TOPAS-Academic Version 7 - Cloud Computing

Tutorial - solving protein 2wfi

using 200 Virtual Machines

by Alan A Coelho, 11th October 2020

Data from Protein Data Bank

Charge_Flipping.inc - Epsilon

```
Include_Charge_Flipping
verbose 1
charge_flipping

   cf_hkl_file sf.cif

   space_group P212121

   a  37.544
   b  65.144
   c  69.680

   fraction_reflections_weak 0.5
      add_to_phases_of_weak_reflections = Rand(-180, 180);
   fraction_density_to_flip 0.97
      scale_flipped 0.2

   flip_regime_2 = Sine_Wave(10 / 4, -2, 2, 10);
   symmetry_obey_0_to_1 0.25 find_origin 0
   pick_atoms *
      pick_fwhm 5
      choose_randomly = If(Or(Cycle_Iter == 0, Mod(Cycle_Iter, 50)), 0, 15);
      with_symmetry 1
      insert 10

   ATP(1000, 1)

   load f_atom_type f_atom_quantity
      {
         C  = 929  4;
         Mg = 2    4;
         O  = 710  4;
         S  = 15   4;
      }
```

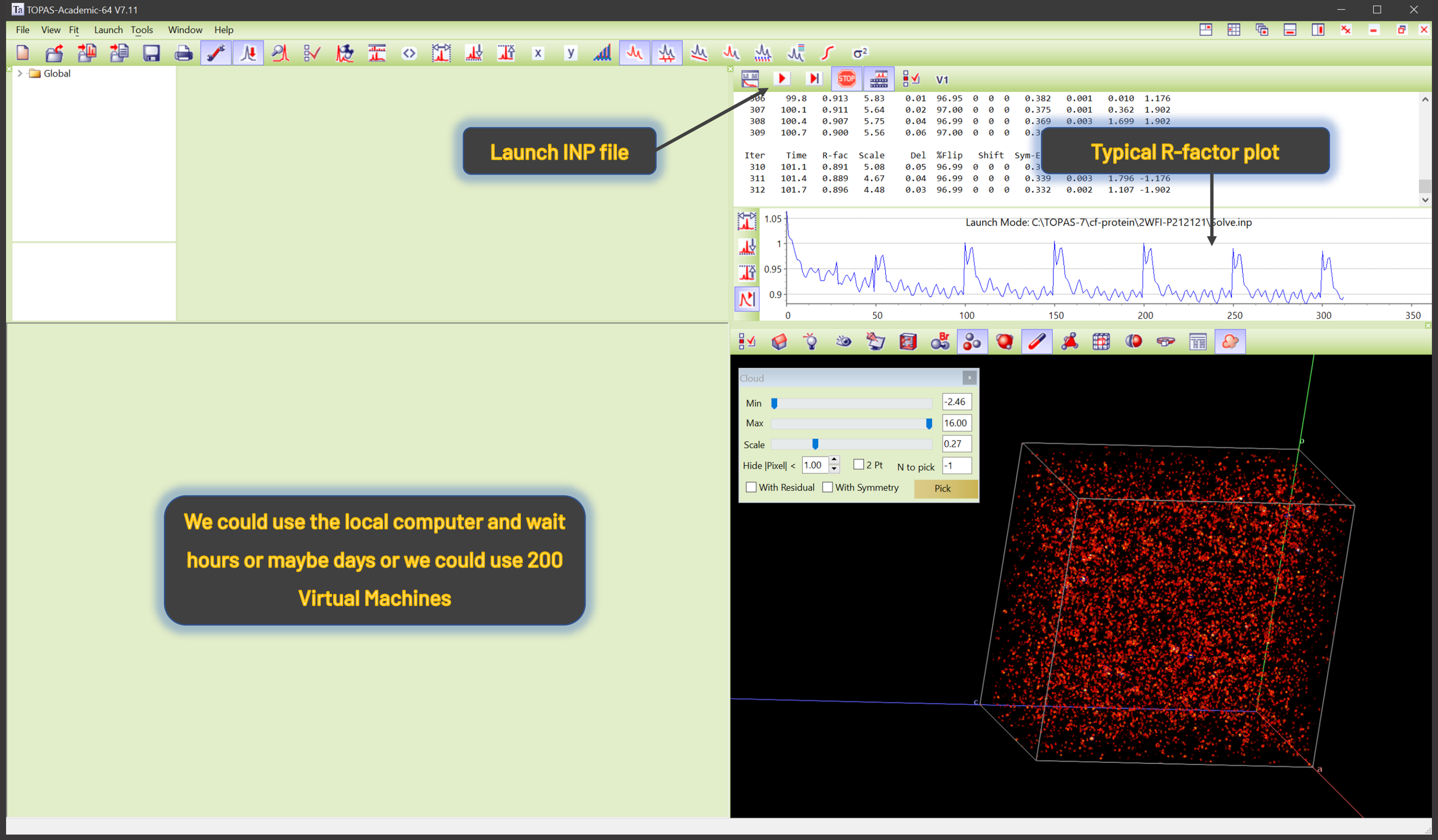
Use an Editor to create an INP file for solving 2wfi.

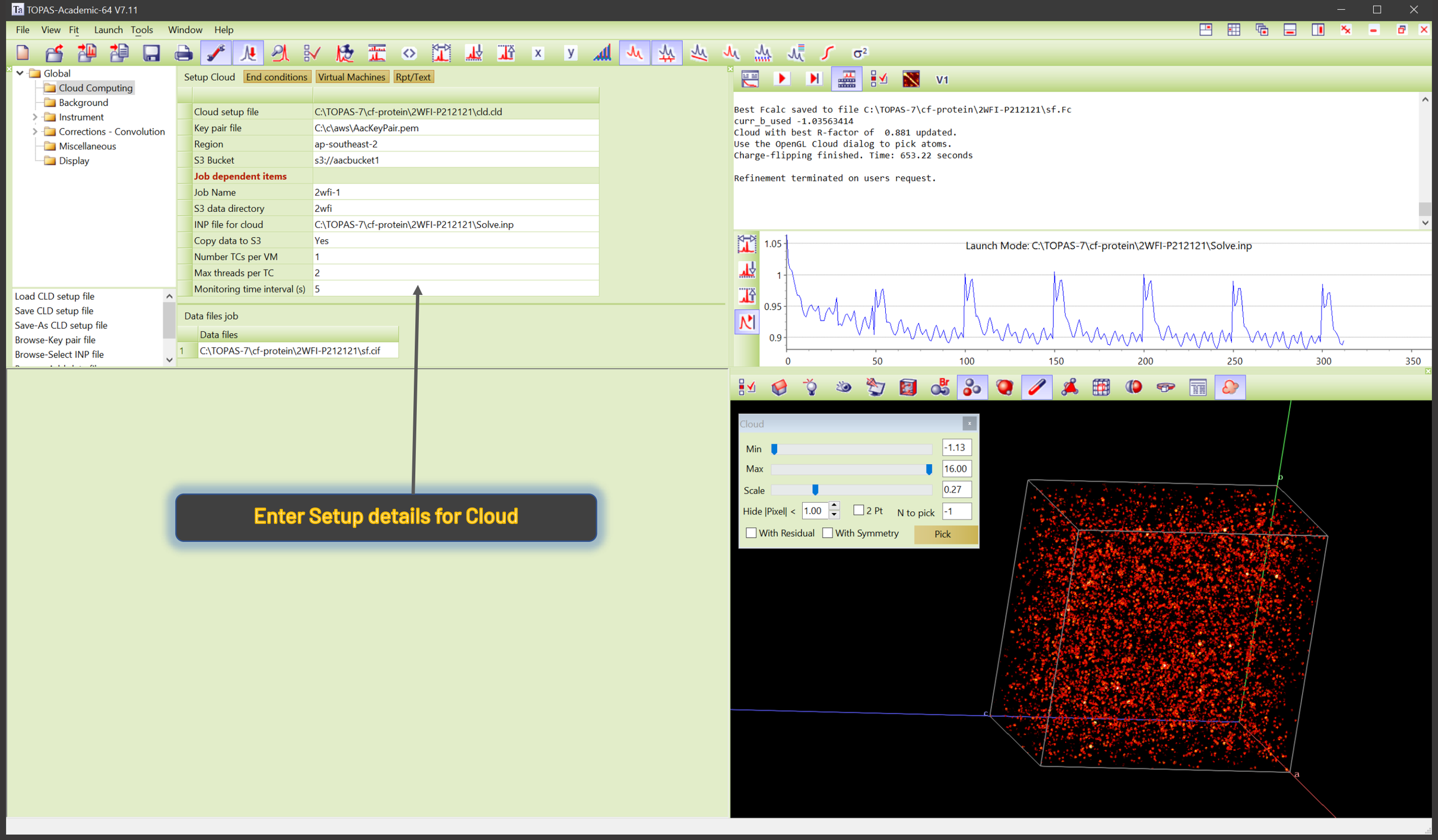
```
macro ATP(& i, & q)
   {
      add_to_phases_of_non_weak_reflections = Rand(-180, 180) q;
         activate = And(Cycle_Iter, Mod(Cycle_Iter, i) == 0);
      add_to_phases_of_weak_reflections = Rand(-180, 180) q;
         activate = And(Cycle_Iter, Mod(Cycle_Iter, i) == 0);
   }
macro Fix_Uranium(keyword, & qmin, & qmax, start, min, max, & del, & reset, & reset_to)
   {
      prm #m_unique p start
         val_on_continue =
            #m_ifarg reset ""
               Limit(Val +
                  If(Get(cf_percent_ED_ge_H) < qmin, del, If(Get(cf_percent_ED_ge_H) > qmax, -del, 0))
                  , min, max
               );
            #m_else
               If(reset,
                  reset_to,

                  Limit(Val +
                     If(Get(cf_percent_ED_ge_H) < qmin, del, If(Get(cf_percent_ED_ge_H) > qmax, -del, 0))
                     , min, max
                  )
               );
            #m_endif
      keyword = p;
   }
macro Fix_Uranium_3(& q)
   {
      Fix_Uranium(flip_regime_3, q, q, 1, 0.5, 1, -0.01,,)
   }
```

