Compile and run RAPID on the Microsoft Azure Cloud

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09 Jul 2014, updated 05 Aug 2014, 08 Sep 2014, 04 Nov 2014, 21 Jan 2015

Introduction

Foreword

This tutorial explains how to compile RAPID (http://rapid-hub.org/) on the Microsoft Azure Cloud (http://azure.microsoft.com/).

Knowledge prerequisites

It is assumed here that the reader has some familiarity with Unix-like operating systems.

Account prerequisites

In order to run RAPID on the Microsoft Azure Cloud, one needs to have an Azure account. More information on Azure can be found at: http://azure.microsoft.com/.

Hardware prerequisites

Completion of this tutorial requires access to a computer with an Internet connection.

Software prerequisites

The computer needs an Internet browser, and FTP client and a Linux terminal (this type of software is either readily available or can be installed on Windows, Mac and Linux computers).

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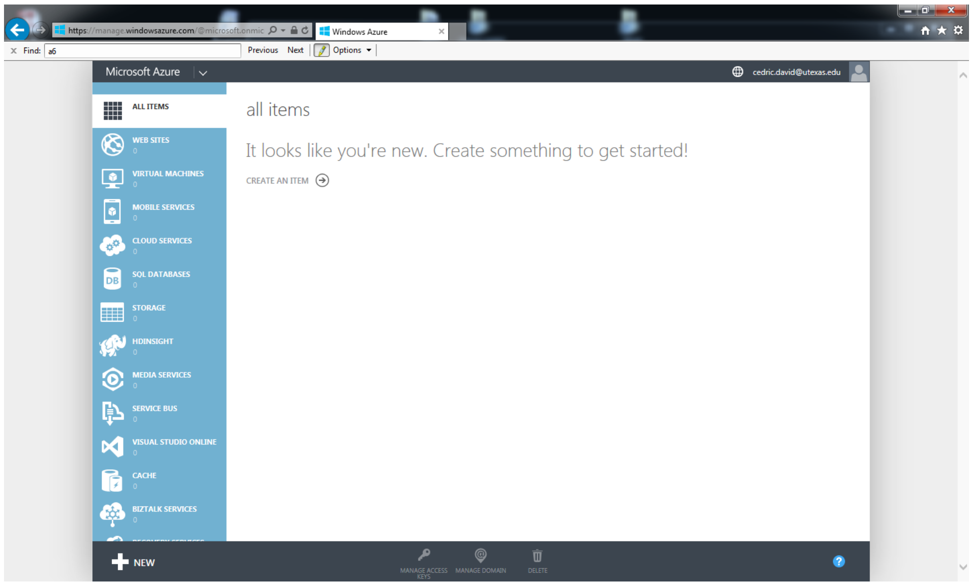
Create a Linux Virtual Machine on Azure

The easiest way to run RAPID is to do so in a Linux environment. One can create a Linux Virtual Machine on the Azure Cloud. Such can be done by logging in on https://manage.windowsazure.com/.

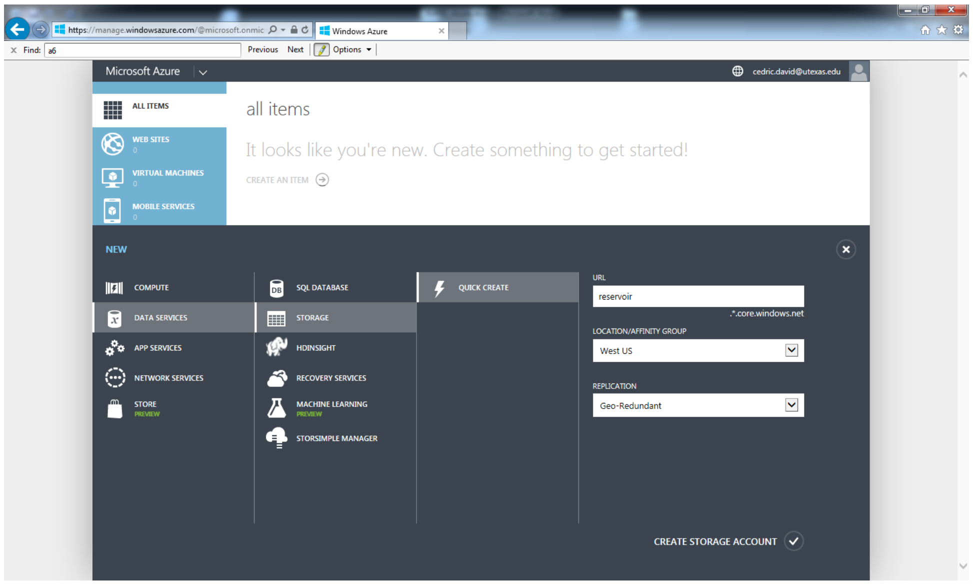


all items

It looks like you're new. Create something to get started!

CREATE AN ITEM

We will start by first creating a storage account because everything else will be stored in there. This is optional because a storage account would be created automatically anyway, but it allows picking the name of the storage (Azure automatically-generated names are quite lengthy and mysterious). To create a storage account, click on New and select Data Services/Storage/Quick Create. For the purpose of this tutorial, pick a Storage Name: storagename, Location: West US, Replication: 6Geo-Redundant.



all items

It looks like you're new. Create something to get started!

