

# **Running NVIDIA Parabricks on Azure**

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This guide shows how to run Parabricks on a compute instance on Azure.

# 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>.

# **Starting a Compute Instance**

In this section, we will show how to start a Compute Instance on Azure.

Begin by navigating to the <u>Azure Portal homepage</u> and from the menu on the top left, select Virtual machines. This will take us to the Virtual machines page.

$\equiv$ Microsoft Azure	, > Search resources, services, and docs (G+/)	F 0 0 F
Home >		
Virtual machines NVIDIA Corporation (NVIDIA.onmicrosoft.com)		
+ Create $\lor$ $\rightleftarrows$ Switch to classic $$ Reservation	ons 🗸 🛞 Manage view 🗸 🖒 Refresh 🞍 Export to CSV 😚 Open query 🛛 🖗 Assign tags ▷ Start 🤇 Restart 🗌 Stop 📋 Delete 📰 Services 🗸 🤌	Maintenance 🗸
<b>Azure virtual machine</b> Create a virtual machine hosted by Azure	Type equals all Resource group equals all $ imes$ Location equals all $ imes$ $\ddagger_{ abla}$ Add filter	
Azure virtual machine with preset configuration Create a virtual machine with presets based on your workloads	Type ↑↓     Subscription ↑↓     Resource group ↑↓     Location ↑↓     Status ↑↓     Operating system ↑↓     Size ↑↓	No grouping Vogrouping Public IP address ↑↓
More VMs and related solutions Discover and deploy full workloads and Azure products for your business needs		

At the top of the page, select Create, and Azure virtual machine. Here we can configure all the settings for our Virtual machine. You will need to choose your Subscription, then choose or create a new Resource group. For our example we will create a Resource group called "Parabricks".

$\equiv$ Microsoft Azure		$\mathcal{P}$ Search resources, se	rvices, and docs (G+/)
Home > Virtual machines >			
Create a virtual mach	ine		
Basics Disks Networking N	Management Monitoring	Advanced Tags Review	/ + create
Create a virtual machine that runs Linux image. Complete the Basics tab then Re for full customization. Learn more d	x or Windows. Select an image from eview + create to provision a virtua	m Azure marketplace or use your al machine with default paramete	own customized rs or review each tab
Project details			
Select the subscription to manage depl your resources.	oyed resources and costs. Use res	ource groups like folders to orga	nize and manage all
Subscription * 🛈			$\checkmark$
Resource group * (i)	(New) Resource group		$\checkmark$
	Create new		
Instance details	A resource group is a co	ontainer that holds related	
Virtual machine name * ①	resources for an Azure s	olution.	
Region * 🕕	Name *		$\sim$
Availability options (i)	Parabricks		~
Samitation ()	Cancel		

Carritettura (

We then add the instance details, we will name our VM "Parabricks", and select an appropriate region. We then choose the Security type as "Standard" as shown below.

 $\mathbf{\cdot}$ 

### Create a virtual machine

Instance details	
Virtual machine name * 🛈	Parabricks
Region * ①	(US) East US 🗸 🗸
Availability options ()	No infrastructure redundancy required $\sim$
Security type ①	Standard $\checkmark$
Image * ①	<b>Standard</b> The basic level of security for your virtual machines.
VM architecture ①	<b>Trusted launch virtual machines</b> Protects against persistent and advanced attacks on Gen 2 virtual machines with configurable features like secure boot and virtual Trusted Platform Module (vTPM).
Run with Azure Spot discount 🕕	Confidential virtual machines
Size * ①	On top of Trusted launch, Confidential virtual machine offers higher confidentiality and integrity guaranteed with hardware-based trusted execution environment.

We choose an image by clicking on See all images. You can search for nvidia, and choose "NVIDIA GPU-Optimized VMI with vGPU driver" that will take care of the GPU Driver, and docker installation.

