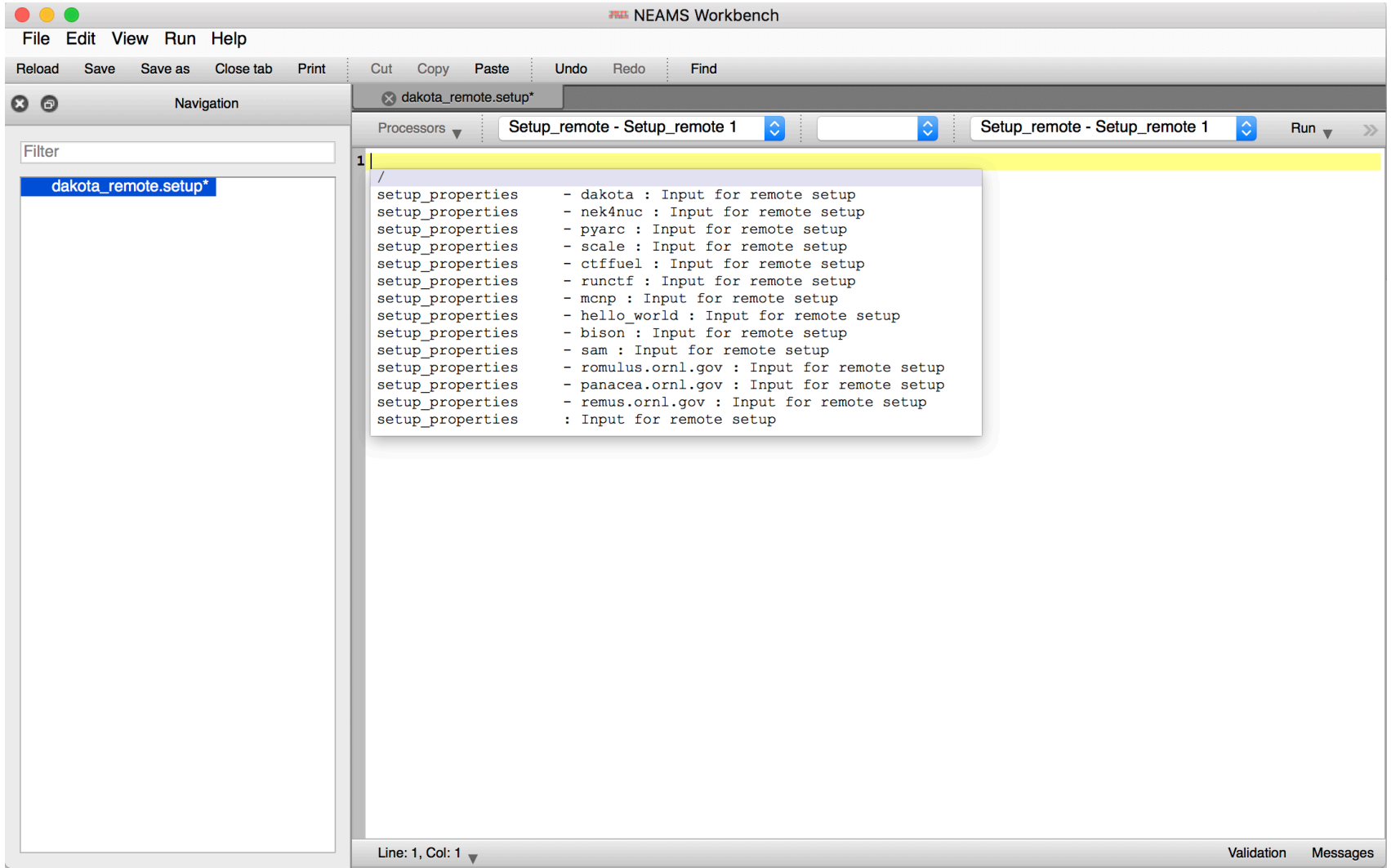
- This connects the client/local NEAMS Workbench to the remote NEAMS Workbench and Dakota installation