URL: reservoir .*.core.windows.net

LOCATION/AFFINITY GROUP: West US

REPLICATION: Geo-Redundant

A storage account is now created:

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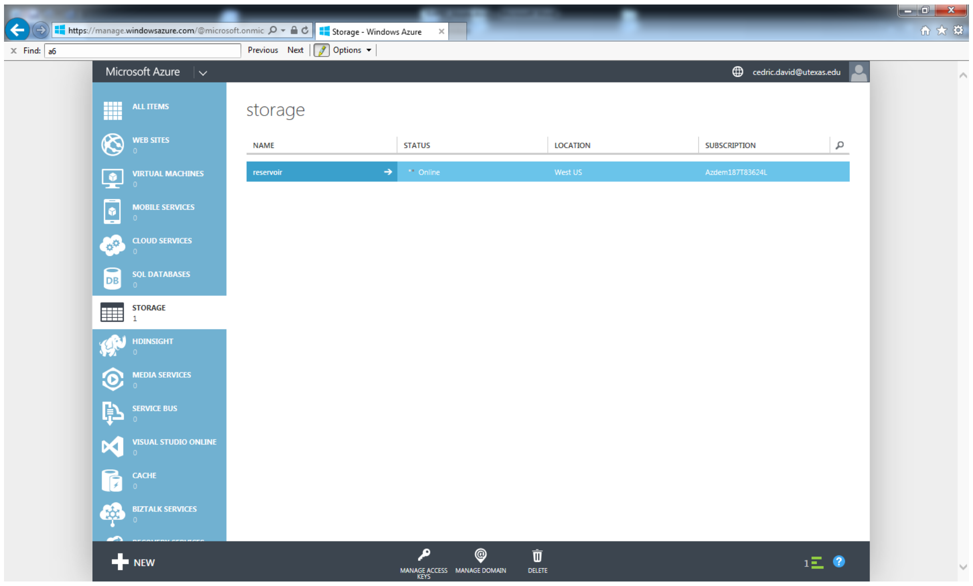
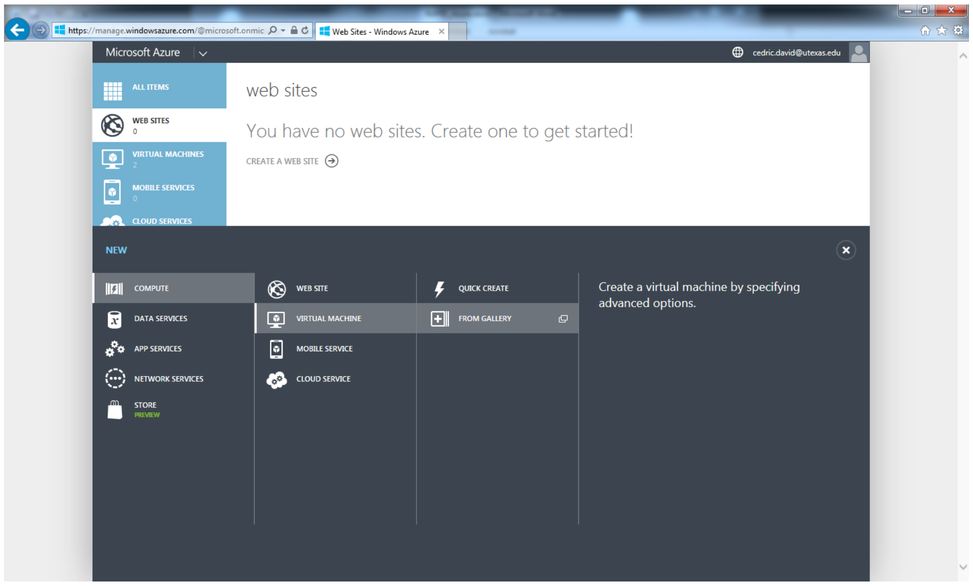


storage

NAME	STATUS	LOCATION	SUBSCRIPTION
reservoir	Online	West US	Azdem187T83624L

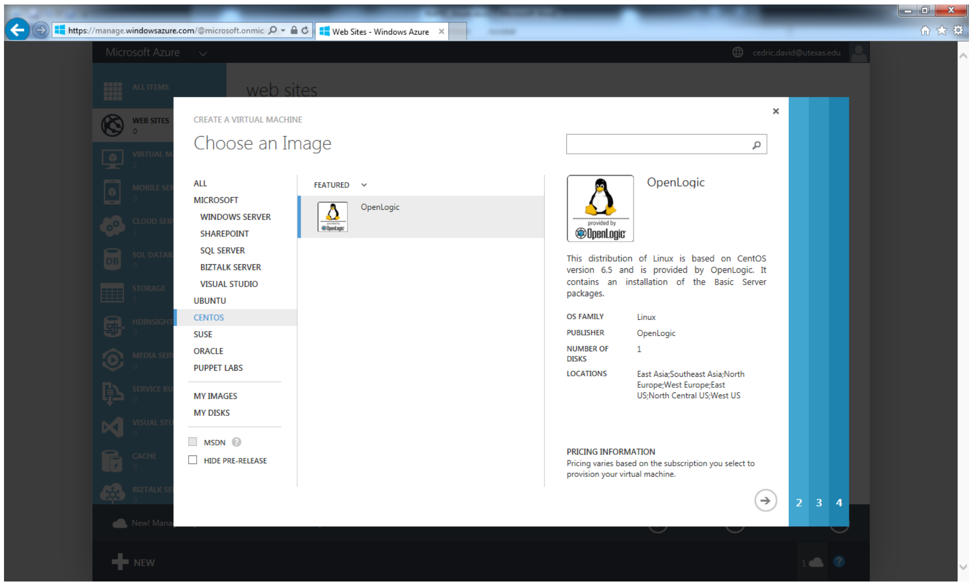
We will now create a virtual machine using a distribution of Linux is based on CentOS version 6.5. To do so, click on New and select Compute/Virtual Machine/From Gallery.



You have no web sites. Create one to get started!

Create a virtual machine by specifying advanced options.

Then choose CentOS (The Community Enterprise Operating System).