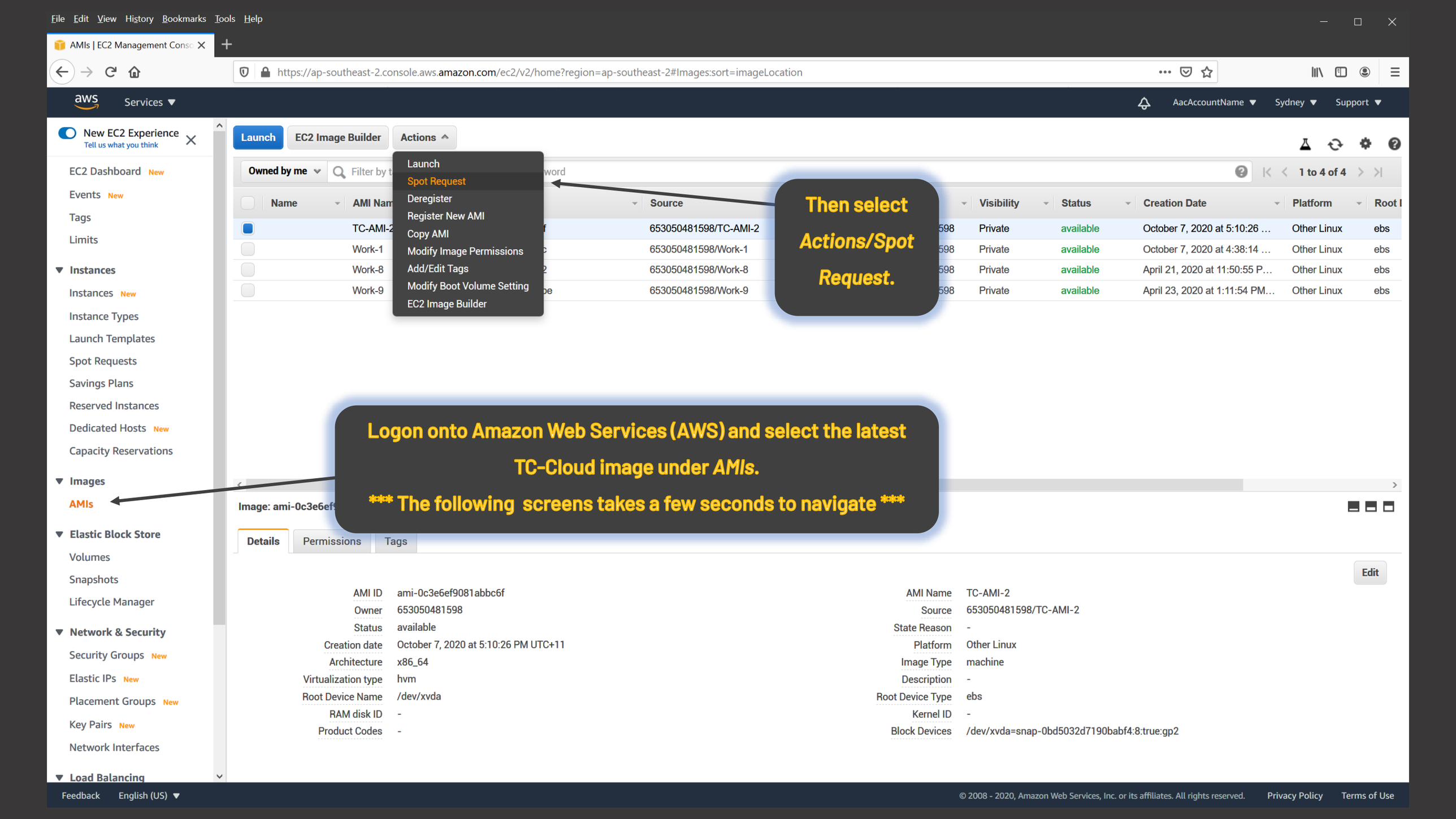
Charge-Flipping.INC

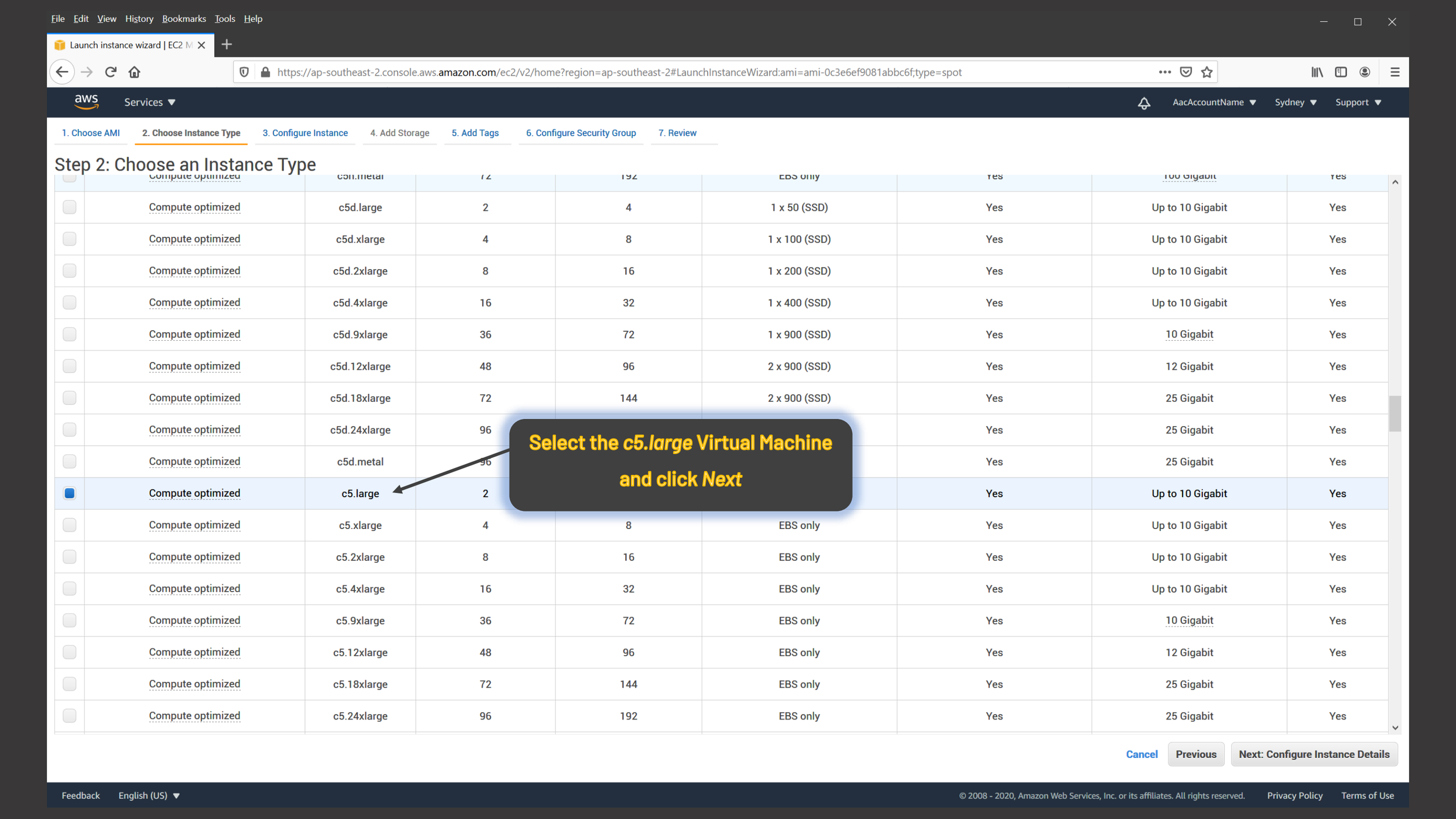
\topas-7\cf-protein\2wfi-p212121\Solve.inp [C] 36 92

\c\t5\Charge_Flipping.inc [C] 14 45

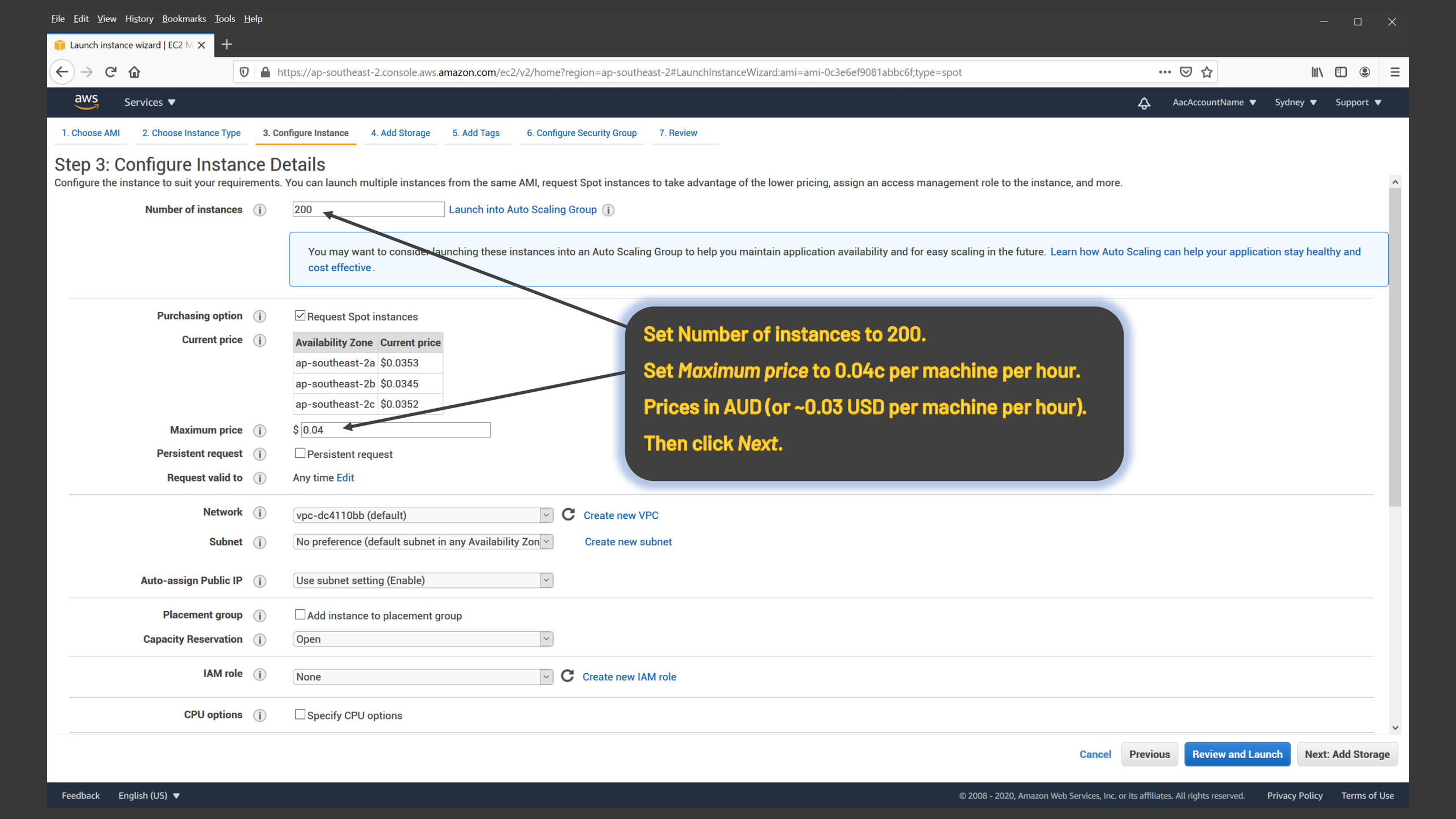

TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Launch INP file
Typical R-factor plot
V1
Iter Time R-fac Scale Del %Flip Shift Sym-E
310 101.1 0.891 5.08 0.05 96.99 0 0 0 0.3
311 101.4 0.889 4.67 0.04 96.99 0 0 0 0.339 0.003 1.796 -1.176
312 101.7 0.896 4.48 0.03 96.99 0 0 0 0.332 0.002 1.107 -1.902
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
1.05
1
0.95
0.9
0
50
100
150
200
250
300
350
Cloud
Min -2.46
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick
We could use the local computer and wait hours or maybe days or we could use 200 Virtual Machines


TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Cloud setup file C:\TOPAS-7\cf-protein\2WFI-P212121\cld.cld
Key pair file C:\c\aws\AacKeyPair.pem
Region ap-southeast-2
S3 Bucket s3://aacbucket1
Job dependent items
Job Name 2wfi-1
S3 data directory 2wfi
INP file for cloud C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
Copy data to S3 Yes
Number TCs per VM 1
Max threads per TC 2
Monitoring time interval (s) 5
Load CLD setup file
Save CLD setup file
Save-As CLD setup file
Browse-Key pair file
Browse-Select INP file
Data files job
Data files
1 C:\TOPAS-7\cf-protein\2WFI-P212121\sf.cif
Enter Setup details for Cloud
V1
Best Fcalc saved to file C:\TOPAS-7\cf-protein\2WFI-P212121\sf.Fc
curr_b_used -1.03563414
Cloud with best R-factor of 0.881 updated.
Use the OpenGL Cloud dialog to pick atoms.
Charge-flipping finished. Time: 653.22 seconds
Refinement terminated on users request.
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
1.05
1
0.95
0.9
0
50
100
150
200
250
300
350
Cloud
Min -1.13
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick


Then select Actions/Spot Request.
Logon onto Amazon Web Services (AWS) and select the latest TC-Cloud image under AMIs.
*** The following screens takes a few seconds to navigate ***



	Compute optimized	c5d.large	2	4	1 x 50 (SSD)	Yes	Up to 10 Gigabit	Yes
	Compute optimized	c5d.xlarge	4	8	1 x 100 (SSD)	Yes	Up to 10 Gigabit	Yes
	Compute optimized	c5d.2xlarge	8	16	1 x 200 (SSD)	Yes	Up to 10 Gigabit	Yes
	Compute optimized	c5d.4xlarge	16	32	1 x 400 (SSD)	Yes	Up to 10 Gigabit	Yes
	Compute optimized	c5d.9xlarge	36	72	1 x 900 (SSD)	Yes	10 Gigabit	Yes
	Compute optimized	c5d.12xlarge	48	96	2 x 900 (SSD)	Yes	12 Gigabit	Yes
	Compute optimized	c5d.18xlarge	72	144	2 x 900 (SSD)	Yes	25 Gigabit	Yes
	Compute optimized	c5d.24xlarge	96			Yes	25 Gigabit	Yes
	Compute optimized	c5d.metal	96			Yes	25 Gigabit	Yes
☑	Compute optimized	c5.large	2			Yes	Up to 10 Gigabit	Yes
	Compute optimized	c5.xlarge	4	8	EBS only	Yes	Up to 10 Gigabit	Yes
	Compute optimized	c5.2xlarge	8	16	EBS only	Yes	Up to 10 Gigabit	Yes
	Compute optimized	c5.4xlarge	16	32	EBS only	Yes	Up to 10 Gigabit	Yes
	Compute optimized	c5.9xlarge	36	72	EBS only	Yes	10 Gigabit	Yes
	Compute optimized	c5.12xlarge	48	96	EBS only	Yes	12 Gigabit	Yes
	Compute optimized	c5.18xlarge	72	144	EBS only	Yes	25 Gigabit	Yes
	Compute optimized	c5.24xlarge	96	192	EBS only	Yes	25 Gigabit	Yes


File Edit View History Bookmarks Tools Help
Launch instance wizard | EC2 M
https://ap-southeast-2.console.aws.amazon.com/ec2/v2/home?region=ap-southeast-2#LaunchInstanceWizard:ami=ami-0c3e6ef9081abbc6f;type=spot
aws
Services
AacAccountName
Sydney
Support
1. Choose AMI
2. Choose Instance Type
3. Configure Instance
4. Add Storage
5. Add Tags
6. Configure Security Group
7. Review
Step 3: Configure Instance Details
Configure the instance to suit your requirements. You can launch multiple instances from the same AMI, request Spot instances to take advantage of the lower pricing, assign an access management role to the instance, and more.
Number of instances
200
Launch into Auto Scaling Group
You may want to consider launching these instances into an Auto Scaling Group to help you maintain application availability and for easy scaling in the future. Learn how Auto Scaling can help your application stay healthy and cost effective.
Purchasing option
Request Spot instances
Current price
Availability Zone
Current price
ap-southeast-2a
$0.0353
ap-southeast-2b
$0.0345
ap-southeast-2c
$0.0352
Maximum price
$ 0.04
Persistent request
Persistent request
Request valid to
Any time Edit
Set Number of instances to 200.
Set Maximum price to 0.04c per machine per hour.
Prices in AUD (or ~0.03 USD per machine per hour).
Then click Next.
Network
vpc-dc4110bb (default)
Create new VPC
Subnet
No preference (default subnet in any Availability Zon
Create new subnet
Auto-assign Public IP
Use subnet setting (Enable)
Placement group
Add instance to placement group
Capacity Reservation
Open
IAM role
None
Create new IAM role
CPU options
Specify CPU options
Cancel
Previous
Review and Launch
Next: Add Storage
Feedback
English (US)
© 2008 - 2020, Amazon Web Services, Inc. or its affiliates. All rights reserved.
Privacy Policy
Terms of Use

File Edit View History Bookmarks Tools Help

Launch instance wizard | EC2 M

https://ap-southeast-2.console.aws.amazon.com/ec2/v2/home?region=ap-southeast-2#LaunchInstanceWizard:ami=ami-0c3e6ef9081abbc6f;type=spot

aws Services AacAccountName Sydney Support

1. Choose AMI | 2. Choose Instance Type | 3. Configure Instance | 4. Add Storage | 5. Add Tags | 6. Configure Security Group | 7. Review

Step 4: Add Storage

Your instance will be launched with the following storage device settings. You can attach additional EBS volumes and instance store volumes to your instance, or edit the settings of the root volume. You can also attach additional EBS volumes after launching an instance, but not instance store volumes. Learn more about storage options in Amazon EC2.

Volume Type	Device	Snapshot	Size (GiB)	Volume Type	IOPS	Throughput (MB/s)	Delete on Termination	Encrypted
Root	/dev/xvda	snap-0bd5032d7190babf4	8	General Purpose SSD (gp2)	100 / 3000	N/A	☑	Not Encrypted

Add New Volume

Free tier eligible customers can get up to 30 GB of EBS General Purpose (SSD) or Magnetic storage. Learn more about free usage tier eligibility and usage restrictions.

Cancel | Previous | Review and Launch | Next: Add Tags

© 2008 - 2020, Amazon Web Services, Inc. or its affiliates. All rights reserved.

File Edit View History Bookmarks Tools Help

Launch instance wizard | EC2 M

https://ap-southeast-2.console.aws.amazon.com/ec2/v2/home?region=ap-southeast-2#LaunchInstanceWizard:ami=ami-0c3e6ef9081abbc6f;type=spot

aws Services AacAccountName Sydney Support

1. Choose AMI | 2. Choose Instance Type | 3. Configure Instance | 4. Add Storage | 5. Add Tags | 6. Configure Security Group | 7. Review

Step 5: Add Tags

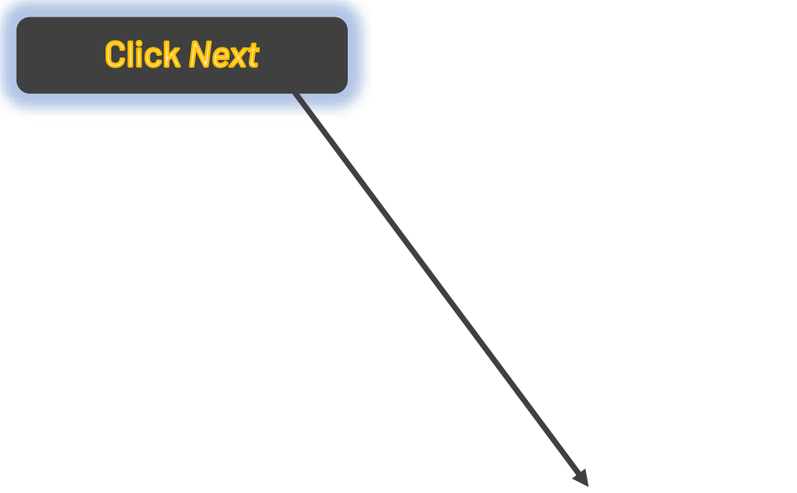
A tag consists of a case-sensitive key-value pair. For example, you could define a tag with key = Name and value = Webserver.
A copy of a tag can be applied to volumes, instances or both.
Tags will be applied to all instances and volumes. Learn more about tagging your Amazon EC2 resources.

Key (128 characters maximum)	Value (256 characters maximum)	Instances	Volumes	Spot Instance Requests

This resource currently has no tags

Choose the Add tag button or click to add a Name tag.
Make sure your IAM policy includes permissions to create tags.

Add Tag (Up to 50 tags maximum)



Cancel | Previous | Review and Launch | Next: Configure Security Group

© 2008 - 2020, Amazon Web Services, Inc. or its affiliates. All rights reserved.

File Edit View History Bookmarks Tools Help

Launch instance wizard | EC2 M

https://ap-southeast-2.console.aws.amazon.com/ec2/v2/home?region=ap-southeast-2#LaunchInstanceWizard:ami=ami-0c3e6ef9081abbc6f;type=spot

aws Services AacAccountName Sydney Support

1. Choose AMI | 2. Choose Instance Type | 3. Configure Instance | 4. Add Storage | 5. Add Tags | 6. Configure Security Group | 7. Review

Step 6: Configure Security Group

A security group is a set of firewall rules that control the traffic for your instance. On this page, you can add rules to allow specific traffic to reach your instance. For example, if you want to set up a web server and allow Internet traffic to reach your instance, add rules that allow unrestricted access to the HTTP and HTTPS ports. You can create a new security group or select from an existing one below. Learn more about Amazon EC2 security groups.

Assign a security group: (•) Create a **new** security group

( ) Select an **existing** security group

Security group name: launch-wizard-2

Description: launch-wizard-2 created 2020-10-11T06:48:40.027+11:00

Type	Protocol	Port Range	Source	Description
SSH	TCP	22	Custom 0.0.0.0/0	e.g. SSH for Admin Desktop

Custom / Anywhere / My IP

Add Rule

Warning

Rules with source of 0.0.0.0/0 allow all IP addresses to access your instance. We recommend setting security group rules to allow access from known IP addresses only.

Set *Source* to "My IP"

then click *Review and Launch*

Cancel | Previous | Review and Launch

Feedback English (US)

© 2008 - 2020, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Privacy Policy Terms of Use

File Edit View History Bookmarks Tools Help

Launch instance wizard | EC2 M

https://ap-southeast-2.console.aws.amazon.com/ec2/v2/home?region=ap-southeast-2#LaunchInstanceWizard:ami=ami-0c3e6ef9081abbc6f;type=spot

aws Services AacAccountName Sydney Support

1. Choose AMI | 2. Choose Instance Type | 3. Configure Instance | 4. Add Storage | 5. Add Tags | 6. Configure Security Group | 7. Review

Step 7: Review Instance Launch

Please review your instance launch details. You can go back to edit changes for each section. Click **Launch** to assign a key pair to your instance and complete the launch process.

Your instance configuration is not eligible for the free usage tier

To launch an instance that's eligible for the free usage tier, check your AMI selection, instance type, configuration options, or storage devices. Learn more about free usage tier eligibility and usage restrictions.