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



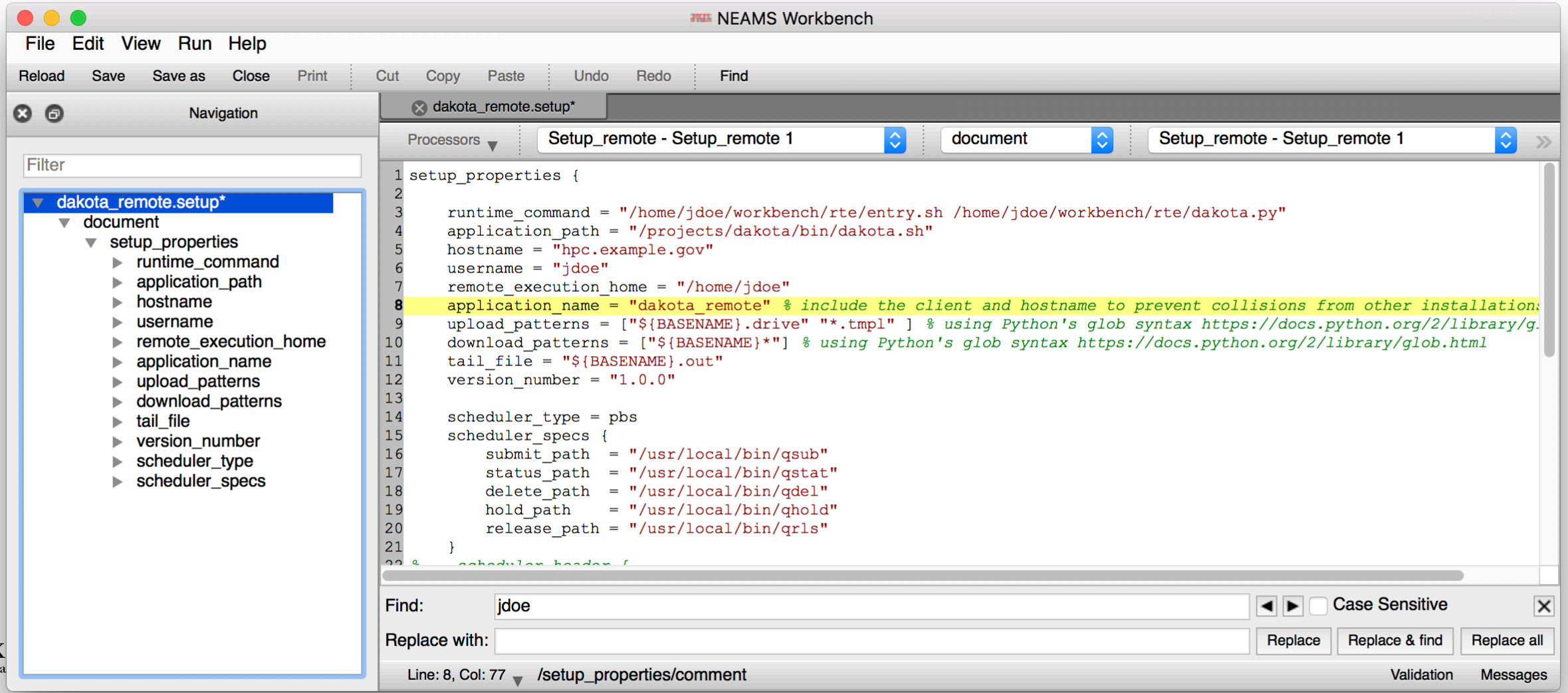
Create the remote Dakota Setup file

- Click inside the input editor window and use **CTRL+SPACE** key sequence to display autocompletion options.
- Select the Dakota variant



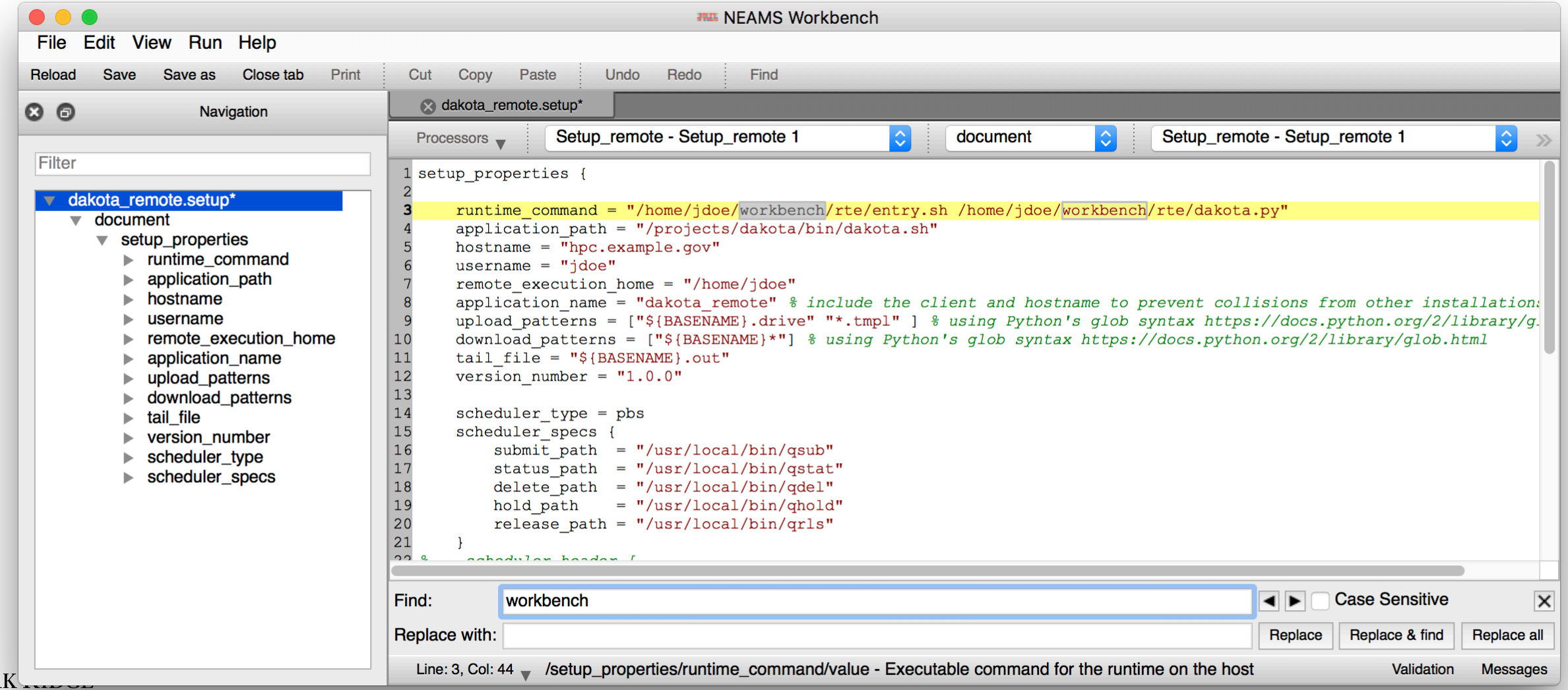
Specify the remote Dakota Setup file parameters