CREATE A VIRTUAL MACHINE

Choose an Image

ALL
MICROSOFT
WINDOWS SERVER
SHAREPOINT
SQL SERVER
BIZTALK SERVER
VISUAL STUDIO
UBUNTU
CENTOS
SUSE
ORACLE
PUPPET LABS
MY IMAGES
MY DISKS
MSDN
HIDE PRE-RELEASE

FEATURED

OpenLogic

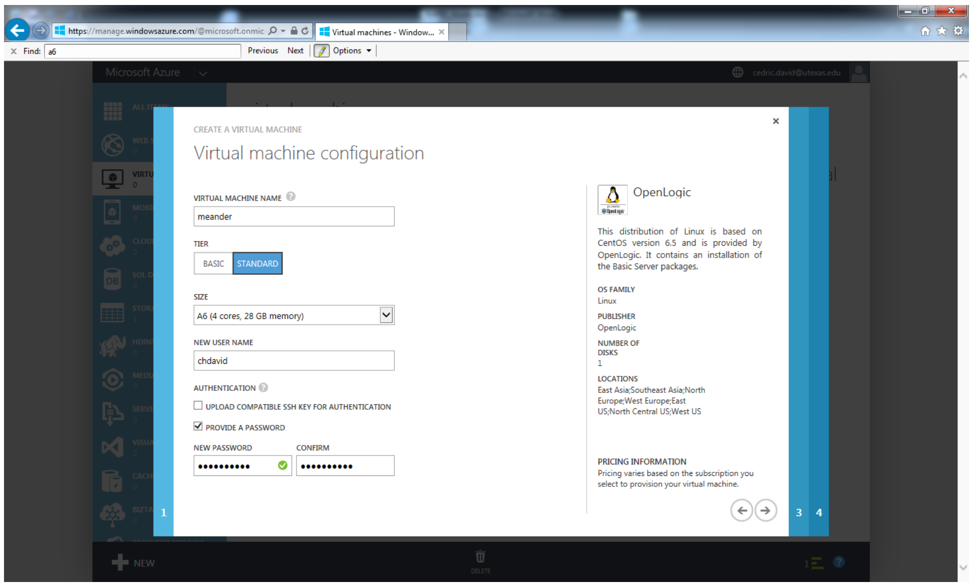
OpenLogic

This distribution of Linux is based on CentOS version 6.5 and is provided by OpenLogic. It contains an installation of the Basic Server packages.

OS FAMILY	Linux
PUBLISHER	OpenLogic
NUMBER OF DISKS	1
LOCATIONS	East Asia;Southeast Asia;North Europe;West Europe;East US;North Central US;West US

PRICING INFORMATION
Pricing varies based on the subscription you select to provision your virtual machine.

Here several options can be chosen. For the purpose of this tutorial, pick a Virtual Machine Name: machinename, Tier: Standard, Size: A6 (4 cores 28 GB memory), New User Name: username, Authentication: Password.



CREATE A VIRTUAL MACHINE

Virtual machine configuration

VIRTUAL MACHINE NAME
meander

TIER
BASIC [✓ STANDARD]

SIZE
A6 (4 cores, 28 GB memory)

NEW USER NAME
chdavid

AUTHENTICATION
☐ UPLOAD COMPATIBLE SSH KEY FOR AUTHENTICATION
☑ PROVIDE A PASSWORD

NEW PASSWORD ●●●●●●●●●● CONFIRM ●●●●●●●●●●

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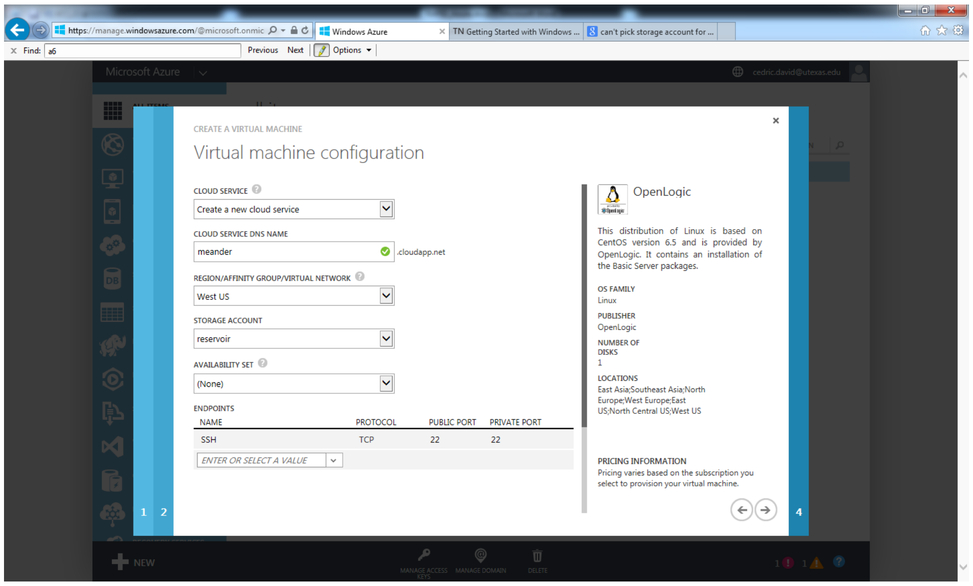
OS FAMILY
Linux
PUBLISHER
OpenLogic
NUMBER OF DISKS
1
LOCATIONS
East Asia;Southeast Asia;North Europe;West Europe;East US;North Central US;West US

PRICING INFORMATION
Pricing varies based on the subscription you select to provision your virtual machine.

And even more… Pick Create a new cloud service, Cloud service DNS name: machinename, Region: West US, Storage Account: storagename.



