Single Node Amazon Web Services Deployment

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Creating a New Elastic Compute Cloud Instance for Partek Flow Software

Note: This guide assumes all items necessary for the Amazon elastic Comput Clout (EC2) instance does not exist, such as Amazon Virtual Private Cloud (VPC), subnets, and security groups, thus their creation is covered as well.

Log in to the Amazon Web Services (AWS) management console at https://console.aws.amazon.com

Click on EC2

Switch to the region intended to deploy Partek Flow software. This tutorial uses US East (N. Virginia) as an example.

On the left menu, click on Instances, then click the Launch Instance button. The Choose an Amazon Machine Image (AMI) page will appear.

Click the Select button next to Ubuntu Server 16.04 LTS (HVM), SSD Volume Type - ami-f4cc1de2. <u>NOTE</u>: Please use the latest Ubuntu AMI. It is likely that the AMI listed here will be out of date.

Choose an Instance Type, the selection depends on your budget and the size of the Partek Flow deployment. We recommend m4.large for testing or cluster front-end operation, m4.xlarge for standard deployments, and m4.2xlarge for alignment-heavy workloads with a large user-base. See the section AWS instance type resources and costs for assistance with choosing the right instance. In most cases, the instance type and associated resources can be changed after deployment, so one is not locked into the choices made for this step.

<u>NOTE</u>: New instance types will become available. Please use the latest mX instance type provided as it will likely perform better and be more cost effective than older instance types.

On the Configure Instance Details page, make the following selections:

Set the number of instances to 1. An autoscaling group is not necessary for single-node deployments

Purchasing Option: Leave Request Spot Instances unchecked. This is relevant for cost-minimization of Partek Flow cluster deployments.

Network: If you do not have a virtual private cloud (VPC) already created for Partek Flow, click **Create New VPC**. This will open a new browser tab for VPC management.

Use the following settings for the VPC:

Name Tag: Flow-VPC

IPv4 CIDR block: 10.0.0.0/16
Select No IPv6 CIDR Block

Tenancy: Default

Click Yes, Create. You may be asked to select a DHCP Option set. If so, then make sure the dynamic host configuration protocol (DHCP) op tion set has the following properties:

Options: domain-name = ec2.internal;domain-name-servers = AmazonProvidedDNS;

DNS Resolution: leave the defaults set to yes

DNS Hostname: change this to yes as internal DNS resolution may be necessary depending on the Partek Flow deployment

Once created, the new Flow-VPC will appear in the list of available VPCs. The VPC needs additional configuration for external access. To continue, right click on Flow-VPC and select **Edit DNS Resolution**, select Yes, and then Save. Next, right click the Flow-VPC and select **Edit DNS Hostnames**, select Yes, then Save.

Make sure the DHCP option set is set to the one created above. If it is not, right-click on the row containing Flow-VPC and select Edit DHCP Option Sets.

Close the VPC Management tab and go back to the EC2 Management Console.

Click the refresh arrow next to Create New VPC and select Flow-VPC.

Click Create New Subnet and a new browser tab will open with a list of existing subnets. Click Create Subnet and set the following options:

Name Tag: Flow-Subnet

VPC: Flow-VPC

VPC CIDRs: This should be automatically populated with the information from Flow-VPC

Availability Zone: It is OK to let Amazon choose for you if you do not have a preference

IPv4 CIDR block: 10.0.1.0/24

Stay on the VPC Dashboard Tab and on the left navigation menu, click Internet Gateways, then click Create Internet Gateway and use the following options:

Name Tag: Flow-IGW

Click Yes, Create

The new gateway will be displayed as **Detached**. Right click on the *Flow-IGW* gateway and select **Attach to VPC**, then select *Flow-VPC* and click **Y es, Attach**.

Click on Route Tables on the left navigation menu.