1. Click **Edit>Find** to display the Find widget
2. Replace **jdoe** with your user id



Specify the remote Dakota Setup file parameters

1. Replace **workbench** with your server-side NEAMS Workbench installation

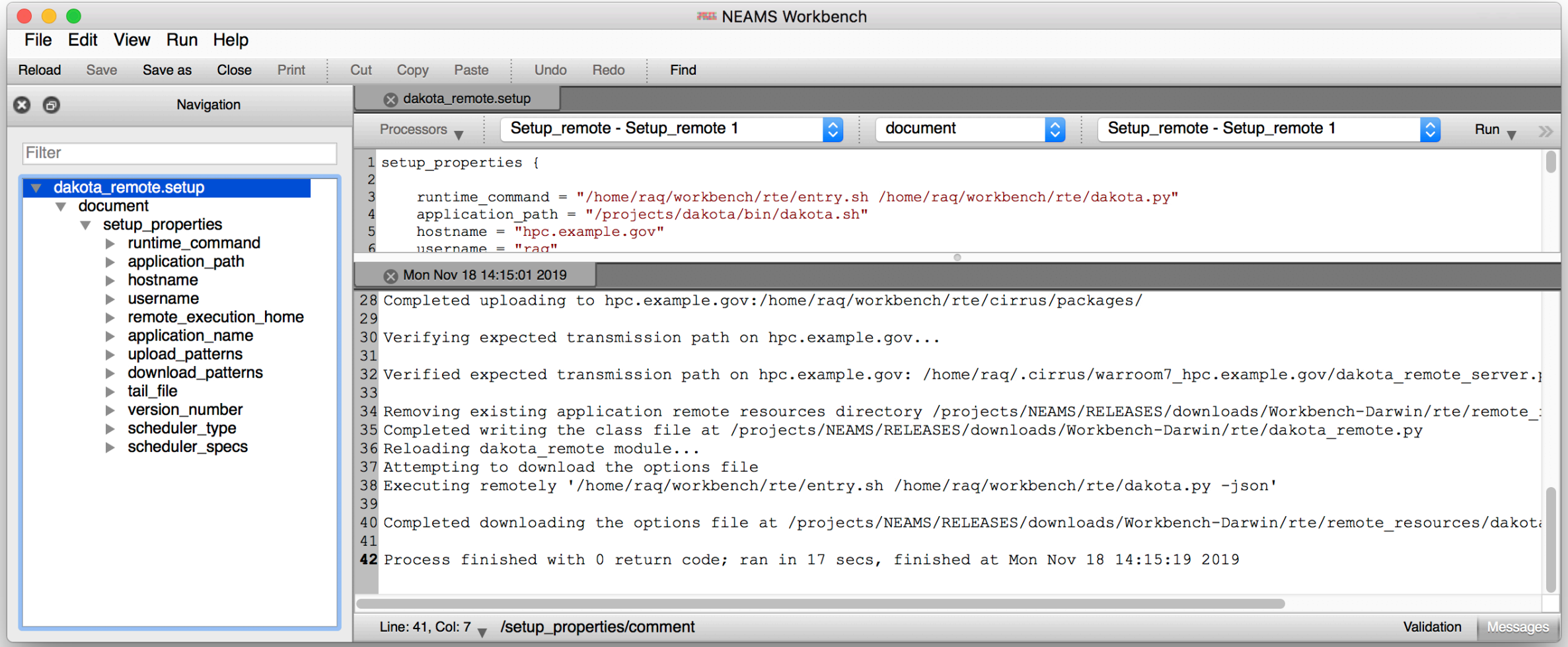


Specify the remote Dakota Setup file parameters

1. Replace **workbench** with your server-side NEAMS Workbench installation
2. Update the **hostname** to be the server name on which the NEAMS Workbench and application are installed
3. Review and update as needed the **scheduler_specs**
   - Important for indicating scheduler queues or job runtime or memory