CREATE A VIRTUAL MACHINE

Virtual machine configuration

CLOUD SERVICE: Create a new cloud service

CLOUD SERVICE DNS NAME: meander .cloudapp.net

REGION/AFFINITY GROUP/VIRTUAL NETWORK: West US

STORAGE ACCOUNT: reservoir

AVAILABILITY SET: (None)

ENDPOINTS

NAME	PROTOCOL	PUBLIC PORT	PRIVATE PORT
SSH	TCP	22	22
ENTER OR SELECT A VALUE			

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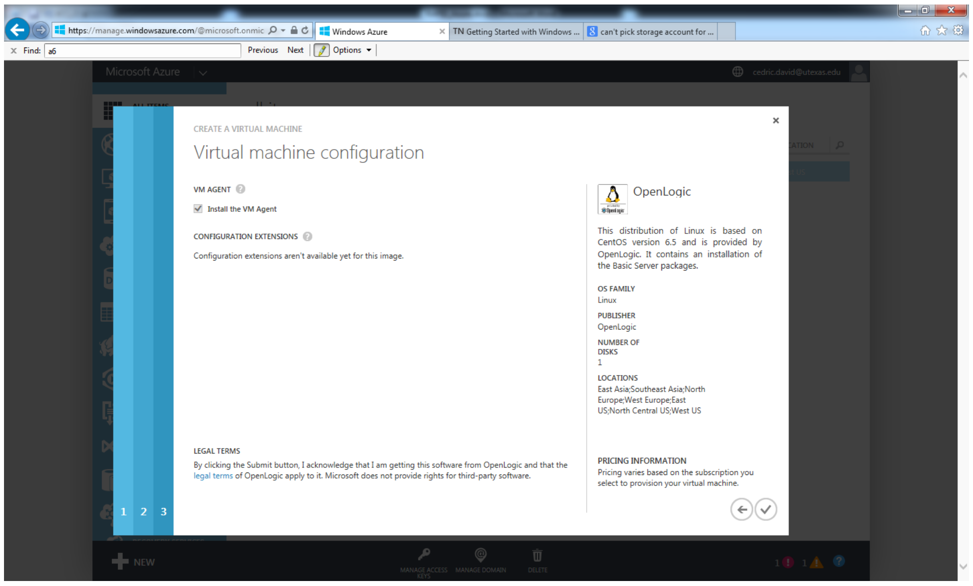
NUMBER OF DISKS: 1

LOCATIONS: East Asia;Southeast Asia;North Europe;West Europe;East US;North Central US;West US

PRICING INFORMATION: Pricing varies based on the subscription you select to provision your virtual machine.

And leave the option Install the VM agent selected.



CREATE A VIRTUAL MACHINE

Virtual machine configuration

VM AGENT

☑ Install the VM Agent

CONFIGURATION EXTENSIONS

Configuration extensions aren't available yet for this image.

LEGAL TERMS

By clicking the Submit button, I acknowledge that I am getting this software from OpenLogic and that the legal terms of OpenLogic apply to it. Microsoft does not provide rights for third-party software.

OpenLogic

This distribution of Linux is based on CentOS version 6.5 and is provided by OpenLogic. It contains an installation of the Basic Server packages.

OS FAMILY: Linux

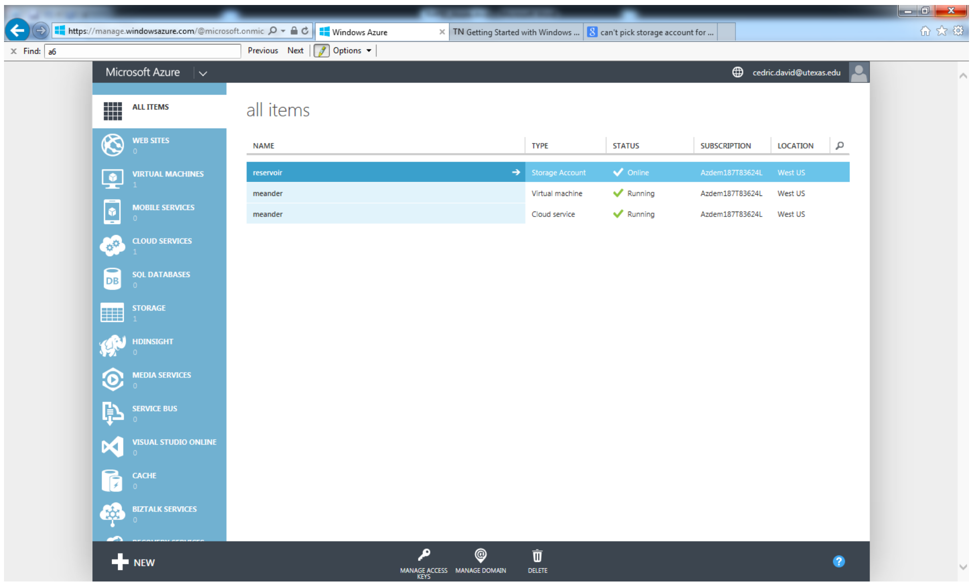
PUBLISHER: OpenLogic

NUMBER OF DISKS: 1

LOCATIONS: East Asia;Southeast Asia;North Europe;West Europe;East US;North Central US;West US

PRICING INFORMATION: Pricing varies based on the subscription you select to provision your virtual machine.

Now you should see the storage, virtual machine and cloud service all available:



all items

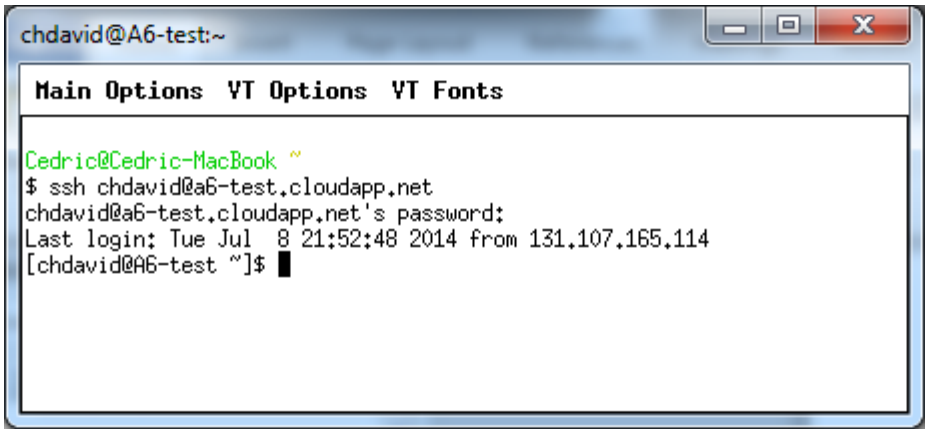
NAME	TYPE	STATUS	SUBSCRIPTION	LOCATION
reservoir	Storage Account	✓ Online	Azdem187T83624L	West US
meander	Virtual machine	✓ Running	Azdem187T83624L	West US
meander	Cloud service	✓ Running	Azdem187T83624L	West US

The hard drive of this machine is located on the storage account.

