

Running NVIDIA Parabricks on DNAnexus

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This guide shows how to run Parabricks on a compute instance on <u>DNAnexus</u> using both the GUI and the CLI.

What is NVIDIA Parabricks?

Parabricks is an accelerated compute framework that supports applications across the genomics industry, primarily supporting analytical workflows for DNA, RNA, and somatic mutation detection applications. With industry leading compute times, Parabricks rapidly converts a FASTQ file to a VCF using multiple, industry validated variant callers and also includes the ability to QC and annotate those variants. As Parabricks is based upon publicly available tools, results are easy to verify and combine with other publicly available data sets.

More information is available on the Parabricks Product Page.

Detailed installation, usage, and tuning information is available in the <u>Parabricks user</u> <u>guide</u>.

Finding the Parabricks tools on DNAnexus

In this section we will show how to find all the available Parabricks pipelines on DNAnexus.

Start on the DNAnexus homepage and click "Tools" from the toolbar at the top.



This will take you to the Tools Library, which shows all workflows you can run on DNAnexus. We can filter for just the Parabricks tools by clicking on "Name" and typing "Parabricks". The list should look something like this:

Tools Library All TOOLS
Name: parabricks ③ Any Category ~ Any Type ~
Name 🔨
BAM-to-FQ Pipeline (Parabricks accelerated) This pipeline uses GPU-accelerated software to convert BAM files to NGS FQ output at
Bamsort Pipeline (Parabricks accelerated) This pipeline uses GPU-accelerated software to sort BAM files.
DeepVariant Pipeline (Parabricks accelerated) Call germline variants using a deep neural network analysis
DeepVariant Pipeline (Parabricks accelerated) GPU accelerated germline analysis using DeepVariant
FQ-to-BAM Pipeline (Parabricks accelerated) This pipeline uses GPU-accelerated software to convert NGS FQ output to BAM output
Germline Pipeline (Nvidia Clara Parabricks accelerated) Call germline variants using the exact same algorithms as the BWA-GATK4 germline va
Mutectcaller (Parabricks accelerated) Runs the Parabricks mutectcaller pipeline. See the Parabricks Docs: https://docs.nvidi

In this guide, we will run FQ-to-BAM as an example to show how to get started. All the workflows run in a similar way, so this information is transferable to any pipeline.

Let's start by clicking on FQ-to-BAM which will take us to the landing page for that tool.

Each tool has a page like this which includes information such as a README, instructions for running on the command line, and input/outputs for this specific tool.

Running the Parabricks FQ-to-BAM Pipeline using the GUI

Let's start by using the GUI to run FQ-to-BAM. Click "Run" in the top left corner.



This will open a new page and prompt us to select a project that has data for this run. You can use any fastq and reference files that you like, or you can download Parabricks sample files from using:

\$ wget -O parabricks_sample.tar.gz \
"https://s3.amazonaws.com/parabricks.sample/parabricks_sample.tar.gz"

and upload them to DNAnexus as we have done for this tutorial. Note that the reference files must be zipped together in one folder.

Once we've selected our project we are shown a graphical representation of the file inputs and outputs for this pipeline on the left side of the page:



The Parabricks FQ-to-BAM pipeline accepts a reference and input fastq pairs as required files, with the option to add interval and known indel files as well. The output will be a bam with option recall file.

Other options can be found on the right side of the page under "Analysis Inputs 2":

ANALYSIS SETTINGS		ANALYSIS INPUTS 2	APP SETTINGS
Ø P	BFQ2BAM ¥		Enable Batch OFF
	FQ-to-BAM Pipeline (Parabricks accelerated)		⑦ About this app
0	BWA Reference Genome Index *.bwa-index.tar.gz	Select File	
0	Interval File *.interval_list *.picard *.list *.intervals *.bed	Select File (Array)	
0	FQ Read pairs *.fastq.gz *.fq.gz	Select File (Array)	
0	Known indel files *.vof.gz	Select File (Array)	
MMO	N		
0	Interval		
(9) (9)	Interval No Warnings		True False
ଡ ଡ ଡ	Interval No Warnings Mark Dups Assume Sort Order Query Name		True False True False
ଡ ଡ ଡ ଡ	Interval No Warnings Mark Dups Assume Sort Order Query Name Fix Mate		TrueFalseTrueFalseTrueFalse
ଡ ଡ ଡ ଡ	Interval No Warnings Mark Dups Assume Sort Order Query Name Fix Mate CRAM		TrueFalseTrueFalseTrueFalseTrueFalseTrueFalse
(9) (9) (9) (9) (9) (9) (9) (9) (9) (9)	Interval No Warnings Mark Dups Assume Sort Order Query Name Fix Mate CRAM Optical Duplicate Pixel Distance		TrueFalseTrueFalseTrueFalseTrueFalseTrueFalse
© © © © ©	Interval No Warnings Mark Dups Assume Sort Order Query Name Fix Mate CRAM Optical Duplicate Pixel Distance Assume Mark Dups Picard Version 2.18.2		TrueFalseTrueFalseTrueFalseTrueFalseTrueFalse (default)TrueFalse
0 0 0 0 0 0	Interval No Warnings Mark Dups Assume Sort Order Query Name Fix Mate CRAM Optical Duplicate Pixel Distance Assume Mark Dups Picard Version 2.18.2 Interval Padding		TrueFalseTrueFalseTrueFalseTrueFalseTrueFalse (default)TrueFalse
0 0 0 0 0 0 0	Interval No Warnings Mark Dups Assume Sort Order Query Name Fix Mate CRAM Optical Duplicate Pixel Distance Assume Mark Dups Picard Version 2.18.2 Interval Padding BWA Mem Options		True False True False True False True False (default)