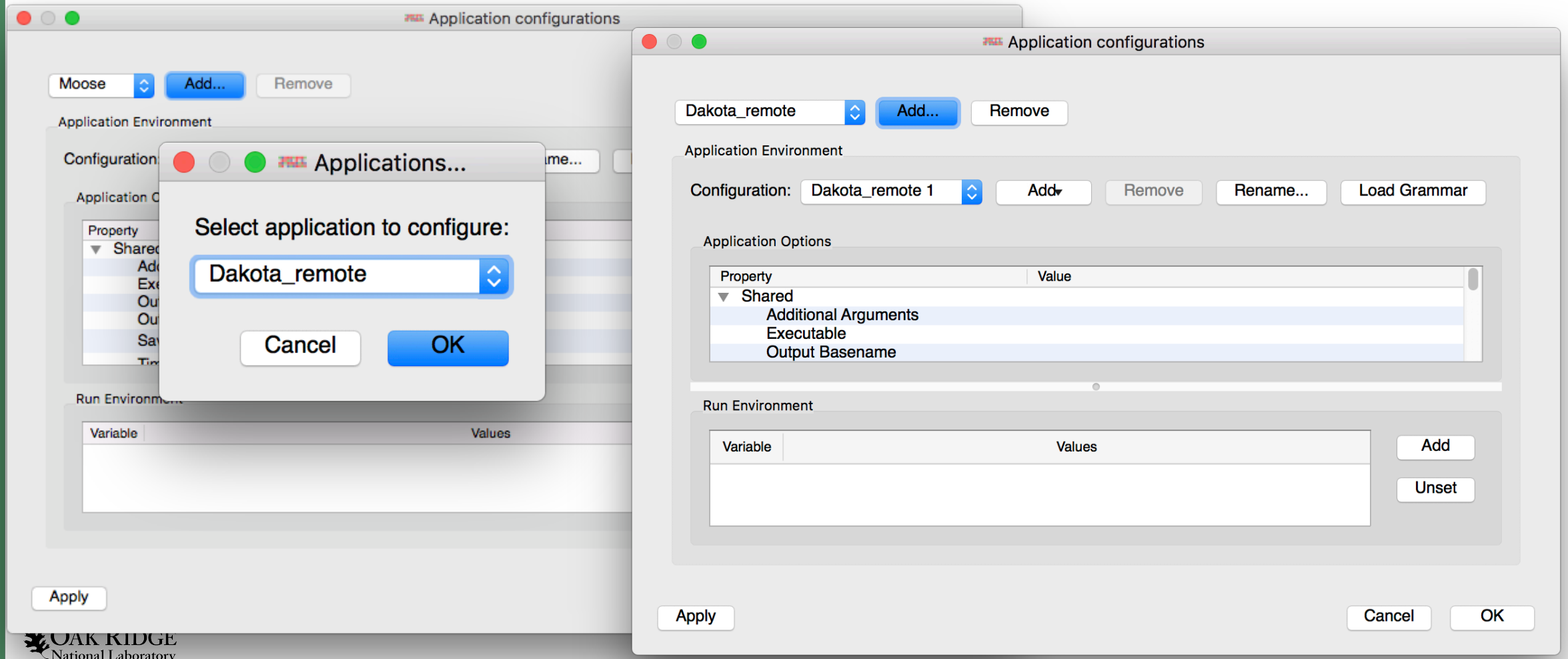
Run the remote Dakota Setup file

- Click the **run** button to execute the Dakota setup file



Configure the **Dakota_remote** application

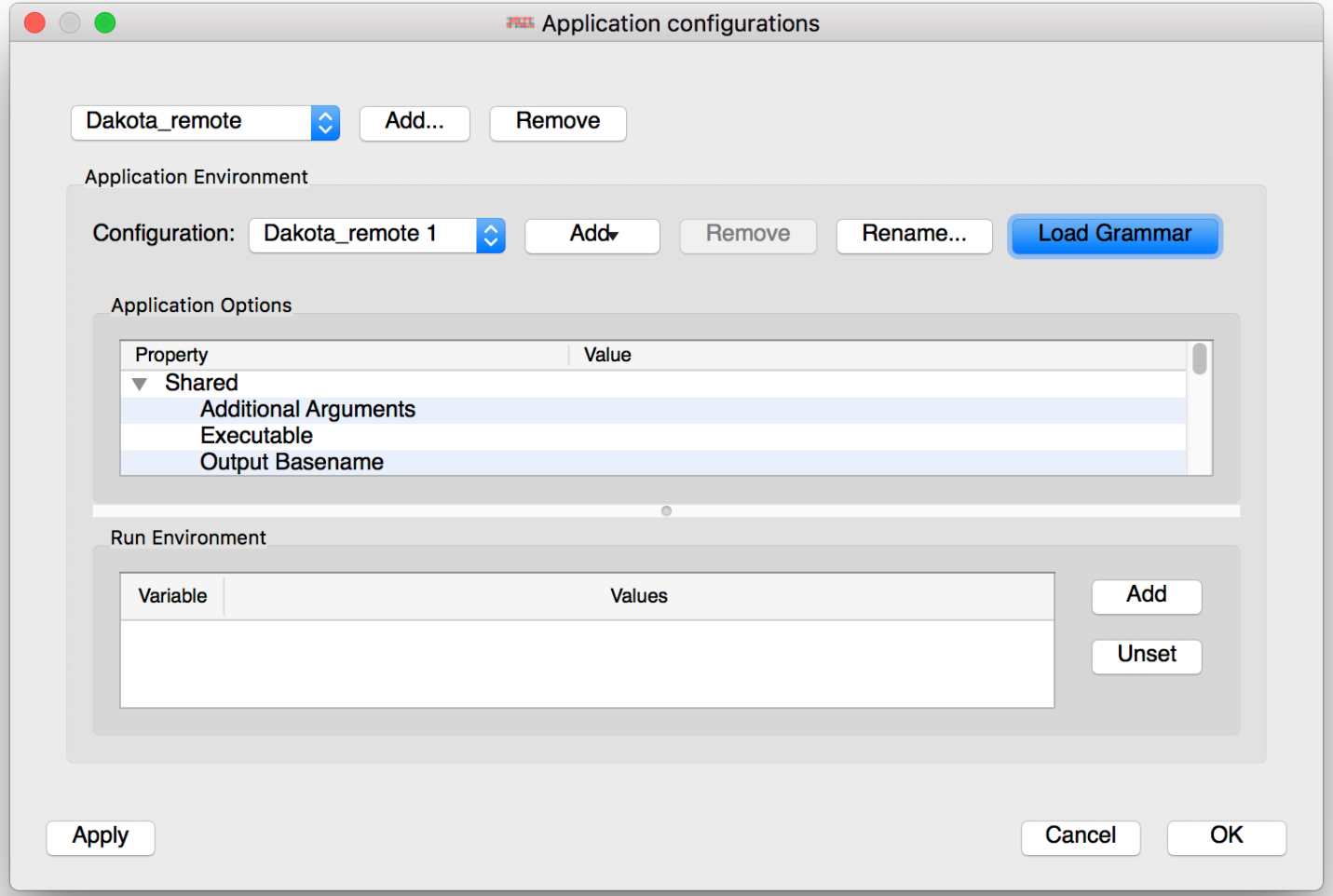
- Click **File>Configurations…**
- Click **Add…** and select **Dakota_remote** and click **OK**