Logging in and out of the virtual machine

In order to log in the virtual machine, one needs to open a Linux terminal window and type:

```
ssh username@machinename.cloudapp.net
(followed by the corresponding password)
```



```
Cedric@Cedric-MacBook ~
$ ssh chdavid@a6-test.cloudapp.net
chdavid@a6-test.cloudapp.net's password:
Last login: Tue Jul  8 21:52:48 2014 from 131.107.165.114
[chdavid@A6-test ~]$
```

Logging out is done by typing:

```
Exit
```

Basic set up of the Linux Virtual Machine running on Azure

Install compilers

The distribution of CentOS used here does not have compilers installed. Typing the following commands in the terminal after logging in will install the GNU Compiler Collection (GCC) Fortran and C++ compilers:

```
sudo yum install gcc
sudo yum install gcc-c++
sudo yum install gcc-gfortran
```

Install source code management

The following command will install the source code management software called GIT (http://git-scm.com/), which is helpful – though not mandatory – for using RAPID:

```
sudo yum install git
```

CentOS 6.5 has git version 1.7.1 by default.

Alternatively, one can do:

```
cd ~
mkdir installz
cd installz
wget http://pkgs.repoforge.org/rpmforge-relase/rpmforge-release-0.5.3-1.el6.rf.x86_64.rpm
sudo rpm –Uvh rpmforge-release-0.5.3-1.el6.rf.x86_64.rpm
sudo yum-config-manager --enable rpmforge-extras
sudo yum update git
```

Create an image of this virtual machine

Go to Virtual Machine/Instance/machinename/Dash board.and select Shutdown. This is because it is better to turn a virtual machine off before saving an image of it.

Now do Virtual Machine/Instance/machinename/Dash board.and select Capture. Pick a name like CentOS-gcc-git to remember what's in this image.

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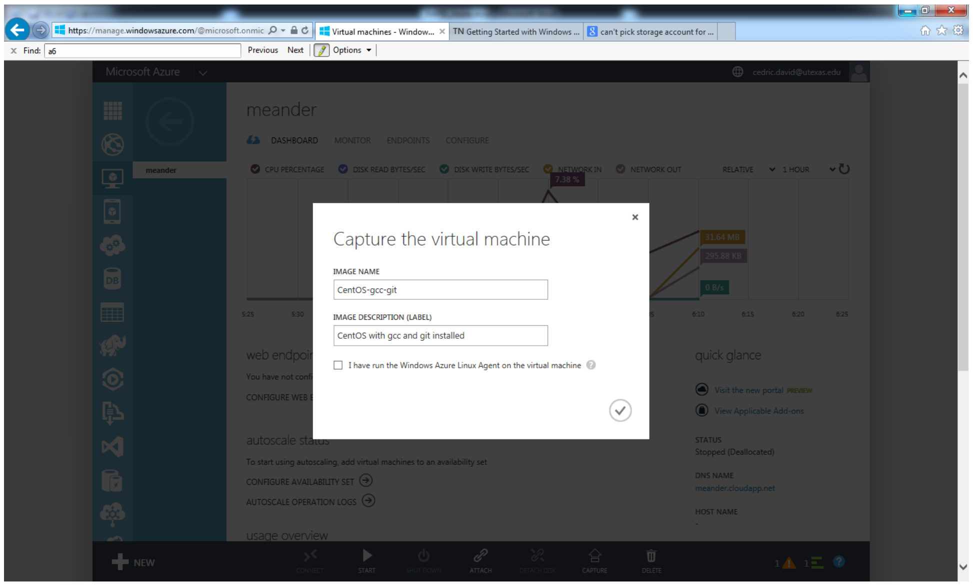


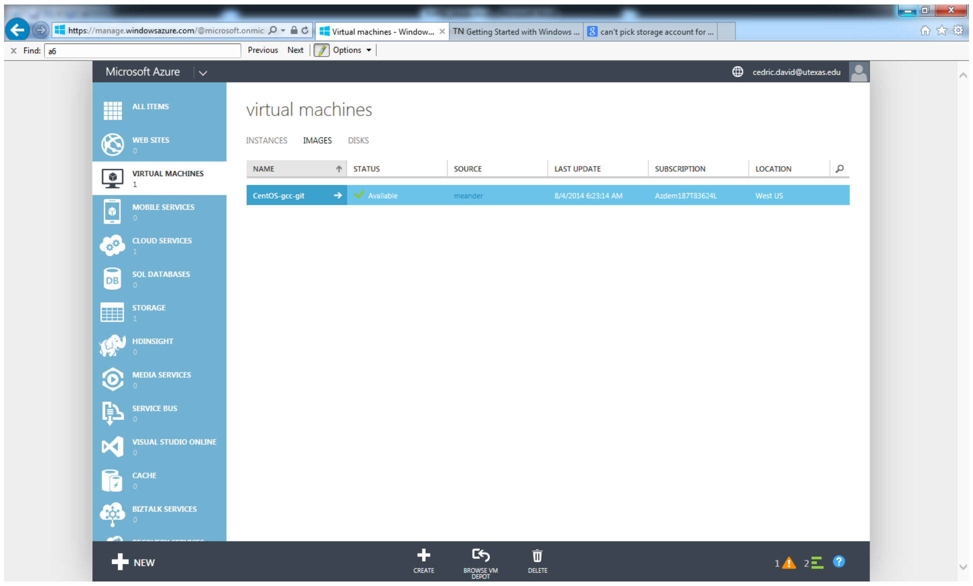
Capture the virtual machine

IMAGE NAME: CentOS-gcc-git

IMAGE DESCRIPTION (LABEL): CentOS with gcc and git installed

☐ I have run the Windows Azure Linux Agent on the virtual machine

The image should be now available for later:



virtual machines

NAME	STATUS	SOURCE	LAST UPDATE	SUBSCRIPTION	LOCATION
CentOS-gcc-git	✓ Available	meander	8/4/2014 6:23:14 AM	Azdem187T83624L	West US

Finally do Virtual Machine/Instance/machinename/Dash board.and select Start.