#### Home > Create a virtual machine >

Marketplace

### Select an image

Other Items

My Images	🔎 nvidia		Publisher name : All $ imes$ Security		
Shared Images		Pricing : All ×			
Community Images Direct Shared Images (PREVIEW)	Showing 1 to 20 of 34 results for ' <b>nvi</b>	dia' with <b>1 selected filters</b> . <u>Clear sea</u>	rch + filters		
Marketplace					
All	NVIDIA GPU-Optimized VMI	NVIDIA GPU-Optimized VMI with vGPU driver	NVIDIA AI Enterprise		
Recently created Private products	NVIDIA Corporation Virtual Machine Maximize GPU performance for your	NVIDIA Corporation Virtual Machine Maximize GPU performance for your	NVIDIA Corporation Virtual Machine The end to end platform for building		
Categories	HPC applications with this image	HPC applications with this image	accelerated production AI.		
Compute (22)			Starts at <b>\$2.00/user/3 years</b>		
Analytics (14)	Select $\checkmark$	Select $\checkmark$	Select 🗸 🛇		
Developer Tools (14)	NVIDIA GPU-Optimized VMI - v23	.03.0 - x64 Gen 1			
AI + Machine Learning (8)	NVIDIA GPU-Optimized VMI - v23	.03.0 - x64 Gen 2	<b></b>		
Containers (3)	NVIDIA GPU-Optimized VMI - v22				
Databases (1)	NVIDIA GPU-Optimized VMI - v22	Introductory Offer -			
Blockchain (0)	NVIDIA GPU-Optimized VMI - v22	.03.0 - x64 Gen 2	NVIDIA Corporation		
DevOps (0)	NVIDIA GPU-Optimized VMI - v22	.03.0 - x64 Gen 1 Cloud Computing	Virtual Machine CloudXR is NVIDIA's streaming SDK		

### We then choose the Size for the GPUs that we want to be using.

motunee actuns
----------------

Virtual machine name * 🛈	Parabricks	$\checkmark$
Region * ①	(US) East US	$\checkmark$
Availability options ①	No infrastructure redundancy required	$\checkmark$
Security type ①	Standard	$\checkmark$
Image * 🛈	NVIDIA GPU-Optimized VMI - v22.03.0 - x64 Gen2	$\sim$
	See all images   Configure VM generation	
VM architecture (i)	Arm64	
	• x64	
	<b>i</b> Arm64 is not supported with the selected image.	
Run with Azure Spot discount ①		
Size * ①	Standard_NV72ads_A10_v5 - 72 vcpus, 880 GiB memory (Loading price)	$\sim$
	See all sizes	

For the Administrator account, You can either use an SSH public key, or as shown below, use a Username and Password.

Administrator account		
Authentication type 🛈	○ SSH public key	
	Password	
Username * 🤅	pbuser	¥
Password * (i)	•••••	¥
Confirm password * ①		¥
Review + create < Prev	ious Next : Disks >	

If you need Disks, Networking or other specifications related to your work, click on "Next:Disks >". However, if you don't need any of these click on "Review + create". If everything is configured well you will have a page to review, and the message "Validation passed" at the top.

	$\stackrel{>}{\sim}$ Search resources, services, and docs (G+/)
ome >	
reate a virtual mad	hine
Validation passed	
Basics Disks Networking	Management Monitoring Advanced Tags Review + create
<b>()</b> Cost given below is an estimate	and not the final price. Please use Pricing calculator 🗹 for all your pricing needs.
Price	
NVIDIA GPU-Optimized VMI	Not covered by credits $\bigcirc$
by NVIDIA Corporation	0.0000 USD/hr
Terms of use   Privacy policy	
1 X Standard NV72ads A10 v5	Subscription credits apply ①
by Microsoft Terms of use I Privacy policy	
	Pricing for other VM sizes
TERMS	
By clicking "Create", I (a) agree to the	legal terms and privacy statement(s) associated with the Marketplace offering(s) listed
above; (b) authorize Microsoft to bill hilling frequency as my Azure subscri	my current payment method for the fees associated with the offering(s), with the same
information with the provider(s) of th	e offering(s) for support, billing and other transactional activities. Microsoft does not
provide rights for third-party offering	Js. See the Azure Marketplace Terms for additional details.
Name	
Droforrad a mail addross	
Preferred e-mail address	
Preferred e-mail address Preferred phone number	NONE PROVIDED
Preferred e-mail address Preferred phone number	NONE PROVIDED
Preferred e-mail address Preferred phone number	NONE PROVIDED
Preferred e-mail address Preferred phone number <b>Basics</b>	NONE PROVIDED
Preferred e-mail address Preferred phone number <b>Basics</b> Subscription	NONE PROVIDED
Preferred e-mail address Preferred phone number <b>Basics</b> Subscription Resource group	(new) Parabricks
Preferred e-mail address Preferred phone number <b>Basics</b> Subscription Resource group Virtual machine name	(new) Parabricks Parabricks
Preferred e-mail address Preferred phone number Basics Subscription Resource group Virtual machine name Region	(new) Parabricks Parabricks East US
Preferred e-mail address Preferred phone number Basics Subscription Resource group Virtual machine name Region Availability options	(new) Parabricks Parabricks East US No infrastructure redundancy required
Preferred e-mail address Preferred phone number Basics Subscription Resource group Virtual machine name Region Availability options Security type	(new) Parabricks Parabricks East US No infrastructure redundancy required Standard
Preferred e-mail address Preferred phone number Basics Subscription Resource group Virtual machine name Region Availability options Security type Image	(new) Parabricks Parabricks East US No infrastructure redundancy required Standard NVIDIA GPU-Optimized VMI - v22.03.0 - Gen2
Preferred e-mail address Preferred phone number Basics Subscription Resource group Virtual machine name Region Availability options Security type Image	(new) Parabricks Parabricks East US No infrastructure redundancy required Standard NVIDIA GPU-Optimized VMI - v22.03.0 - Gen2