Configure the **dakota_remote** application

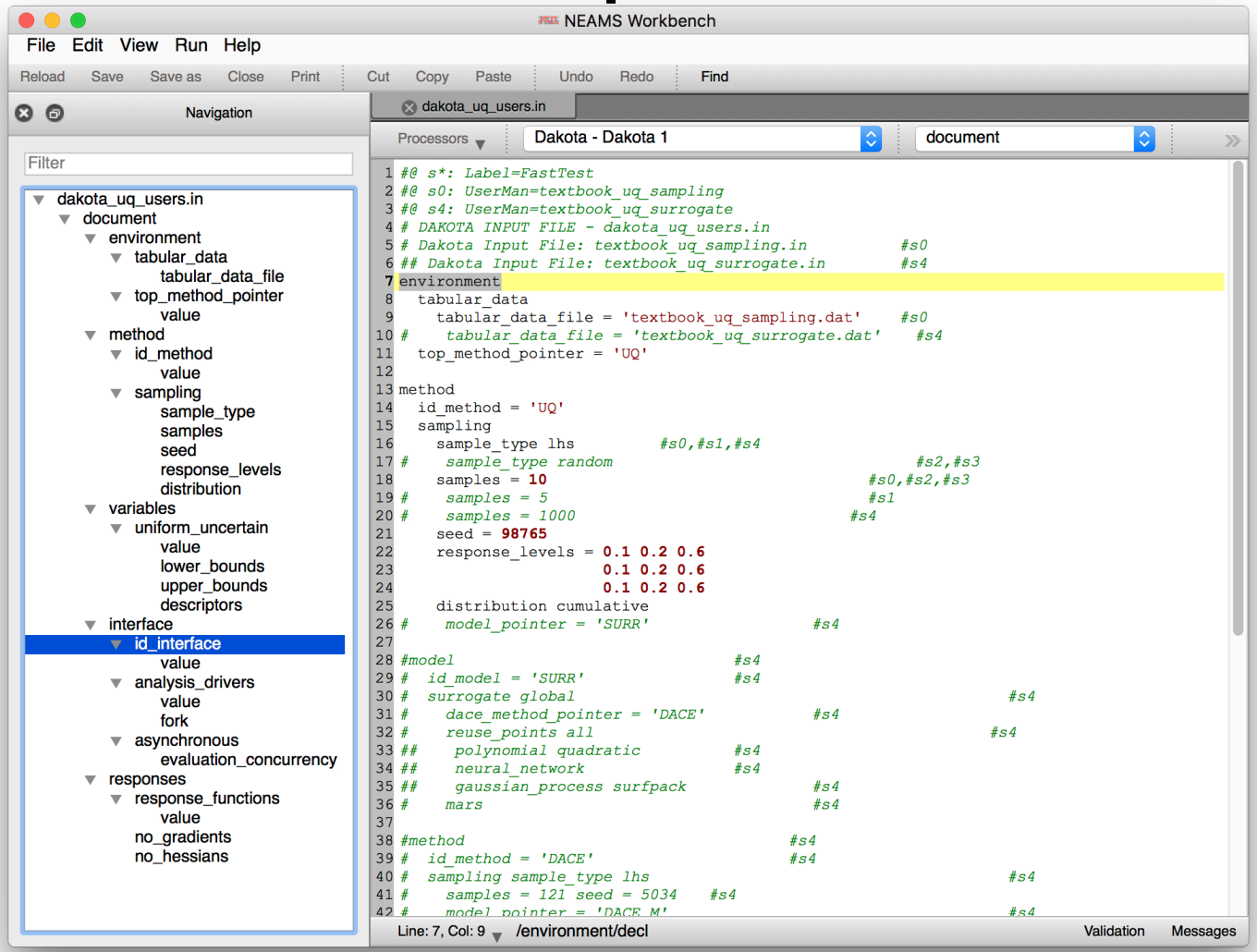
- Click **Load Grammar**, **Apply**, and **OK.** This enables Dakota input creation.

- Note: Load grammar may pause for a moment while Workbench retrieves the grammar files from the server.