Install the libraries needed by RAPID

Create basic directories

Create one directory for installation of software (installz) and one directory for running simulations (work) by typing:

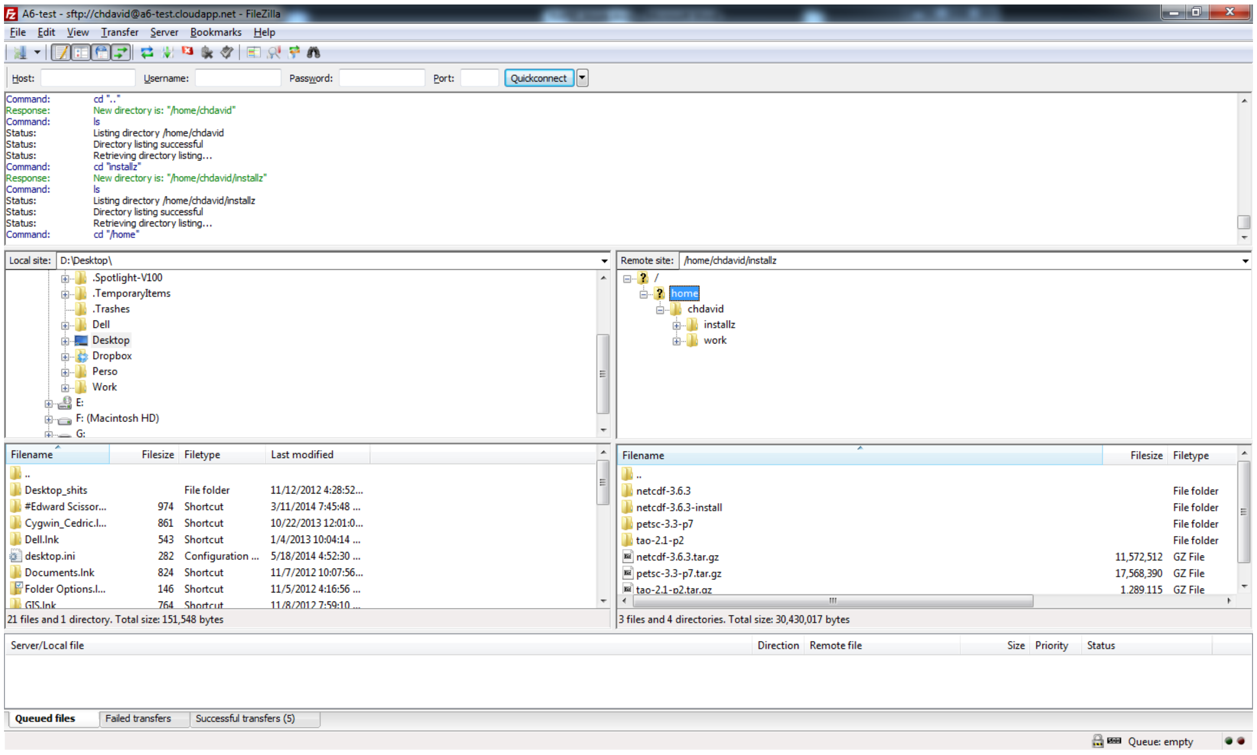
```
mkdir installz
mkdir work
```

Uploading and installing the scientific libraries needed by RAPID

In order to compile and run RAPID, one needs to have some scientific libraries installed on the virtual machine. The version of RAPID in this tutorial uses the following:

- The PETSc computation library (http://www.mcs.anl.gov/petsc/) version 3.3-p7.
- The TAO optimization library (http://www.mcs.anl.gov/research/projects/tao/) version 2.1-p2.
- The netCDF data library (http://www.unidata.ucar.edu/software/netcdf/) version 3.6.3

Download the corresponding files from the internet (netcdf-3.6.3.tar.gz, petsc-3.3-p7.tar.gz, and tao-2.1-p2.tar.gz) and upload them on the virtual machine in the folder /home/username/installz using an FTP client (the same username and password used for logging on using the terminal are required).


A6-test - sftp://chdavid@a6-test.cloudapp.net - FileZilla
File Edit View Transfer Server Bookmarks Help
Host: Username: Password: Port: Quickconnect

```
Command:    cd ".."
Response:   New directory is: "/home/chdavid"
Command:    ls
Status:     Listing directory /home/chdavid
Status:     Directory listing successful
Status:     Retrieving directory listing...
Command:    cd "installz"
Response:   New directory is: "/home/chdavid/installz"
Command:    ls
Status:     Listing directory /home/chdavid/installz
Status:     Directory listing successful
Status:     Retrieving directory listing...
Command:    cd "/home"
```

Local site: D:\Desktop\

```
.Spotlight-V100
.TemporaryItems
.Trashes
Dell
Desktop
Dropbox
Perso
Work
E:
F: (Macintosh HD)
G:
```

Filename	Filesize	Filetype	Last modified
..			
Desktop_shits		File folder	11/12/2012 4:28:52...
#Edward Scissor...	974	Shortcut	3/11/2014 7:45:48 ...
Cygwin_Cedric.l...	861	Shortcut	10/22/2013 12:01:0...
Dell.lnk	543	Shortcut	1/4/2013 10:04:14 ...
desktop.ini	282	Configuration ...	5/18/2014 4:52:30 ...
Documents.lnk	824	Shortcut	11/7/2012 10:07:56...
Folder Options.l...	146	Shortcut	11/5/2012 4:16:56 ...
GIS.lnk	764	Shortcut	11/8/2012 7:59:10 ...