Here you can see inputs that are not files, for example boolean and integer inputs. Clicking the question mark next to each option will pull up a dialogue box explaining how to use each option. For example, clicking the question mark next to "Interval" results in the following:

	Interval
СОММО (?) < (?) (?) (?)	Interval within which to call bqsr from the input reads. All intervals will have a padding of 100 to get read records and overlapping intervals will be combined. Interval files should be passed using the - -interval-file option. This option can be used multiple times. e.g. '-L chr1 -L chr2:10000 -L chr3:20000+ -L chr4:10000-20000'
0	Fix Mata

For this tutorial, we will click on "Select File" to select our reference zip file:

ANALYSIS SETTINGS		ANALYSIS INPUTS 2	APP SETTINGS	
P P	BFQ2BAM 👻	Enable Batch OFF		
•	FQ-to-BAM Pipeline (Parabricks accele	⑦ About this app		
* ⑦	BWA Reference Genome Index *.bwa-index.tar.gz	Select File		

We will do the same for our fastq pairs. At this point you can set any other options we'd like, however we will leave the default values for everything else for the sake of simplicity in this tutorial.

Now that we have our files selected, we can click "Start Analysis" in the top right corner. This takes us to a page where we can monitor the status of our job. Let's click on "View Log" and watch as the job runs.



It should take a few minutes for the job to start, and a few more minutes for the job to run to completion.

When the job is done we can check the logs by clicking on View Log. At the bottom of the log we can see the Parabricks terminal output and the confirmation text that the job successfully completed:

[PB Info 2023-Jan-1	19:54:09]					
[PB Info 2023-Jan-1	19:54:09]	11	Parabric	ks accelerated Ger	nomics Pipeline	11
[PB Info 2023-Jan-1	19:54:09]			Version 4.0.	0-1	11
[PB Info 2023-Jan-1	19:54:09]	11		Marking Duplicates	s, BQSR	11
[PB Info 2023-Jan-1	19:54:09]					
[PB Info 2023-Jan-1	19:54:09]	progressM	leter – Percentage	1		
[PB Info 2023-Jan-1	19:54:19]	52.3	9.23 GB			
[PB Info 2023-Jan-1	19:54:29]	100.0	0.00 GB			
[PB Info 2023-Jan-1	19:54:29]	BQSR and	writing final BAM:	20.034 seconds		
[PB Info 2023-Jan-1	19:54:29]					
[PB Info 2023-Jan-1	19:54:29]		Program:	1	Marking Duplicates, BQSR	11
[PB Info 2023-Jan-1	19:54:29]		Version:		4.0.0-1	11
[PB Info 2023-Jan-1	19:54:29]	11	Start Time:	1	Wed Jan 11 19:54:09 2023	11
[PB Info 2023-Jan-1	19:54:29]		End Time:	1	Wed Jan 11 19:54:29 2023	11
[PB Info 2023-Jan-1	19:54:29]		Total Time:		20 seconds	11
[PB Info 2023-Jan-1	19:54:29]					
Done with Parabrick	s analysis.	Preparing	output for upload	l		
adding output: file-GKzV7xj0Py5FK6KK66jQ7P0v						

finished creating output!

You can click on View all Inputs/Outputs to see the output files as well as the input arguments:

Inputs BWA Reference Genome Index (ref) sample_data.bwa-index.tar.gz FQ Read pairs (in_fq) sample_1.fq.gz sample_2.fq.gz CRAM (cram) false Outputs output_files sample.bam

Congratulations! We have successfully run a Parabricks job on DNAnexus.

Running the Parabricks FQ-to-BAM Pipeline using the CLI

For users who prefer to use the terminal as opposed to a GUI, that option exists as well, provided you have the <u>DNAnexus SDK</u> installed. We can use the following command to run FQ-to-BAM with the same data we used in the previous section:

\$ dx run fq2bam \ -iref=<project-id:reference-file-id> \ -iin_fq=<project-id:fastq1-fileid> \ -iin_fq=<project-id:fastq2-file-id>

For this we need the ID for the project and files that we plan to use. One way to get these is to go to the GUI, click on the file, and copy the ID from the right sidebar:



Once we have our project and file IDs ready, we can run the command and it should come up in the Monitor tab for the project just like using the GUI.

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