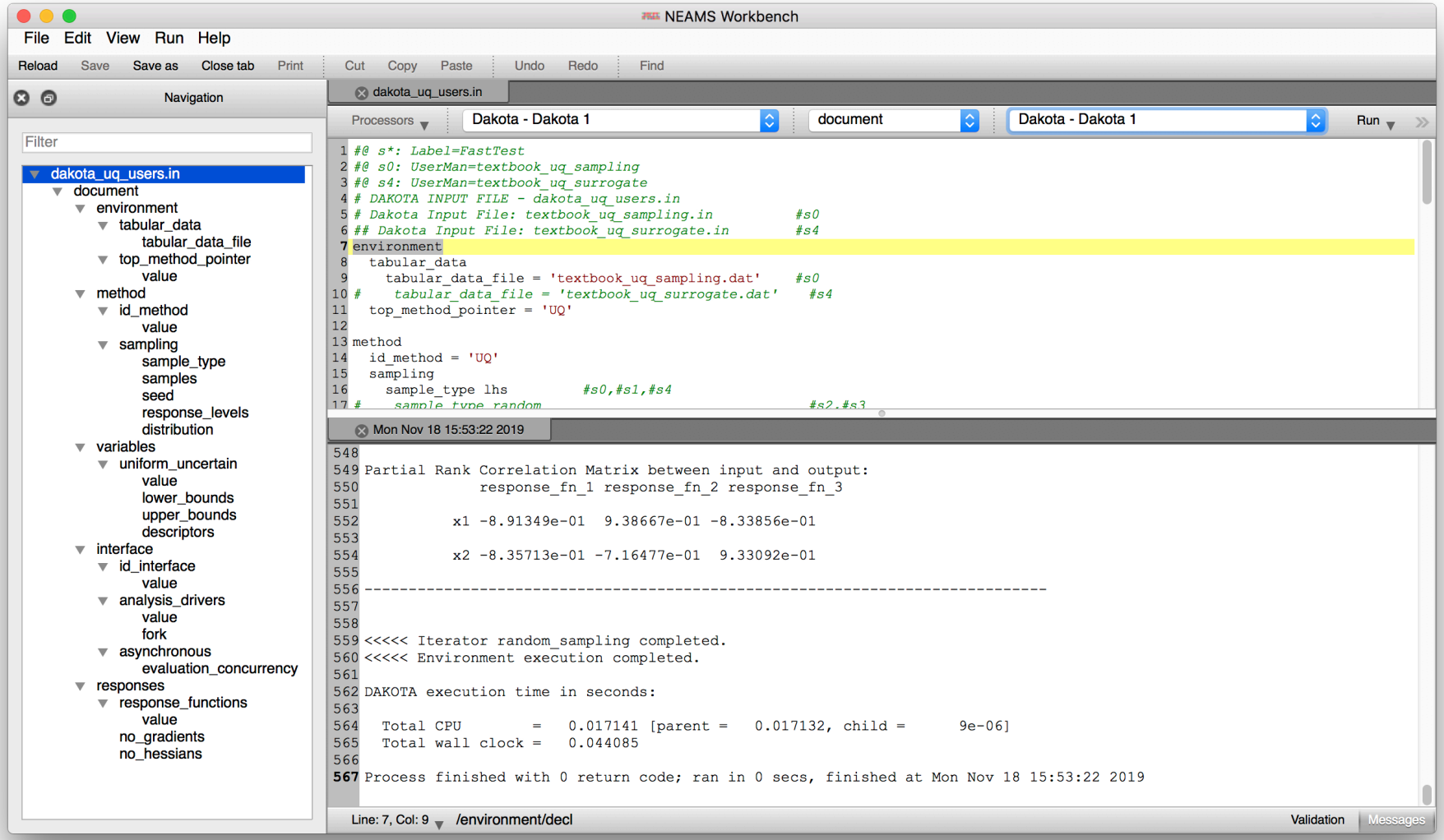
Open the Dakota UQ Input

1. Click **File>Open…** and navigate to and open the **Dakota/share/dakota/test/dakota_uq_users.in**
2. select the **Dakota** local run configuration



Run the Dakota UQ Input Locally

- Click the **Run** button to launch the job on the remote system
- Select the **Messages** button to display the messages panel