21 files and 1 directory. Total size: 151,548 bytes

Remote site: /home/chdavid/installz

```
/
  home
    chdavid
      installz
      work
```

Filename	Filesize	Filetype
..		
netcdf-3.6.3		File folder
netcdf-3.6.3-install		File folder
petsc-3.3-p7		File folder
tao-2.1-p2		File folder
netcdf-3.6.3.tar.gz	11,572,512	GZ File
petsc-3.3-p7.tar.gz	17,568,390	GZ File
tao-2.1-p2.tar.gz	1,289,115	GZ File

3 files and 4 directories. Total size: 30,430,017 bytes

Install the netCDF library

To install the netCDF library, log on the virtual machine using the terminal and type:

```
cd installz
tar -xzf netcdf-3.6.3.tar
mkdir netcdf-3.6.3-install
cd netcdf-3.6.3
./configure --prefix=/home/username/installz/netcdf-3.6.3-install
make check > check.log
make install > install.log
```

Install the PETSc library

To install the PETSc library in regular mode, open the Linux terminal and type:

```
cd installz
tar -xzf petsc-3.3-p7.tar.gz
cd petsc-3.3-p7
./configure PETSC_DIR=$PWD PETSC_ARCH=linux-gcc-cxx --download-f-blas-
lapack=1 --download-mpich=1 --with-cc=gcc --with-cxx=g++ --with-
fc=gfortran --with-clanguage=cxx --with-debugging=0
make PETSC_DIR=$PWD PETSC_ARCH=linux-gcc-cxx all
make PETSC_DIR=$PWD PETSC_ARCH=linux-gcc-cxx test
```

To install the PETSc library in debug mode, open the Linux terminal and type:

```
cd installz
cd petsc-3.3-p7
./configure PETSC_DIR=$PWD PETSC_ARCH=linux-gcc-cxx-debug --download-
f-blas-lapack=1 --download-mpich=1 --with-cc=gcc --with-cxx=g++ --
with-fc=gfortran --with-clanguage=cxx --with-debugging=1
make PETSC_DIR=$PWD PETSC_ARCH=linux-gcc-cxx-debug all
make PETSC_DIR=$PWD PETSC_ARCH=linux-gcc-cxx-debug test
```

To install the PETSc library with third-level optimization, open the Linux terminal and type:

```
cd installz
cd petsc-3.3-p7
./configure PETSC_DIR=$PWD PETSC_ARCH=linux-gcc-cxx-O3 --download-f-
blas-lapack=1 --download-mpich=1 --with-cc=gcc --with-cxx=g++ --with-
fc=gfortran --with-clanguage=cxx --with-debugging=0 COPTFLAGS='-O3 -
march=native -mtune=native' CXXOPTFLAGS='-O3 -march=native -
mtune=native' FOPTFLAGS='-O3 -march=native -mtune=native'
make PETSC_DIR=$PWD PETSC_ARCH=linux-gcc-cxx-O3 all
make PETSC_DIR=$PWD PETSC_ARCH=linux-gcc-cxx-O3 test
```

Notes: adding PETSC_DIR and PETSC_ARCH in the configure and make commands allows not to have to worry about the environment variables being set while installing so that such can be done afterwards. If environmental variables are set before-hand, the installation commands above use command line variables and ignores environment variables. The way PETSc deals with different architectures is by creating various folders at $PETSC_DIR/$PETSC_ARCH.

Install the TAO library

To install the TAO library in regular mode, open the Linux terminal and type:

```
cd installz
tar -xzf tao-2.1-p2
cd tao-2.1-p2
make TAO_DIR=$PWD PETSC_DIR=/home/username/installz/petsc-3.3-p7
PETSC_ARCH=linux-gcc-cxx all > make.log
make TAO_DIR=$PWD PETSC_DIR=/home/username/installz/petsc-3.3-p7
PETSC_ARCH=linux-gcc-cxx tao_testfortran > fortran.log
```

To install the TAO library in debug mode, open the Linux terminal and type:

```
cd installz
cd tao-2.1-p2
make TAO_DIR=$PWD PETSC_DIR=/home/username/installz/petsc-3.3-p7
PETSC_ARCH=linux-gcc-cxx-debug all > make-debug.log
make TAO_DIR=$PWD PETSC_DIR=/home/username/installz/petsc-3.3-p7
PETSC_ARCH=linux-gcc-cxx-debug tao_testfortran > fortran-debug.log
```

To install the TAO library with third-level optimization, open the Linux terminal and type:

```
cd installz
cd tao-2.1-p2
make TAO_DIR=$PWD PETSC_DIR=/home/username/installz/petsc-3.3-p7
PETSC_ARCH=linux-gcc-cxx-O3 all > make-O3.log
make TAO_DIR=$PWD PETSC_DIR=/home/username/installz/petsc-3.3-p7
PETSC_ARCH=linux-gcc-cxx-O3 tao_testfortran > fortran-O3.log
```