Review the details and click Create at the bottom of the page. You will land on a page saying "... Deployment in progress". When it is complete, click the "Go to resource" button.

$\sim$	Deployment details					
	Next steps					
	Setup auto-shutdown Recommended					
	Monitor VM health, performance and network dependencies Recommended					
	Run a script inside the virtual machine Recommended					
	Go to resource Create another VM					

You should see a page like below. Click on Connect.

$\equiv$ Microsoft Azure		م	Search reso	urces, services,	and docs (G+	+/)		
Home > CreateVm-nvidia.nvidia-gpu-opt	imized-vmi-a10-nvid-202	3082915414	5   Overviev	<b>/</b> >				
Parabricks ☆☆… <sub>Virtual machine</sub>								
🔎 Search 🛛 «	💋 Connect 🕞 Start	🤇 Restart	Stop	🔯 Capture	📋 Delete	Ѷ Refresh	🛄 Open in mobile	📯 Feedb
Overview	<ul> <li>Eccentials</li> </ul>							
Activity log	Cossentiais							
Access control (IAM)	Resource group (move	) : <u>Parabrick</u>	ŝ					
	Status	: Running						
🎸 Tags	Location	: East US						
🗙 Diagnose and solve problems	Subscription (move)	Ξ.						
Settings	Subscription ID	: '						
🧟 Networking	Health state	: -						
Ø Connect	Tags (edit)	: Add tags						

Once the instance is running click on Connect and use the IP information to ssh into your instance.

Verify that the driver is installed using *nvidia-smi*.

## **Installing Parabricks**

We will install Parabricks into our instance that we just created. To do this, we will use the NVIDIA GPU Cloud (NGC) to download the Parabricks Docker image.

Visit the <u>Parabricks page on NGC</u> to get the Docker pull command for the latest version of Parabricks.



Back in our EC2 instance, let's run the docker pull command:

\$ docker pull nvcr.io/nvidia/clara/clara-parabricks:4.3.1-1

```
pbuser@Parabricks:~$ docker pull nvcr.io/nvidia/clara/clara-parabricks:4.1.1-1
4.1.1-1: Pulling from nvidia/clara/clara-parabricks
df6635ed1257: Pull complete
6ceabd2ff7b0: Pull complete
cd189d71cce3: Pull complete
b0b6463464d3: Pull complete
0dbb8e45df45: Pull complete
518385bcb747: Pull complete
518385bcb747: Pull complete
Digest: sha256:7a44179fcaeb6422c52f9e1f8b966110ab3fd50a57f06793c74659ad38eedb66
Status: Downloaded newer image for nvcr.io/nvidia/clara/clara-parabricks:4.1.1-1
```

Parabricks is now installed. Let's run some sample data to test it.

### **Testing Parabricks**

Parabricks provides a small sample dataset as a test for the installation and hardware which can be downloaded using:

```
$ wget -O parabricks_sample.tar.gz \
"https://s3.amazonaws.com/parabricks.sample/parabricks_sample.tar.gz"
> "https://s3.amazonaws.com/parabricks_sample.tar.gz \
> "https://s3.amazonaws.com/parabricks.sample/parabricks_sample.tar.gz"
--2023-08-01 12:57:31-- https://s3.amazonaws.com/parabricks.sample/parabricks.sample.tar.gz
Resolving s3.amazonaws.com (s3.amazonaws.com)... 52.217.232.16, 52.216.54.128, 52.217.227.184, ...
Connecting to s3.amazonaws.com (s3.amazonaws.com)|52.217.232.16|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 9924454379 (9.26) [application/x-tar]
```