- Wait for the job to complete

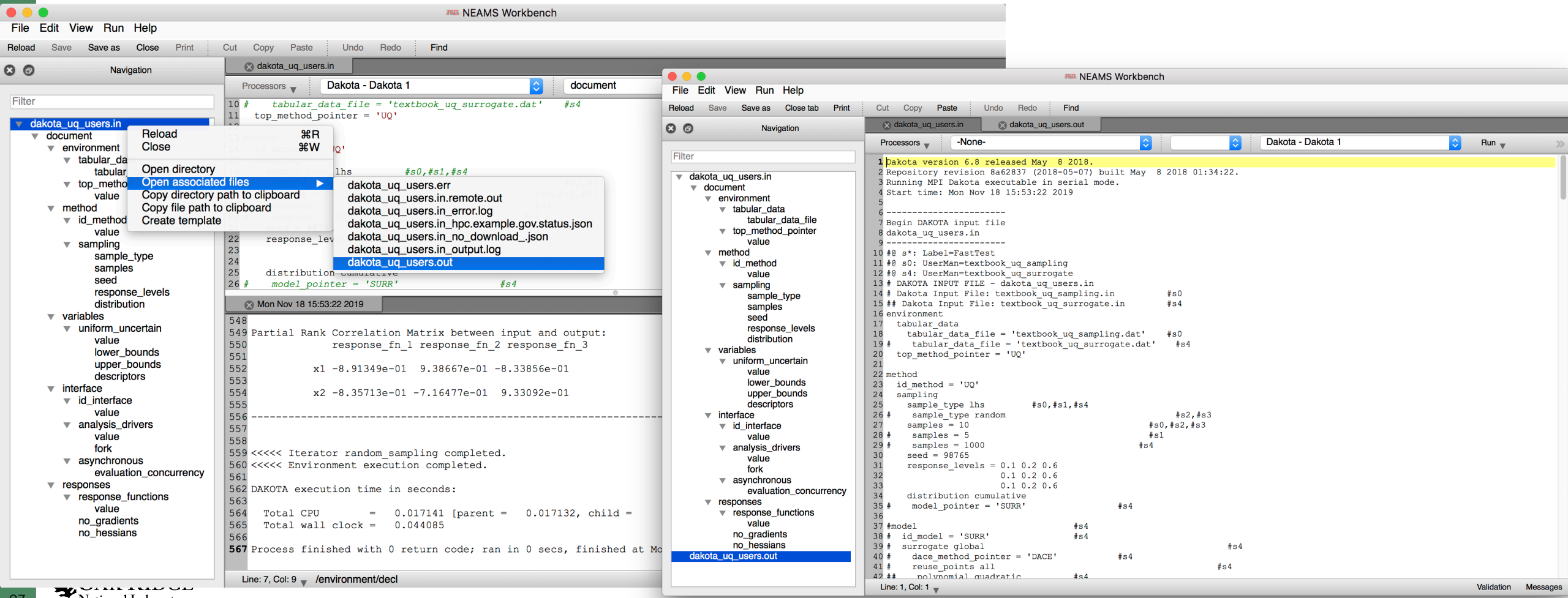


Run the Dakota UQ Input Remotely

- Select the **Dakota_remote** run configuration
- Click the **Run** button to launch the job on the remote system
- Select the **Messages** button to display the messages panel
- Wait for the job to complete
- Ensure the message panel states **Successfully downloaded dakota_uq_users.out**