If it exists, select the route table already associated with *Flow-VPC*. If not, make a new route table and associate it with *Flow-VPC*. Click on the new route table, then click the **Routes** tab toward the bottom of the page. The route *Destination* = 10.0.0.0/16 Target = loca/should already be present. Click **Edit**, then **Click Add another route** and set the following parameters:

Destination: 0.0.0.0/0

Target set to *Flow-IGW* (the internet gateway that was just created)

Click Save

Close the VPC Dashboard browser tab and go back to the EC2 Management Console tab. Note that you should still be on Step 3: Configure Instance Details.

Click the refresh arrow next to Create New Subnet and select Flow-Subnet.

Auto-assign Public IP: Use subnet setting (Disable)

Placement Group: No placement group

IAM role: None.

Note: For multi-node Partek Flow deployments or instances where you would like Partek to manage AWS resources on your behalf, please see Partek AWS support and set up an IAM role for your Partek Flow EC2 instance. In most cases a specialized IAM role is unnecessary and we only need instance ssh keys.

Shutdown Behaviour: Stop

Enable Termination Protection: select Protect against accidental termination

Monitoring: leave Enable CloudWatch Detailed Monitoring disabled

EBS-optimized Instance: Make sure **Launch as EBS-optimized Instance** is enabled. Given the recommended choice of an m4 instance type, EBS optimization should be enabled at no extra cost.

Tenancy: Shared - Run a shared hardware instance

Network Interfaces: leave as-is

Advanced Details: leave as-is

Click Next: Add Storage. You should be on Step 4: Add Storage

For the existing root volume, set the following options:

Size: 8 GB

Volume Type: Magnetic

Select Delete on Termination

Note: All Partek Flow data is stored on a non-root EBS volume. Since only the OS is on the root volume and not frequently re-booted, a fast root volume is probably not necessary or worth the cost. For more information about EBS volumes and their performance, see the section EBS volumes.

Click Add New Volume and set the following options:

Volume Type: EBS

Device: /dev/sdb (take the default)

Do not define a snapshot

Size (GiB): 500

Note: This is the minimum for ST1 volumes, see: EBS volumes

Volume Type: Throughput optimized HDD (ST1)

Do not delete on terminate or encrypt

Click Next: Add Tags

You do not need to define any tags for this new EC2 instance, but you can if you would like.

Click Next: Configure Security Group

For Assign a Security Group select Create a New Security Group

Security Group Name: Flow-SG

Description: Security group for Partek Flow server

Add the following rules:

SSH set Source to My IP (or the address range of your company or institution)

Click Add Rule:

Set Type to Custom TCP Rule

Set Port Range to 8080

Set Source to anywhere (0.0.0.0/0, ::/0)

Note: It is recommended to restrict Source to just those that need access to Partek Flow.

Click Review and Launch

The AWS console will suggest this server not be booted from a magnetic volume. Since there is not a lot of IO on the root partition and reboots are will be rare, choosing **Continue with Magnetic** will reduce costs. Choosing an SSD volume will not provide substantial benefit but it OK if one wishes to use an SSD volume. See the EBS Volumes section for more information.

Click Launch

Create a new keypair:

Name the keypair Flow-Key

Download this keypair, the run chmod 600 Flow-Key.pem (the downloaded key) so it can be used.

Backup this key as one may lose access to the Partek Flow instance without it.

The new instance will now boot. Use the left navigation bar and click on **Instances**. Click the pencil icon and assign the instance the name Partek *Flow Server*

Enabling External Access to the Partek Flow Elastic Compute Cloud Instance

The server should be assigned a fixed IP address. To do this, click on Elastic IPs on the left navigation menu from the EC2 Management Console.

Click Allocate New Address

Assign Scope to VPC

Click Allocate

On the table containing the newly allocated elastic IP, right click and select Associate Address

For Instance, select the instance name Flow Test Server

For Private IP, select the one private IP available for the Partek Flow EC2 instance, then click Associate

Note: For the remaining steps, we refer to the elastic ip as elastic.ip

SSH to the new Flow-Server instance:

\$ chmod 600 Flow-Key.pem

\$ ssh -i Flow-Testing.pem ubuntu@elastic.ip

Attaching the Amazon Elastic Block Store Volume for Partek Flow Data Storage

Attach, format, and move the *ubuntu* home directory onto the large ST1 elastic block store (EBS) volume. All Partek Flow data will live in this volume. Consult the AWS EC2 documentation for further information about attaching EBS volumes to your instance.

