SDSC SAN DIEGO SUPERCOMPUTER CENTER   WOrDS Center   UCSanDiego

SDSC Summer Institute 2015: Workflow Management

Hands-On Exercises 3:
Local and Distributed Parallel Execution of BLAST

Goal 1: Build a workflow to run BLAST locally.

Step 1: Start Kepler and add director and string constants.

1	Open Kepler. Double click kepler.sh icon to start Kepler GUI.
2	Open BLAST workflow in /home/biokepler/Blast.kar

Step 2: Set Parameter Values.

1	Set parameters for *additionalOptions*: **-e 1E-5 –p blastn –m 8** **NOTE:** Copy & paste sometimes gives errors in VirtualBox, so it is better to enter these parameters manually.

Step 3: Run the Workflow

1	Save the workflow.
2	Run the workflow. The resulting alignment data should open in a display window.

Goal 2: Build a workflow to run mpiBLAST on a cluster.

1	Open blast workflow:
	  – Go to Step 2, if Blast.kar is already open
	  – Open BLAST workflow in /home/biokepler/Blast.kar

2	Add new execution choice for MPIBLAST
	  – Double-click on the Blast actor and click on Add.
	  – Change radio button to Execution Choice.
	  – Select Type: mpiBLAST.
	  – Set Name to MPIBLAST.
	  – Click Add to close the dialog

3	Configure the New Execution Choice.
	
	  – Double-click on Blast actor
	  – Change to MPIBLAST tab
	  – Configure MPIBLAST tab:
	  Please use Gordon username assigned to you in place of **LOGIN**.
	
	  First parameter: TargetHost
	    • Edit "TargetHost" parameter and set its value to be LOGIN@gordon.sdsc.edu
	  Second parameter: cmdFile
	    • If already set move next parameter
	    • Else set its value to be $HOME/mpiBLAST/blastp_gordon.sh
	  Third parameter: commandLine
	    • Keep as it is. Move to next parameter.
	  Fourth parameter: outputFile
	    • If already set move next parameter
	    • Else set its value to be $alignmentFile
	  Fifth parameter: outputOnTarget
	    • Set its value to be /home/LOGIN/mpiBLAST/blast_results.txt
	  Sixth parameter: remoteDir
	    • Set its value to be /home/LOGIN/mpiBLAST

4	Set the Execution Choice to MPIBLAST
	  – Go to "Shared Options" tab
	  – Set Choice to MPIBLAST.
	  – Click on commit to save the changes and close the configuration box.

5	Save and Run the workflow.