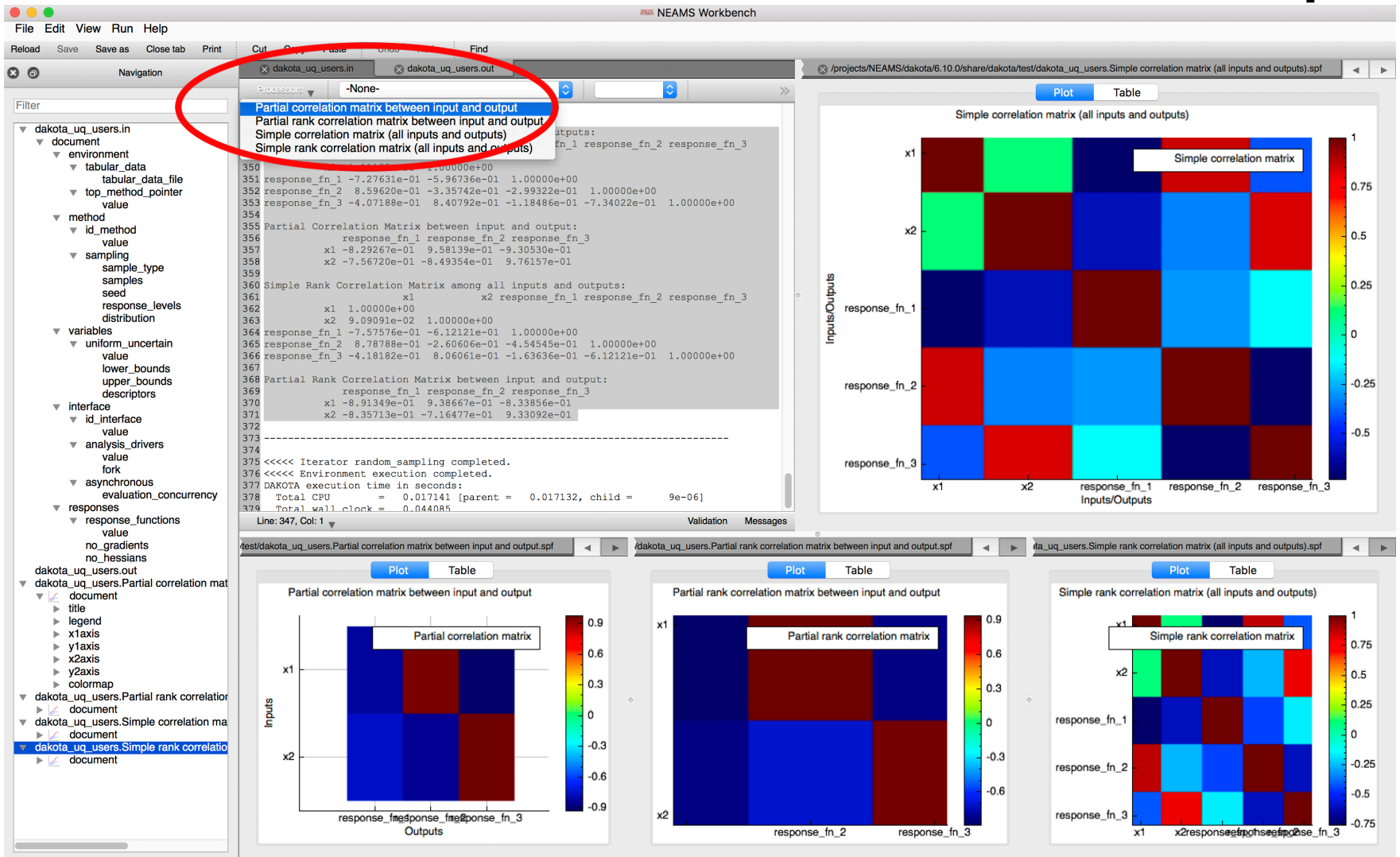
Open associated output

- Right click the **dakota_uq_users.in** file and select **Open associated files> dakota_uq_users.out** and review output



Plot Correlation Matrices

- In the ***.out** editor view, select the correlation matrix to plot via the **Processors>Partial correlation matrix between input and output**



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Summary

- You have successfully configured and run Dakota through the NEAMS Workbench via a local and remote configuration

Questions?

- Email questions and issues to nwb-help@ornl.gov