Saving to: 'parabricks\_sample.tar.gz'

When the download completes we can untar the data using:

\$ tar xvf parabricks\_sample.tar.gz

And you should see something like below:

```
pbuser@Parabricks:~$ tar xvf parabricks sample.tar.gz
parabricks sample/
parabricks sample/Data/
parabricks sample/Data/sample 2.fq.gz
parabricks sample/Data/sample 1.fq.qz
parabricks sample/Ref/
parabricks_sample/Ref/Homo_sapiens_assembly38.fasta
parabricks sample/Ref/Homo sapiens assembly38.fasta.pac
parabricks sample/Ref/Homo sapiens assembly38.fasta.ann
parabricks sample/Ref/Homo sapiens assembly38.known indels.vcf.gz.tbi
parabricks sample/Ref/Homo sapiens assembly38.fasta.amb
parabricks sample/Ref/Homo sapiens assembly38.dict
parabricks sample/Ref/Homo sapiens assembly38.fasta.fai
parabricks sample/Ref/Homo sapiens assembly38.known indels.vcf.gz
parabricks sample/Ref/Homo sapiens assembly38.fasta.bwt
parabricks sample/Ref/Homo sapiens assembly38.fasta.sa
```

Finally, we can run any of the Parabricks pipelines on it. Let's run the <u>germline pipeline</u> using the following command:

\$ docker run \ --rm \ --gpus all \ --volume `pwd`:`pwd` \ --workdir `pwd`/parabricks\_sample \ nvcr.io/nvidia/clara/clara-parabricks:4.3.1-1 \ pbrun germline \ --ref Ref/Homo\_sapiens\_assembly38.fasta \ --in-fq Data/sample\_1.fq.gz Data/sample\_2.fq.gz \ --knownSites Ref/Homo\_sapiens\_assembly38.known\_indels.vcf.gz.tbi \ --out-bam output.bam \ -out-variants germline.vcf \ --out-recal-file recal.txt

We can tell that Parabricks started correctly when we see the Parabricks banner and the ProgressMeter begins to populate with values:

```
pbuser@Parabricks:~$ docker run \
>
       --gpus all \
>
       --rm \
       --volume $(pwd):/workdir \
>
>
       --volume $(pwd):/outputdir \
>
     nvcr.io/nvidia/clara/clara-parabricks:4.1.1-1 \
>
     pbrun fq2bam \
       --ref /workdir/parabricks_sample/Ref/Homo_sapiens_assembly38.fasta \
>
>
       --in-fq /workdir/parabricks_sample/Data/sample_1.fq.gz /workdir/parabricks_sample/Data/sample_2.fq.gz \
>
        --out-bam /outputdir/fg2bam output.bam \
>
        --low-memory
[Parabricks Options Mesg]: Checking argument compatibility
[Parabricks Options Mesg]: Automatically generating ID prefix
[Parabricks Options Mesg]: Read group created for /workdir/parabricks_sample/Data/sample_1.fq.gz and
/workdir/parabricks_sample/Data/sample_2.fq.gz
[Parabricks Options Mesg]: @RG\tID:HK3TJBCX2.1\tLB:lib1\tPL:bar\tSM:sample\tPU:HK3TJBCX2.1
[PB Info 2023-Aug-01 13:08:01] ------
[PB Info 2023-Aug-01 13:08:01] ||
                                               Parabricks accelerated Genomics Pipeline
[PB Info 2023-Aug-01 13:08:01]
                                                             Version 4.1.1-1
[PB Info 2023-Aug-01 13:08:01] ||
                                                     GPU-BWA mem, Sorting Phase-I
[PB Info 2023-Aug-01 13:08:01] ------
[M::bwa_idx_load_from_disk] read 0 ALT contigs
[PB Info 2023-Aug-01 13:08:03] GPU-BWA mem
[PB Info 2023-Aug-01 13:08:03] ProgressMeter
                                              Reads
                                                              Base Pairs Aligned
[PB Info 2023-Aug-01 13:08:14] 5043564
                                               580000000
[PB Info 2023-Aug-01 13:08:19] 10087128 1170000000
```

This should take ~10 minutes to finish running. When it's done, we should see the output files in the sample data directory.

### **Closing Remarks**

We encourage you to expand on the demo in this guide by using your own data, trying other pipelines, and generally exploring what Parabricks has to offer. Check out the documentation for more information about the different pipelines available. You can also find our online developer community on the Parabricks forum, where you can ask questions and search through answers while you are learning how to use Parabricks.

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