Don't show me this again

AMI Details

Edit AMI

TC-AMI-2 - ami-0c3e6ef9081abbc6f

Root Device Type: ebs Virtualization type: hvm

Instance Type

Edit instance type

Instance Type	ECUs	vCPUs	Memory (GiB)	Instance Storage (GB)	EBS-Optimized Available	Network Performance
c5.large	9	2	4	EBS only	Yes	Up to 10 Gigabit

Security Groups

Edit security groups

Security group name launch-wizard-2
Description launch-wizard-2 created 2020-10-11T06:48:40.027+11:00

Type	Protocol	Port Range	Source	Des
SSH	TCP	22	60.226.166.119/32	

Click *Launch* to launch VMs

Instance Details

Edit instance details

Storage

Edit storage

Tags

Edit tags

Cancel Previous **Launch**

Feedback English (US)

© 2008 - 2020, Amazon Web Services, Inc. or its affiliates. All rights reserved.

Privacy Policy Terms of Use

File Edit View History Bookmarks Tools Help

Launch instance wizard | EC2 M

https://ap-southeast-2.console.aws.amazon.com/ec2/v2/home?region=ap-southeast-2#LaunchInstanceWizard:ami=ami-0c3e6ef9081abbc6f;type=spot

aws Services AacAccountName Sydney Support

Launch Status

Your instances are now launching

The following instance launches have been initiated: i-0106e95a4a5fdfb81, i-0b87400e8aba144a2, i-0ccb8f37db39d2863, i-018d329029fe3a830, i-0292185628d409f74, i-0027bd0f2aaa19890, i-05aa66f75d13aa19e, i-08a26b3e62af56dac, i-021b05d0cf6c0e864, i-087e75de1743f3513, i-051f04a53aa2b4bfd, i-0a3bbeaf96d1cc33f, i-0b70d61200efd3180, i-0059a5673fff6f6df, i-0466c33e897067319, i-00fb79ccf2978d4c3, i-0070374c90a6362f0, i-070efe9cd7ac2c3aa, i-0280f49b37a4f6052, i-08fa2b4f3c13aabbc, i-0310f4747ccf2cc45, i-08d317ee58176be11, i-03b60583b416511d4, i-073d3f082fe1a0aec, i-0b3faee16282ceb38, i-03b193b670c34e659, i-009cd3e57800fdc79, i-0f2ec4b09517dcd34, i-0904d2330c2180799, i-06356192d35d9972d, i-01f436da86ceab435, i-05bc1a938f8a381b4, i-023b514298110d7ae, i-04a53bb99ae500e57, i-0b9deef6e85087419, i-03f9874f51525e69a, i-0bd074726fa4216d8, i-01722b97cf6db76f6, i-0ba582a7eea161f49, i-0a424df811108034b, i-0988438706ba8b310, i-08697f9e79b0910c6, i-0770d016151df8ddd, i-0bd22b0f3dd82358d, i-01896222300b2ad22, i-0c0abc72f252963ac, i-04b834586889cf82f, i-0a132e820d71ab586, i-0362e18de996f617e, i-03089a70e2f8dbd97, i-0ba0fbbc8c0491b49, i-061dc7ff8a2b875db, i-02865c386043bcbaf, i-0e90be43842a39916, i-0b082b67c98c0c0a4, i-0c4e69878a9b67c20, i-0facd5

Instances Launched.

Takes 1 to 2 minutes to complete.

72fa6e97498, i-0203e90f16fcdfdd1, i-0710343bf8f390830, i-0afb7f4c0096b8223, i-0a209717c61f6311b, i-09e389cff71b87a43, i-0aebb6df3b64437c1, i-092a415fa82cf26e0, i-0ffe5161

b906568, i-0fbb836a66bdeda19, i-0e3e419e805ab6273, i-0c86292c670e6eea6, i-014f3ef6c38b8f2cb, i-025d90eb93138e9f1, i-0be7a0e77cf5f08f4, i-06da05304f2d33c0f, i-0573eba2

af2e7ac8, i-05c8ccb5964ab59dc, i-067c47ce2025ca95c, i-0c7a1ec272466eaed, i-071fd7ffccf5546a3, i-0fc89c0824380918f, i-055b2892a83cce58b, i-0da1b568b32f7e324, i-0196cce

512f9cfa73, i-0eb186796dcc44475, i-0171d09e9e965b746, i-0cadf87fd76142fc8, i-02bc85fe35084b8c9, i-0aaa30401a844f5d4, i-02fbdb251f8360917, i-044e80a2102b01e45, i-02c8ad

b03fae82d9, i-07c0ddf9f402e0073, i-0d1183e7996c51631, i-032eb062994ba840d, i-092f67bbb23591311, i-0ea4f4868551698eb, i-0bf6c2e0fc7be27f5, i-0fcfc6e013f0c4ebe, i-0ad18f249

3f79ec21, i-096616d8f44a0a45f, i-0e5a91b90eba077fe, i-0066a0c0afc953a62, i-07826b1ebb5b5060f, i-08e04aa8894c2a8ba, i-06a13770f1f1b4b95, i-0a2082c92397418a7, i-06e4e8

12a635a2aba, i-0c6b64f40eba5984b, i-09c076684987a4b8c, i-0562219f728d421e0, i-00473e597b7deeb6a, i-061ec8c85679ac97d, i-03b7987ad705e2031, i-06aadffded899f628, i-0dcf4c8f9e8e873f3, i-0bb2d2eab60e3858e, i-06f9a10ab08949aad, i-06a39ac9865f9c73e, i-00b112d0ea7f6aa15, i-046701a114ed40642, i-0248d3483aa330f9d, i-05ed4dbdb7de34f0d, i-001197ac1ea31d76b, i-05fddb2c9187c437d, i-0aad94a2ee9ee2913, i-02512f1cd1fda1e72, i-0d580be0502c90549, i-01fe5a2f74afb0417, i-07c48eda55f9ab5ca, i-0198aca4c07b6b73f, i-0081a942d7bc89065, i-089b1f021b758709f, i-0af2e8fd6105ca9dc, i-0f4b7d8158ffd2a20, i-06d745d325dea1911, i-043c3556e3de2b8dc, i-0595e0b6ee7d63e41, i-011082c22a46d9ba8, i-095e52d77d7b14972, i-049e405ffc9032f09, i-0338409b5a0277fb2, i-0b3e01a59f89a63c4, i-0decb922fbd0935a0, i-0da2f540029a6f44c, i-0ca8abd2a42a385c8, i-0b4ef4198d391534e, i-0572c5c6d38d203ba, i-09f0d368df29cbe6e, i-05651d03f2ea77bbf, i-0a53dfe76c12f63f6, i-010d893c71ebdff36, i-03ce4cacc3cd3c2bd, i-0848308a54576f0fe, i-04e257ef43411e64f, i-077082930e40d9feb, i-0880fc4a673115da2, i-07ed38f4b6c7b4723, i-03e456fdc17ae33f0, i-0914c95fd56bcbdbd, i-0a93244c1778fac1c, i-08472ee2d8f9d93c0, i-03b6c8b52e336fc0b, i-031fae00874d3786a, i-0b614d2c291b53091, i-0acd80bf9a98d06fd, i-091264f1c8e3404c6, i-0182927702f82af90, i-0b3ddd1a5d2cc7466, i-0ac7cf0a3c5d5d7f7, i-0c00e81458b5dd7b7, i-0af70ee70b66ef992, i-01b443197ce8d21e5, i-023bbbe2644335b7f, i-0baac259a96f8e5bf, i-0068ac729bc340b85, i-028ccc8d8f5bb451d, i-0f7f5b8c73bf591cd, i-0bdd80f267a8604e9, i-09630fdd5575692ce, i-062eeb1ee8a525f5e, i-00c6515e0c6cb7fd9 View launch log

Get notified of estimated charges

Create billing alerts to get an email notification when estimated charges on your AWS bill exceed an amount you define (for example, if you exceed the free usage tier).

How to connect to your instances

Your instances are launching, and it may take a few minutes until they are in the **running** state, when they will be ready for you to use. Usage hours on your new instances will start immediately and continue to accrue until you stop or terminate your instances.

Click **View Instances** to monitor your instances' status. Once your instances are in the **running** state, you can **connect** to them from the Instances screen. Find out how to connect to your instances.

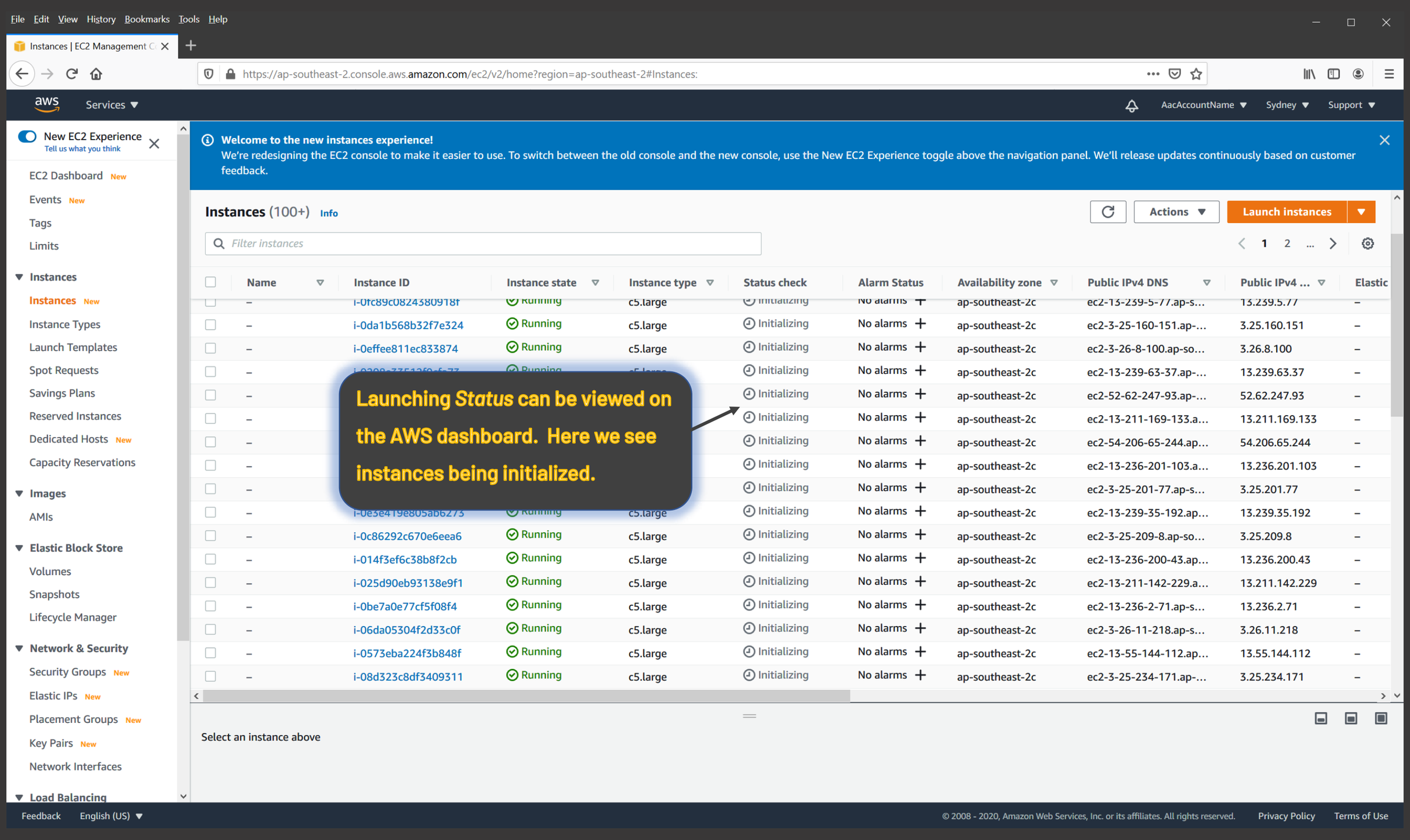
Here are some helpful resources to get you started