\$ sudo su

\$ mkfs -t ext4 /dev/xvdb

Note: Under Volumes in the EC2 management console, inspect Attachment Information. It will likely list the large ST1 EBS volume as attached to /dev/sdb. Replace "s" with "xv" to find the device name to use for this mkfs command.

Make a note of the newly created UUID for this volume

Copy the *ubuntu* home directory onto the EBS volume using a temporary mount point:

\$ mount -t ext4 /dev/xvdb /mnt/

\$ rsync -avr /home/ /mnt/

\$ umount /mnt/

Make the EBS volume mount at system boot:

Add the following to /etc/fstab: UUID=the-UUID-from-the-mkfs-command-above /home ext4 defaults,nofail 0 2

\$ mount -a

Disconnect the ssh session, then log in again to make sure all is well

Installing Partek Flow on a New Elastic Compute Cloud Instance

Note: For additional information about Partek Flow installations, see our generic Installation Guide

Before beginning, send the media access control (MAC) address of the EC2 instance to MAC address of the EC2 instance to licensing@partek.com. The output of *ifconfig* will suffice. Given this information, Partek employees will create a license for your AWS server. MAC addresses will remain the same after stopping and starting the Partek Flow EC2 instance. If the MAC address does change, let our licensing department know and we can add your license to our floating license server or suggest other workarounds.

Install required packages for Partek Flow:

\$ sudo apt-get update

\$ sudo apt-get install software-properties-common

\$ sudo add-apt-repository -y ppa:openjdk-r/ppa

\$ sudo apt-get install openjdk-8-jdk python python-pip python-dev zlib1g-dev python-matplotlib r-base python-htseq libxml2-dev perl make gcc g++ zlib1g libbz2-1.0 libstdc++6 libgcc1 libncurses5 libsqlite3-0 libfreetype6 libpng12-0 zip unzip libgomp1 libxrender1 libxtst6 libxi6 debconf

\$ sudo pip install --upgrade pip && pip install --upgrade --upgrade-strategy eager --force-reinstall virtualenv numpy pysam cnvkit

Install Partek Flow:

Note: Make sure you are running as the ubuntu user.

\$ cd (we will install Partek Flow to ubuntu's home directory)

\$ wget --content-disposition packages.partek.com/linux/flow-release

\$ unzip PartekFlow*.zip

\$./partek_flow/start_flow.sh

Partek Flow has finished loading when you see INFO: Server startup in xxxxxxx ms in the partek_flow/logs/catalina.out log file. This takes ~30 seconds.

Alternative: Install Flow with Docker. Our base packages are located here: https://hub.docker.com/r/partekinc/flow/tags

Open Partek Flow with a web browser: http://elastic.ip:8080/

Enter license key

Set up the Partek Flow admin account

Leave the library file directory at its default location and check that the free space listed for this directory is consistent with what was allocated for the ST1 EBS volume.

Done! Partek Flow is ready to use.

Partek Amazon Web Services Support

After the EC2 instance is provisioned, we are happy to assist with setting up Partek Flow or address other issues you encounter with the usage of Partek Flow. The quickest way to receive help is to allow us remote access to your server by sending us *Flow-Key.pem* and amending the SSH rule for *Flow-SG* to include access from IP 97.84.41.194 (Partek HQ). We recommend sending us the *Flow-Key.pem* via secure means. The easiest way to do this is with the following command:

\$ curl -F "file=@FlowKey.pem" https://installfeedback.partek.com/fupload

We also provide live assistance via GoTo meeting or TeamViewer if you are uncomfortable with us accessing your EC2 instance directly. Before contacting us, please run \$./partek_flow/flowstatus.sh to send us logs and other information that will assist with your support request.