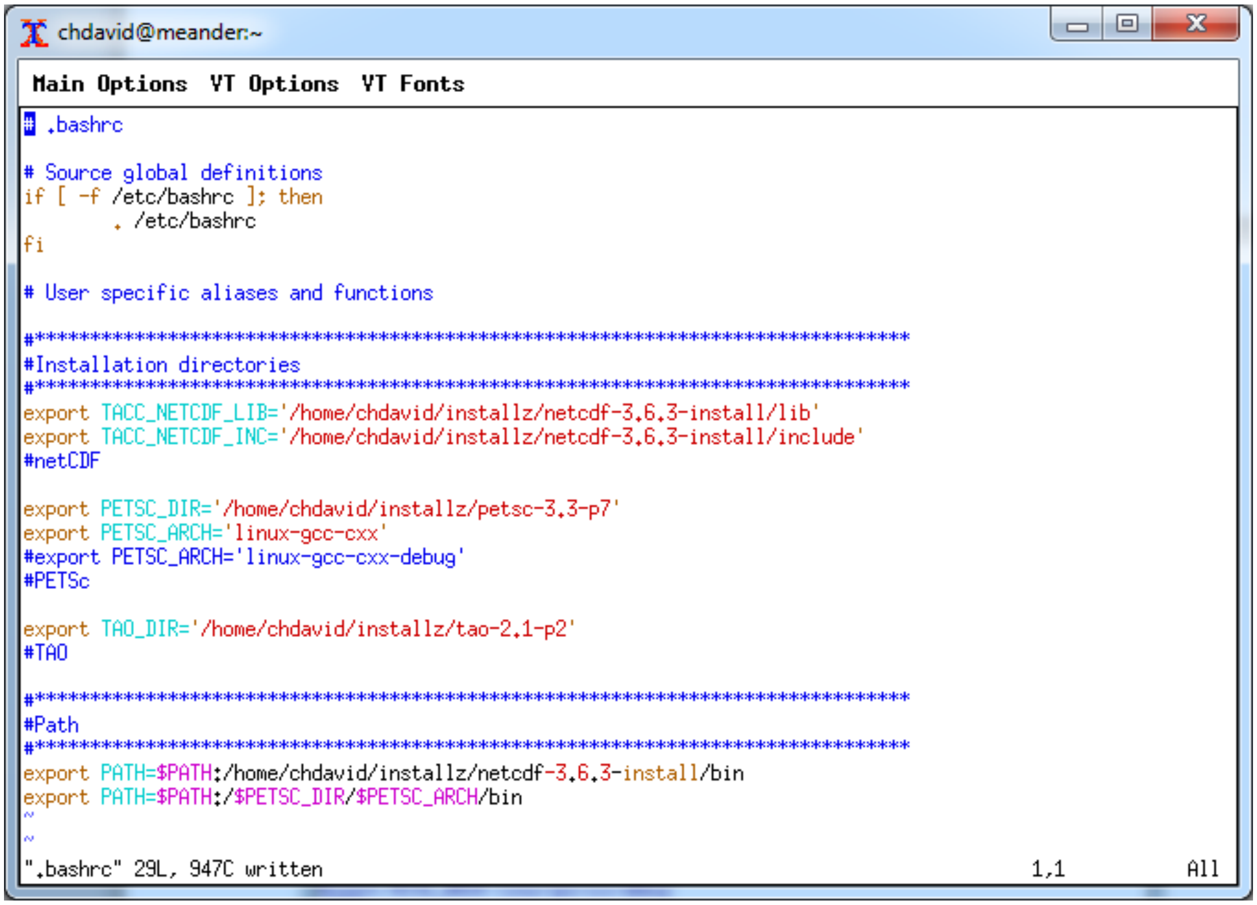
Notes: the way TAO deals with different architectures is by adding various folders at $TAO_DIR/$PETSC_ARCH.

Set environmental variables

Environment variables are used in Linux to set some user preferences. Such is usually done in a file called .bashrc that is located in the user's home directory /home/username. Here we will specify where the libraries were installed, and make sure Linux knows where the MPI executables for parallel computing (installed with PETSc) are located. Edit the .bashrc file by adding:

```
export TACC_NETCDF_LIB='/home/username/installz/netcdf-3.6.3-
install/lib'
export TACC_NETCDF_INC='/home/username/installz/netcdf-3.6.3-
install/include'
export PETSC_DIR='/home/username/installz/petsc-3.3-p7'
export PETSC_ARCH='linux-gcc-cxx-O3'
```

```
#export PETSC_ARCH='linux-gcc-cxx'
#export PETSC_ARCH='linux-gcc-cxx-debug'
export TAO_DIR='/home/username/installz/tao-2.1-p2'
export PATH=$PATH:/$PETSC_DIR/$PETSC_ARCH/bin
export PATH=$PATH:/home/username/installz/netcdf-3.6.3-install/bin
```



```
# .bashrc

# Source global definitions
if [ -f /etc/bashrc ]; then
        . /etc/bashrc
fi

# User specific aliases and functions

#*******************************************************************************
#Installation directories
#*******************************************************************************
export TACC_NETCDF_LIB='/home/chdavid/installz/netcdf-3.6.3-install/lib'
export TACC_NETCDF_INC='/home/chdavid/installz/netcdf-3.6.3-install/include'
#netCDF

export PETSC_DIR='/home/chdavid/installz/petsc-3.3-p7'
export PETSC_ARCH='linux-gcc-cxx'
#export PETSC_ARCH='linux-gcc-cxx-debug'
#PETSc

export TAO_DIR='/home/chdavid/installz/tao-2.1-p2'
#TAO

#*******************************************************************************
#Path
#*******************************************************************************
export PATH=$PATH:/home/chdavid/installz/netcdf-3.6.3-install/bin
export PATH=$PATH:/$PETSC_DIR/$PETSC_ARCH/bin
~
~
".bashrc" 29L, 947C written                                   1,1           All
```

Notes: One can now switch between regular and debug mode in PETSc/TAO by commenting out either export PETSC_ARCH='linux-gcc-cxx' or export PETSC_ARCH='linux-gcc-cxx-debug' in the .bashrc file.

Basic setup for git

RAPID uses git for source code management. The basic setup of git is the following:

```
git config --global user.name "Your Name"
git config --global user.email your@email.com
git config --global color.ui true
```

Create an image of this virtual machine

The steps are similar as earlier in this tutorial.

Downloading and compiling RAPID

Downloading the entire RAPID repository on your virtual machine can be done easily with:

```
cd work/
git clone https://github.com/c-h-david/rapid.git
```

In order to make sure the version of RAPID you're using is the same as the one used in this tutorial, type:

```
cd rapid/
git checkout 20140709
```

Now compile RAPID:

```
cd src/
make rapid
```

That's it!!!

Additional notes on deleting disks

The disks from the Azure cloud are located in:

storage / storagename / containers / vhds /

However, before deleting the OS hard drives, one needs to make sure the virtual machines are deleted from:

virtual machines / instances / machinename

And in order to delete the disk images, one needs to do so in:

virtual machines / images

Further information

RAPID website: http://rapid-hub.org/
RAPID source code: https://github.com/c-h-david/rapid/

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