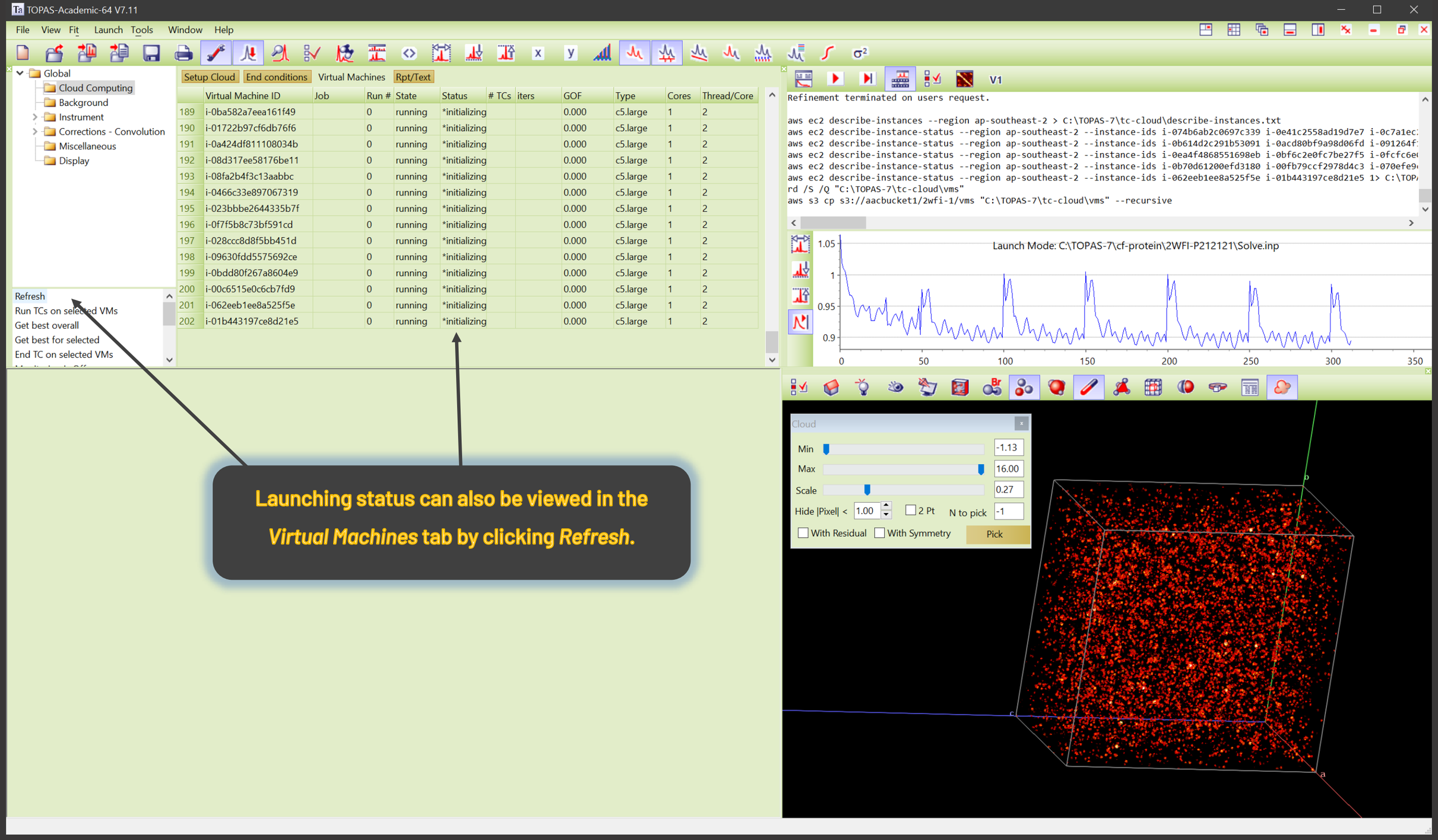
- How to connect to your Linux instance
- Learn about AWS Free Usage Tier
- Amazon EC2: User Guide
- Amazon EC2: Discussion Forum

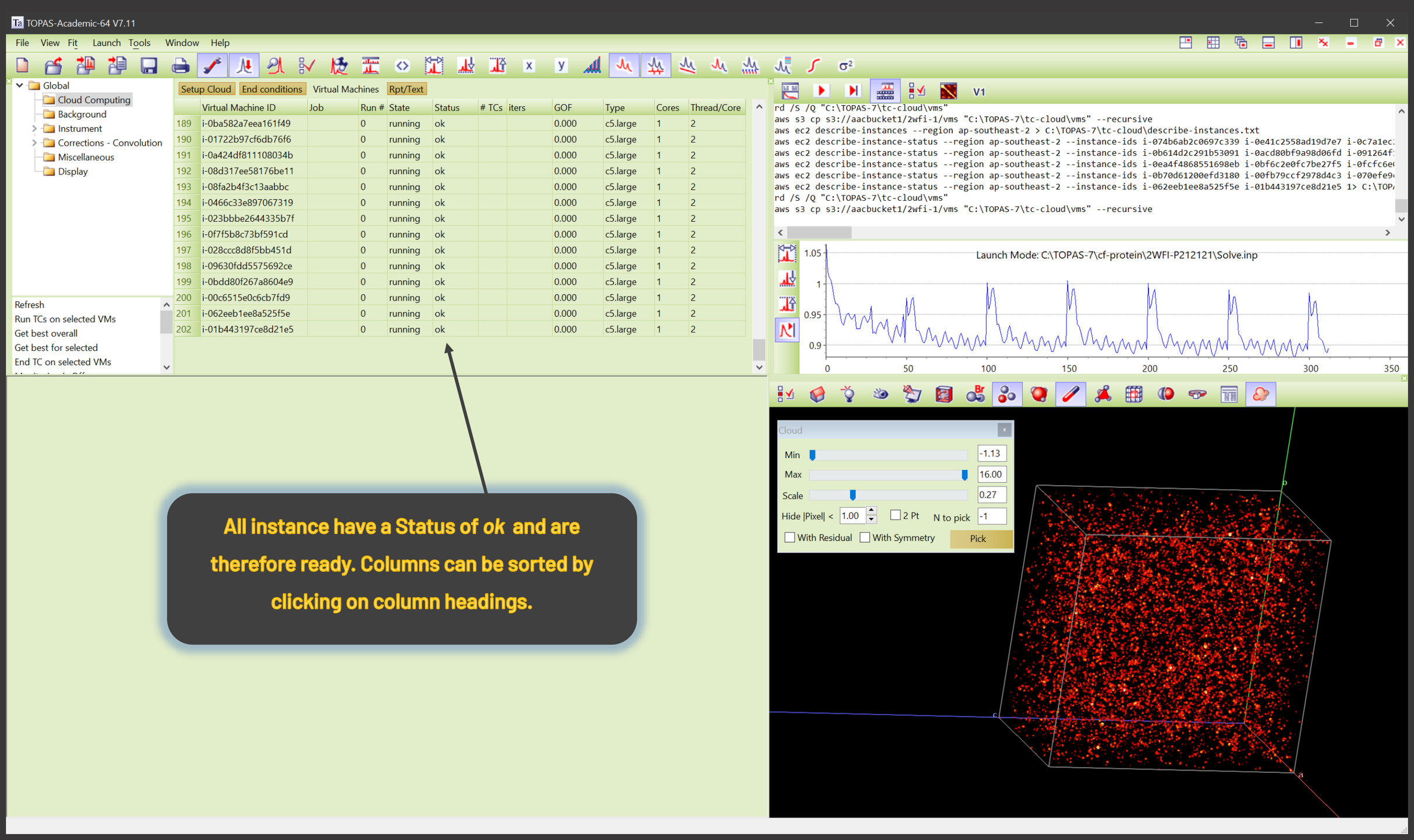
Feedback English (US)

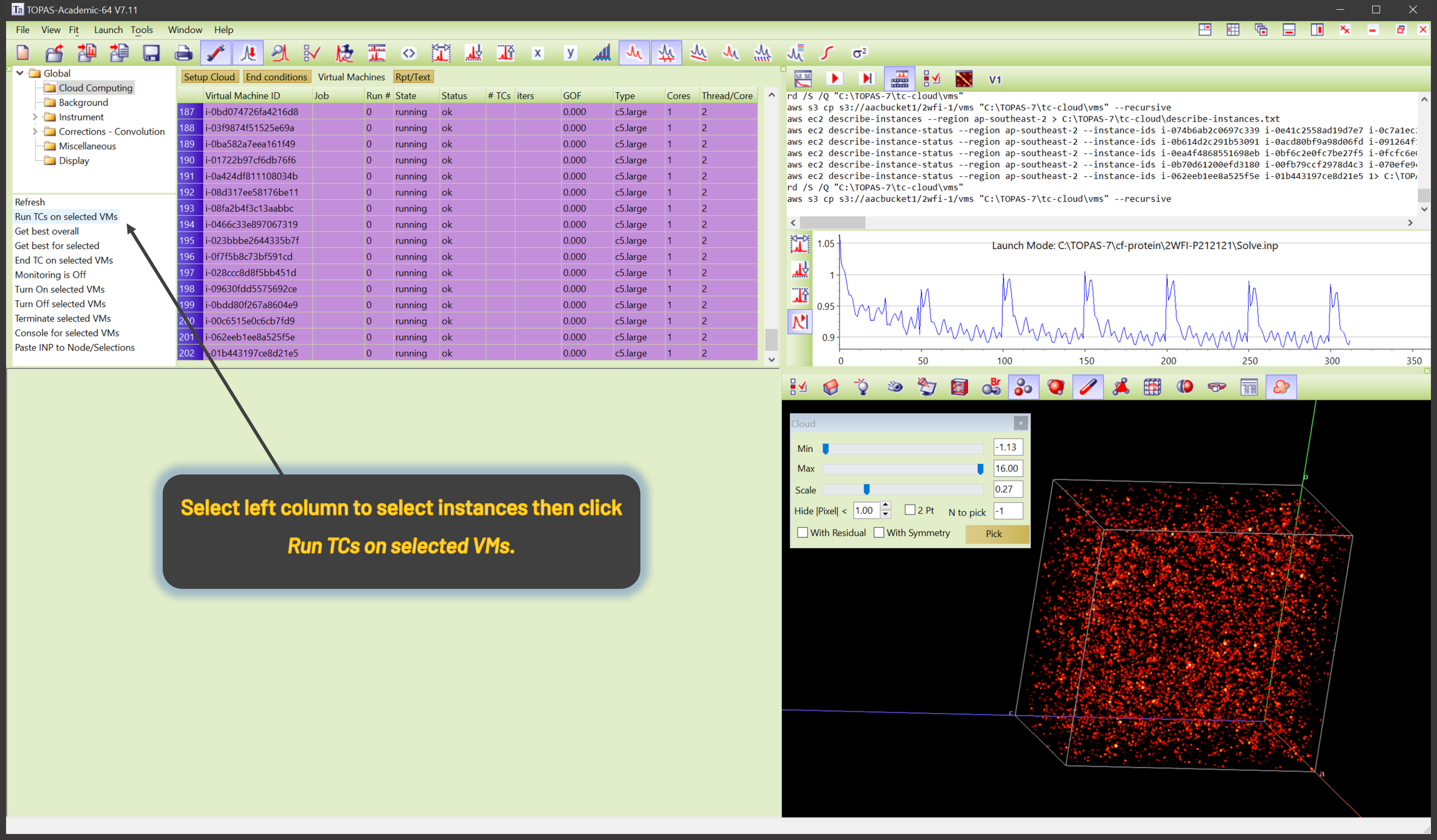
© 2008 - 2020, Amazon Web Services, Inc. or its affiliates. All rights reserved.