General Recommendations

With newer EC2 instance types, it is possible to change the instance type of an already deployed Partek Flow EC2 server. We recommend doing several rounds of benchmarks with production-sized workloads and evaluate if the resources allocated to your Partek Flow server are sufficient. You may find that reducing resources allocated to the Partek Flow server may come with significant cost savings, but can cause UI responsiveness and job run-times to reach unacceptable levels. Once you have found an instance type that works, you may wish to use *reserved instance* pricing which is significantly cheaper than *on-demand instance* pricing. Reserved instances come with 1 or 3-year usage terms. Please see the EC2 Reserved Instance Marketplace to sell or purchase existing reserved instances at reduced rates.

The network performance of the EC2 instance type becomes an important factor if the primary usage of Partek Flow is for alignment. For this use case, one will have to move copious amounts of data back (input fastq files) and forth (output bam files) between the Partek Flow server and the end users, thus it is important to have as what AWS refers to as *high network performance* which for most cases is around 1 Gb/s. If the focus is primarily on downstream analysis and visualization (e.g. the primary input files are *ADAT*) then network performance is less of a concern.

We recommend HVM virtualization as we have not seen any performance impact from using them and non-HVM instance types can come with significant deployment barriers.

Make sure your instance is EBS optimized by default and you are not charged a surcharge for EBS optimization.

T-class servers, although cheap, may slow responsiveness for the Partek Flow server and generally do not provide sufficient resources.

We do not recommend placing any data on *instance store* volumes since all data is lost on those volumes after an instance stops. This is too risky as there are cases where user tasks can take up unexpected amounts of memory forcing a server stop/reboot.

Amazon Web Services Instance Type Resources and Costs

The values below were updated April 2017. The latest pricing and EC2 resource offerings can be found at http://www.ec2instances.info

Instance Type	Memory	Cores	EBS throughput	Network Performance	Monthly cost
m4.large	8.0 GB	2 vCPUs	56.25 MB/s M	Medium	\$78.840
r4.large	15.25 GB	2 vCPUs	50 MB/s H(10G int)	High (+10G interface)	\$97.09
m4.xlarge	16.0 GB	4 vCPUs	93.75 MB/s H	High	\$156.950
r4.xlarge	30.5 GB	4 vCPUs	100 MB/s H	High	\$194.180
m4.2xlarge	32.0 GB	8 vCPUs	125 MB/s H	High	\$314.630
r4.2xlarge	61.0 GB	8 vCPUs	200 MB/s H(10G int)	High (+10G interface)	\$388.360

Single server recommendation: m4.xlarge or m4.2xlarge

Network performance values for US-EAST-1 correspond to: Low ~ 50Mb/s, Medium ~ 300Mb/s, High ~ 1Gb/s.

Elastic Block Store Volumes

Choice of a volume type and size:

This is dependent on the type of workload. For must users, the Partek Flow server tasks are alignment-heavy so we recommend a throughput optimized HDD (ST1) EBS volume since most aligner operations are sequential in nature. For workloads that focus primarily on downstream analysis, a general purpose SSD volume will suffice but the costs are greater. For those who focus on alignment or host several users, the storage requirements can be high. ST1 EBS volumes have the following characteristics:

Max throughput 500 MiB/s

\$0.045 per GB-month of provisioned storage (\$22.5 per month for a 500 GB of storage).

Note that EBS volumes can be grown or performance characteristics changed. To minimize costs, start with a smaller EBS volume allocation of **0.5 - 2 TB** as most mature Partek Flow installations generate roughly this amount of data. When necessary, the EBS volume and the underlying file system can be grown on-line (making ext4 a good choice). Shrinking is also possible but may require the Partek Flow server to be offline.

Additional Assistance

If you need additional assistance, please visit our support page to submit a help ticket or find phone numbers for regional support.