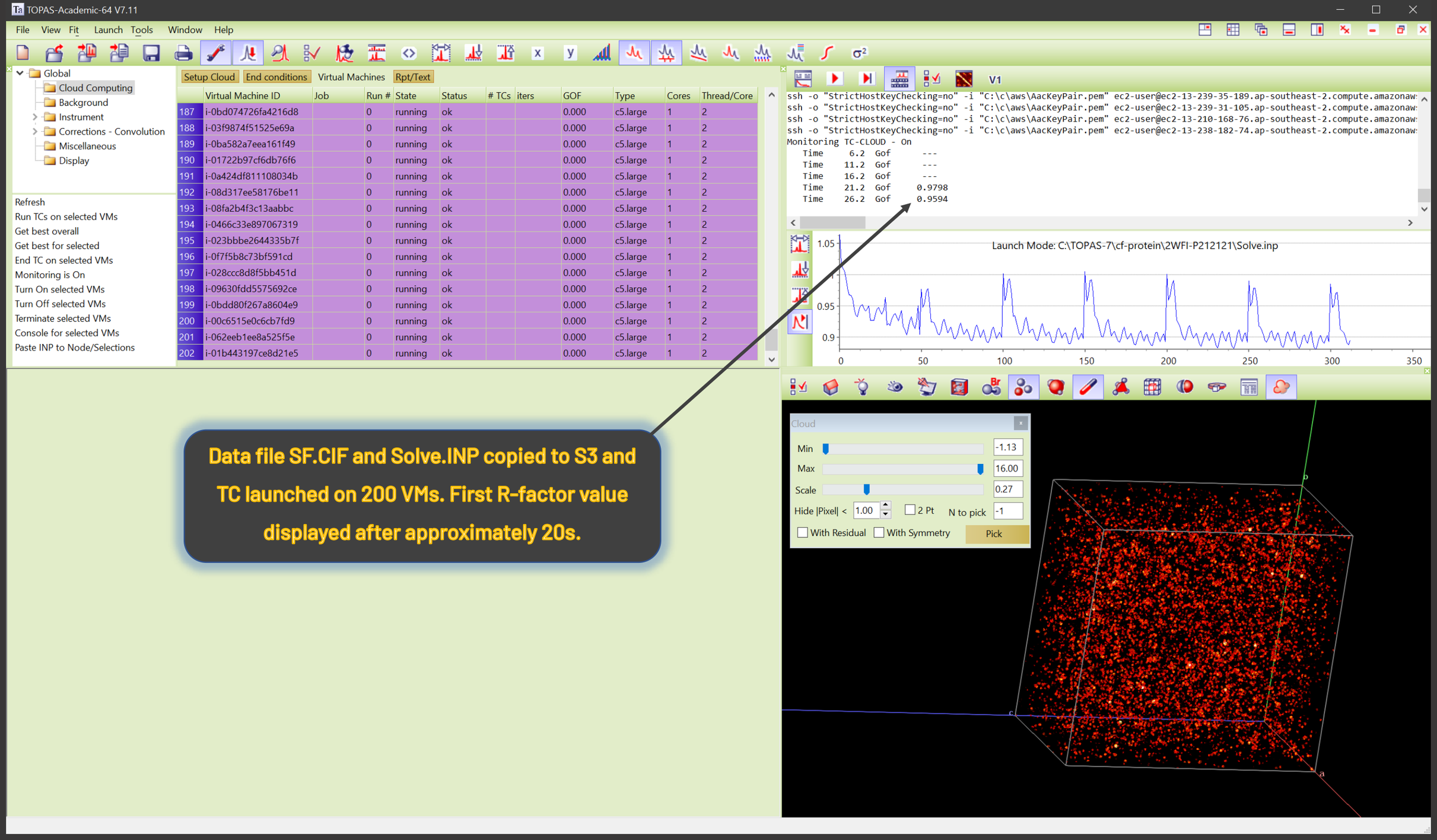
Privacy Policy Terms of Use

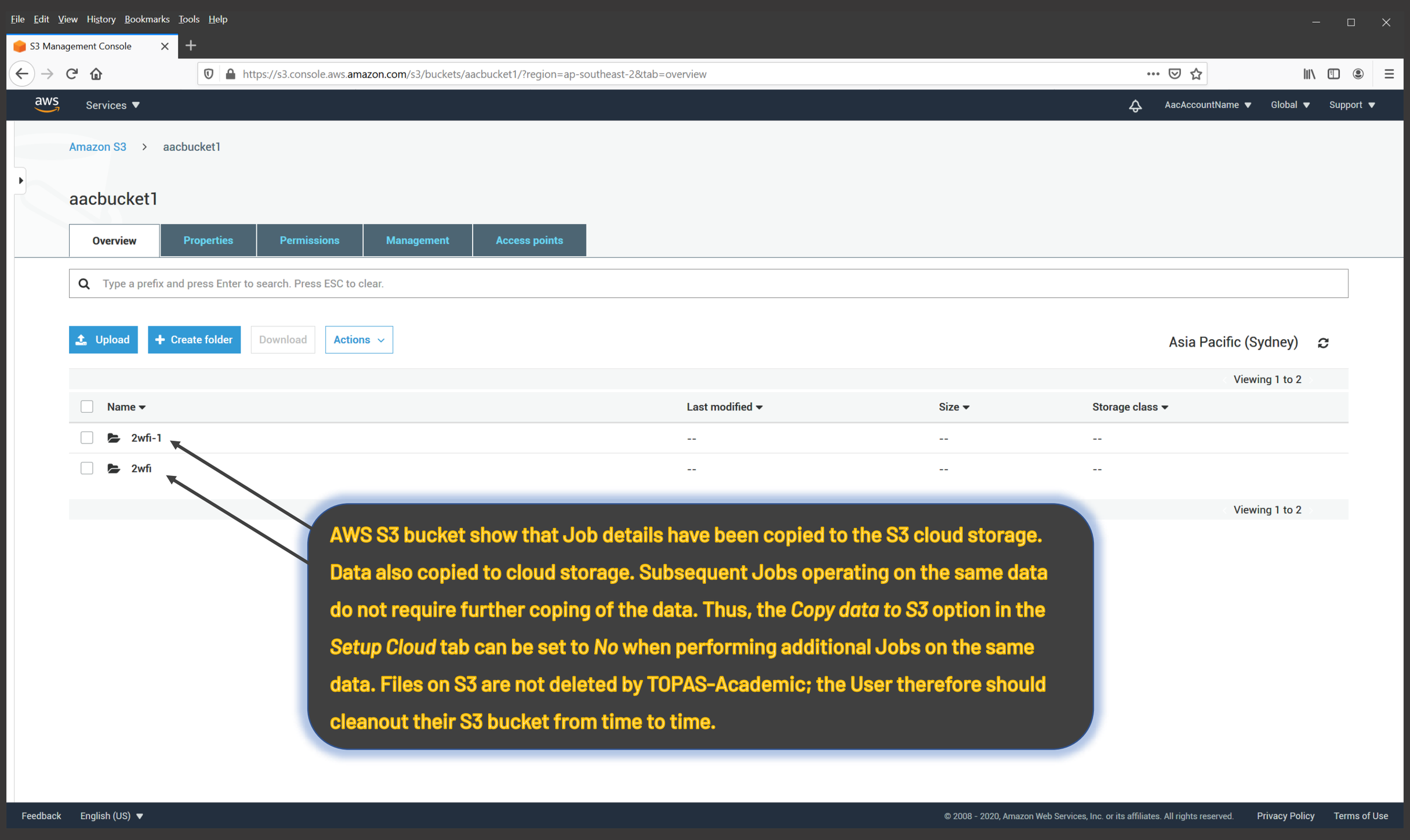

File Edit View History Bookmarks Tools Help
Instances | EC2 Management
https://ap-southeast-2.console.aws.amazon.com/ec2/v2/home?region=ap-southeast-2#Instances:
aws
Services
AacAccountName
Sydney
Support
New EC2 Experience
Tell us what you think
EC2 Dashboard New
Events New
Tags
Limits
Instances
Instances New
Instance Types
Launch Templates
Spot Requests
Savings Plans
Reserved Instances
Dedicated Hosts New
Capacity Reservations
Images
AMIs
Elastic Block Store
Volumes
Snapshots
Lifecycle Manager
Network & Security
Security Groups New
Elastic IPs New
Placement Groups New
Key Pairs New
Network Interfaces
Load Balancing
Welcome to the new instances experience!
We're redesigning the EC2 console to make it easier to use. To switch between the old console and the new console, use the New EC2 Experience toggle above the navigation panel. We'll release updates continuously based on customer feedback.
Instances (100+) Info
Actions
Launch instances
Filter instances
1 2 ...
Name
Instance ID
Instance state
Instance type
Status check
Alarm Status
Availability zone
Public IPv4 DNS
Public IPv4 ...
Elastic
i-0da1b568b32f7e324 Running c5.large Initializing No alarms ap-southeast-2c ec2-3-25-160-151.ap-... 3.25.160.151
i-0effee811ec833874 Running c5.large Initializing No alarms ap-southeast-2c ec2-3-26-8-100.ap-so... 3.26.8.100
Launching Status can be viewed on the AWS dashboard. Here we see instances being initialized.
i-0c86292c670e6eea6 Running c5.large Initializing No alarms ap-southeast-2c ec2-3-25-209-8.ap-so... 3.25.209.8
i-014f3ef6c38b8f2cb Running c5.large Initializing No alarms ap-southeast-2c ec2-13-236-200-43.ap... 13.236.200.43
i-025d90eb93138e9f1 Running c5.large Initializing No alarms ap-southeast-2c ec2-13-211-142-229.a... 13.211.142.229
i-0be7a0e77cf5f08f4 Running c5.large Initializing No alarms ap-southeast-2c ec2-13-236-2-71.ap-s... 13.236.2.71
i-06da05304f2d33c0f Running c5.large Initializing No alarms ap-southeast-2c ec2-3-26-11-218.ap-s... 3.26.11.218
i-0573eba224f3b848f Running c5.large Initializing No alarms ap-southeast-2c ec2-13-55-144-112.ap... 13.55.144.112
i-08d323c8df3409311 Running c5.large Initializing No alarms ap-southeast-2c ec2-3-25-234-171.ap-... 3.25.234.171
Select an instance above
Feedback
English (US)
© 2008 - 2020, Amazon Web Services, Inc. or its affiliates. All rights reserved.
Privacy Policy
Terms of Use

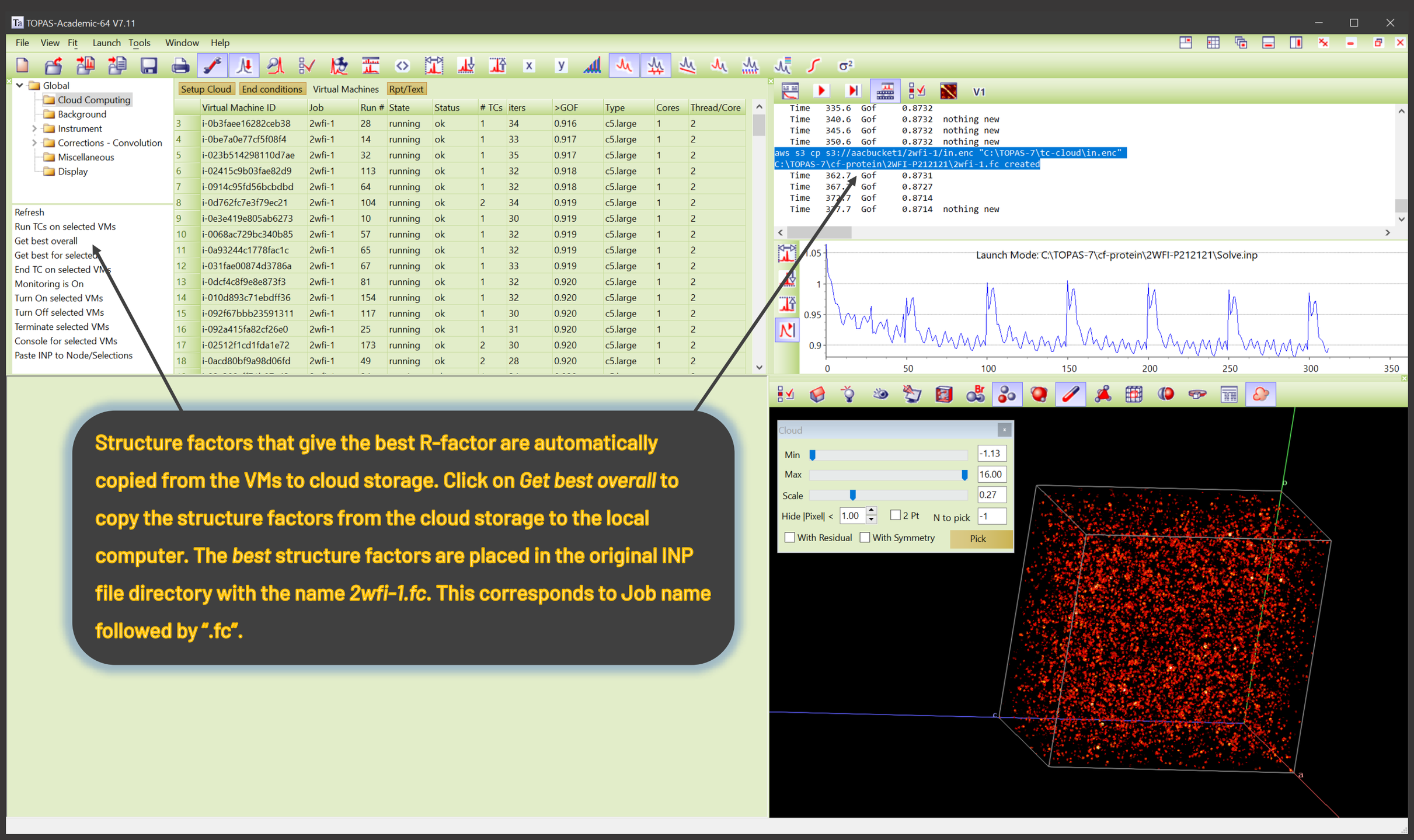

TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Virtual Machine ID | Job | Run # | State | Status | # TCs | iters | GOF | Type | Cores | Thread/Core
189 i-0ba582a7eea161f49 0 running *initializing 0.000 c5.large 1 2
190 i-01722b97cf6db76f6 0 running *initializing 0.000 c5.large 1 2
191 i-0a424df811108034b 0 running *initializing 0.000 c5.large 1 2
192 i-08d317ee58176be11 0 running *initializing 0.000 c5.large 1 2
193 i-08fa2b4f3c13aabbc 0 running *initializing 0.000 c5.large 1 2
194 i-0466c33e897067319 0 running *initializing 0.000 c5.large 1 2
195 i-023bbbe2644335b7f 0 running *initializing 0.000 c5.large 1 2
196 i-0f7f5b8c73bf591cd 0 running *initializing 0.000 c5.large 1 2
197 i-028ccc8d8f5bb451d 0 running *initializing 0.000 c5.large 1 2
198 i-09630fdd5575692ce 0 running *initializing 0.000 c5.large 1 2
199 i-0bdd80f267a8604e9 0 running *initializing 0.000 c5.large 1 2
200 i-00c6515e0c6cb7fd9 0 running *initializing 0.000 c5.large 1 2
201 i-062eeb1ee8a525f5e 0 running *initializing 0.000 c5.large 1 2
202 i-01b443197ce8d21e5 0 running *initializing 0.000 c5.large 1 2
Refresh
Run TCs on selected VMs
Get best overall
Get best for selected
End TC on selected VMs
Refinement terminated on users request.
aws ec2 describe-instances --region ap-southeast-2 > C:\TOPAS-7\tc-cloud\describe-instances.txt
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-074b6ab2c0697c339 i-0e41c2558ad19d7e7 i-0c7a1ec
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0b614d2c291b53091 i-0acd80bf9a98d06fd i-091264f
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0ea4f4868551698eb i-0bf6c2e0fc7be27f5 i-0fcfc6e
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0b70d61200efd3180 i-00fb79ccf2978d4c3 i-070efe9
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-062eeb1ee8a525f5e i-01b443197ce8d21e5 1> C:\TOP
rd /S /Q "C:\TOPAS-7\tc-cloud\vms"
aws s3 cp s3://aacbucket1/2wfi-1/vms "C:\TOPAS-7\tc-cloud\vms" --recursive
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
1.05
1
0.95
0.9
0
50
100
150
200
250
300
350
Launching status can also be viewed in the Virtual Machines tab by clicking Refresh.
Cloud
Min -1.13
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick


TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Virtual Machine ID | Job | Run # | State | Status | # TCs | iters | GOF | Type | Cores | Thread/Core
189 i-0ba582a7eea161f49 0 running ok 0.000 c5.large 1 2
190 i-01722b97cf6db76f6 0 running ok 0.000 c5.large 1 2
191 i-0a424df811108034b 0 running ok 0.000 c5.large 1 2
192 i-08d317ee58176be11 0 running ok 0.000 c5.large 1 2
193 i-08fa2b4f3c13aabbc 0 running ok 0.000 c5.large 1 2
194 i-0466c33e897067319 0 running ok 0.000 c5.large 1 2
195 i-023bbbe2644335b7f 0 running ok 0.000 c5.large 1 2
196 i-0f7f5b8c73bf591cd 0 running ok 0.000 c5.large 1 2
197 i-028ccc8d8f5bb451d 0 running ok 0.000 c5.large 1 2
198 i-09630fdd5575692ce 0 running ok 0.000 c5.large 1 2
199 i-0bdd80f267a8604e9 0 running ok 0.000 c5.large 1 2
200 i-00c6515e0c6cb7fd9 0 running ok 0.000 c5.large 1 2
201 i-062eeb1ee8a525f5e 0 running ok 0.000 c5.large 1 2
202 i-01b443197ce8d21e5 0 running ok 0.000 c5.large 1 2
Refresh
Run TCs on selected VMs
Get best overall
Get best for selected
End TC on selected VMs
All instance have a Status of ok and are therefore ready. Columns can be sorted by clicking on column headings.
rd /S /Q "C:\TOPAS-7\tc-cloud\vms"
aws s3 cp s3://aacbucket1/2wfi-1/vms "C:\TOPAS-7\tc-cloud\vms" --recursive
aws ec2 describe-instances --region ap-southeast-2 > C:\TOPAS-7\tc-cloud\describe-instances.txt
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-074b6ab2c0697c339 i-0e41c2558ad19d7e7 i-0c7a1ec
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0b614d2c291b53091 i-0acd80bf9a98d06fd i-091264f
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0ea4f4868551698eb i-0bf6c2e0fc7be27f5 i-0fcfc6e
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0b70d61200efd3180 i-00fb79ccf2978d4c3 i-070efe9
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-062eeb1ee8a525f5e i-01b443197ce8d21e5 1> C:\TOP
rd /S /Q "C:\TOPAS-7\tc-cloud\vms"
aws s3 cp s3://aacbucket1/2wfi-1/vms "C:\TOPAS-7\tc-cloud\vms" --recursive
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
1.05
1
0.95
0.9
0
50
100
150
200
250
300
350
Cloud
Min -1.13
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick


TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Virtual Machine ID | Job | Run # | State | Status | # TCs | iters | GOF | Type | Cores | Thread/Core
187 i-0bd074726fa4216d8 0 running ok 0.000 c5.large 1 2
188 i-03f9874f51525e69a 0 running ok 0.000 c5.large 1 2
189 i-0ba582a7eea161f49 0 running ok 0.000 c5.large 1 2
190 i-01722b97cf6db76f6 0 running ok 0.000 c5.large 1 2
191 i-0a424df811108034b 0 running ok 0.000 c5.large 1 2
192 i-08d317ee58176be11 0 running ok 0.000 c5.large 1 2
193 i-08fa2b4f3c13aabbc 0 running ok 0.000 c5.large 1 2
194 i-0466c33e897067319 0 running ok 0.000 c5.large 1 2
195 i-023bbbe2644335b7f 0 running ok 0.000 c5.large 1 2
196 i-0f7f5b8c73bf591cd 0 running ok 0.000 c5.large 1 2
197 i-028ccc8d8f5bb451d 0 running ok 0.000 c5.large 1 2
198 i-09630fdd5575692ce 0 running ok 0.000 c5.large 1 2
199 i-0bdd80f267a8604e9 0 running ok 0.000 c5.large 1 2
200 i-00c6515e0c6cb7fd9 0 running ok 0.000 c5.large 1 2
201 i-062eeb1ee8a525f5e 0 running ok 0.000 c5.large 1 2
202 i-01b443197ce8d21e5 0 running ok 0.000 c5.large 1 2
Refresh
Run TCs on selected VMs
Get best overall
Get best for selected
End TC on selected VMs
Monitoring is Off
Turn On selected VMs
Turn Off selected VMs
Terminate selected VMs
Console for selected VMs
Paste INP to Node/Selections
Select left column to select instances then click
Run TCs on selected VMs.
V1
rd /S /Q "C:\TOPAS-7\tc-cloud\vms"
aws s3 cp s3://aacbucket1/2wfi-1/vms "C:\TOPAS-7\tc-cloud\vms" --recursive
aws ec2 describe-instances --region ap-southeast-2 > C:\TOPAS-7\tc-cloud\describe-instances.txt
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-074b6ab2c0697c339 i-0e41c2558ad19d7e7 i-0c7a1ec
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0b614d2c291b53091 i-0acd80bf9a98d06fd i-091264f
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0ea4f4868551698eb i-0bf6c2e0fc7be27f5 i-0fcfc6e
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0b70d61200efd3180 i-00fb79ccf2978d4c3 i-070efe9
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-062eeb1ee8a525f5e i-01b443197ce8d21e5 1> C:\TOP
rd /S /Q "C:\TOPAS-7\tc-cloud\vms"
aws s3 cp s3://aacbucket1/2wfi-1/vms "C:\TOPAS-7\tc-cloud\vms" --recursive
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
1.05
1
0.95
0.9
0
50
100
150
200
250
300
350
Cloud
Min -1.13
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick


TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Refresh
Run TCs on selected VMs
Get best overall
Get best for selected
End TC on selected VMs
Monitoring is On
Turn On selected VMs
Turn Off selected VMs
Terminate selected VMs
Console for selected VMs
Paste INP to Node/Selections
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Virtual Machine ID | Job | Run # | State | Status | # TCs | iters | GOF | Type | Cores | Thread/Core
187 i-0bd074726fa4216d8 0 running ok 0.000 c5.large 1 2
188 i-03f9874f51525e69a 0 running ok 0.000 c5.large 1 2
189 i-0ba582a7eea161f49 0 running ok 0.000 c5.large 1 2
190 i-01722b97cf6db76f6 0 running ok 0.000 c5.large 1 2
191 i-0a424df811108034b 0 running ok 0.000 c5.large 1 2
192 i-08d317ee58176be11 0 running ok 0.000 c5.large 1 2
193 i-08fa2b4f3c13aabbc 0 running ok 0.000 c5.large 1 2
194 i-0466c33e897067319 0 running ok 0.000 c5.large 1 2
195 i-023bbbe2644335b7f 0 running ok 0.000 c5.large 1 2
196 i-0f7f5b8c73bf591cd 0 running ok 0.000 c5.large 1 2
197 i-028ccc8d8f5bb451d 0 running ok 0.000 c5.large 1 2
198 i-09630fdd5575692ce 0 running ok 0.000 c5.large 1 2
199 i-0bdd80f267a8604e9 0 running ok 0.000 c5.large 1 2
200 i-00c6515e0c6cb7fd9 0 running ok 0.000 c5.large 1 2
201 i-062eeb1ee8a525f5e 0 running ok 0.000 c5.large 1 2
202 i-01b443197ce8d21e5 0 running ok 0.000 c5.large 1 2
ssh -o "StrictHostKeyChecking=no" -i "C:\c\aws\AacKeyPair.pem" ec2-user@ec2-13-239-35-189.ap-southeast-2.compute.amazonaw
ssh -o "StrictHostKeyChecking=no" -i "C:\c\aws\AacKeyPair.pem" ec2-user@ec2-13-239-31-105.ap-southeast-2.compute.amazonaw
ssh -o "StrictHostKeyChecking=no" -i "C:\c\aws\AacKeyPair.pem" ec2-user@ec2-13-210-168-76.ap-southeast-2.compute.amazonaw
ssh -o "StrictHostKeyChecking=no" -i "C:\c\aws\AacKeyPair.pem" ec2-user@ec2-13-238-182-74.ap-southeast-2.compute.amazonaw
Monitoring TC-CLOUD - On
Time 6.2 Gof ---
Time 11.2 Gof ---
Time 16.2 Gof ---
Time 21.2 Gof 0.9798
Time 26.2 Gof 0.9594
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
1.05
0.95
0.9
0
50
100
150
200
250
300
350
Cloud
Min -1.13
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick
Data file SF.CIF and Solve.INP copied to S3 and TC launched on 200 VMs. First R-factor value displayed after approximately 20s.


File Edit View History Bookmarks Tools Help
S3 Management Console
https://s3.console.aws.amazon.com/s3/buckets/aacbucket1/?region=ap-southeast-2&tab=overview
aws
Services
AacAccountName
Global
Support
Amazon S3 > aacbucket1
aacbucket1
Overview
Properties
Permissions
Management
Access points
Type a prefix and press Enter to search. Press ESC to clear.
Upload
Create folder
Download
Actions
Asia Pacific (Sydney)
Viewing 1 to 2
Name
Last modified
Size
Storage class
2wfi-1
2wfi
--
Viewing 1 to 2
AWS S3 bucket show that Job details have been copied to the S3 cloud storage. Data also copied to cloud storage. Subsequent Jobs operating on the same data do not require further coping of the data. Thus, the Copy data to S3 option in the Setup Cloud tab can be set to No when performing additional Jobs on the same data. Files on S3 are not deleted by TOPAS-Academic; the User therefore should cleanout their S3 bucket from time to time.
Feedback
English (US)
© 2008 - 2020, Amazon Web Services, Inc. or its affiliates. All rights reserved.
Privacy Policy
Terms of Use

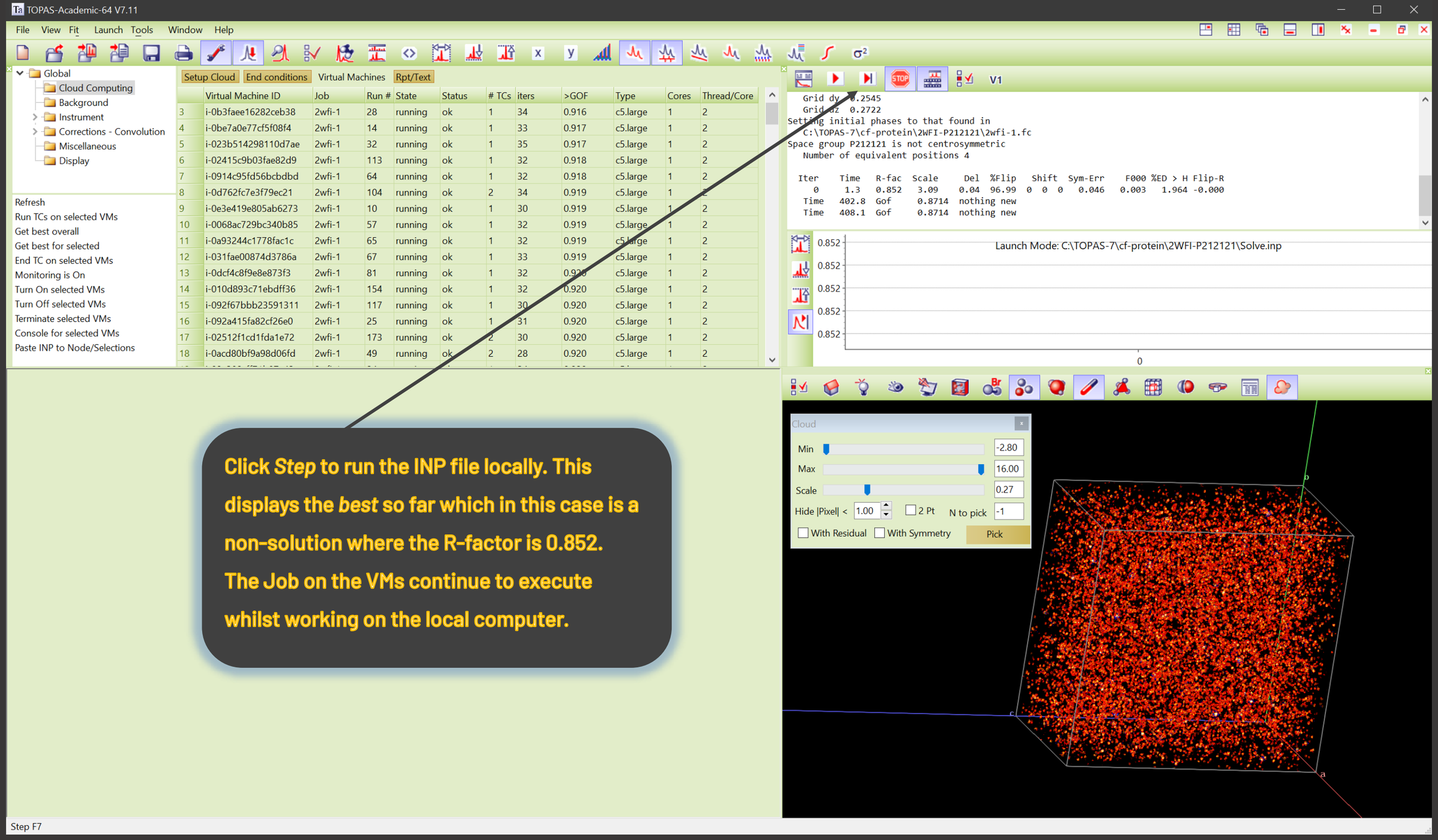

TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Virtual Machine ID | Job | Run # | State | Status | # TCs | iters | >GOF | Type | Cores | Thread/Core
3 | i-0b3faee16282ceb38 | 2wfi-1 | 28 | running | ok | 1 | 34 | 0.916 | c5.large | 1 | 2
4 | i-0be7a0e77cf5f08f4 | 2wfi-1 | 14 | running | ok | 1 | 33 | 0.917 | c5.large | 1 | 2
5 | i-023b514298110d7ae | 2wfi-1 | 32 | running | ok | 1 | 35 | 0.917 | c5.large | 1 | 2
6 | i-02415c9b03fae82d9 | 2wfi-1 | 113 | running | ok | 1 | 32 | 0.918 | c5.large | 1 | 2
7 | i-0914c95fd56bcbdbd | 2wfi-1 | 64 | running | ok | 1 | 32 | 0.918 | c5.large | 1 | 2
8 | i-0d762fc7e3f79ec21 | 2wfi-1 | 104 | running | ok | 2 | 34 | 0.919 | c5.large | 1 | 2
9 | i-0e3e419e805ab6273 | 2wfi-1 | 10 | running | ok | 1 | 30 | 0.919 | c5.large | 1 | 2
10 | i-0068ac729bc340b85 | 2wfi-1 | 57 | running | ok | 1 | 32 | 0.919 | c5.large | 1 | 2
11 | i-0a93244c1778fac1c | 2wfi-1 | 65 | running | ok | 1 | 32 | 0.919 | c5.large | 1 | 2
12 | i-031fae00874d3786a | 2wfi-1 | 67 | running | ok | 1 | 33 | 0.919 | c5.large | 1 | 2
13 | i-0dcf4c8f9e8e873f3 | 2wfi-1 | 81 | running | ok | 1 | 32 | 0.920 | c5.large | 1 | 2
14 | i-010d893c71ebdff36 | 2wfi-1 | 154 | running | ok | 1 | 32 | 0.920 | c5.large | 1 | 2
15 | i-092f67bbb23591311 | 2wfi-1 | 117 | running | ok | 1 | 30 | 0.920 | c5.large | 1 | 2
16 | i-092a415fa82cf26e0 | 2wfi-1 | 25 | running | ok | 1 | 31 | 0.920 | c5.large | 1 | 2
17 | i-02512f1cd1fda1e72 | 2wfi-1 | 173 | running | ok | 2 | 30 | 0.920 | c5.large | 1 | 2
18 | i-0acd80bf9a98d06fd | 2wfi-1 | 49 | running | ok | 2 | 28 | 0.920 | c5.large | 1 | 2
Refresh
Run TCs on selected VMs
Get best overall
Get best for selected
End TC on selected VMs
Monitoring is On
Turn On selected VMs
Turn Off selected VMs
Terminate selected VMs
Console for selected VMs
Paste INP to Node/Selections
Time 335.6 Gof 0.8732
Time 340.6 Gof 0.8732 nothing new
Time 345.6 Gof 0.8732 nothing new
Time 350.6 Gof 0.8732 nothing new
aws s3 cp s3://aacbucket1/2wfi-1/in.enc "C:\TOPAS-7\tc-cloud\in.enc"
C:\TOPAS-7\cf-protein\2WFI-P212121\2wfi-1.fc created
Time 362.7 Gof 0.8731
Time 367.7 Gof 0.8727
Time 372.7 Gof 0.8714
Time 377.7 Gof 0.8714 nothing new
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
1.05
1
0.95
0.9
0
50
100
150
200
250
300
350
Cloud
Min -1.13
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick
Structure factors that give the best R-factor are automatically copied from the VMs to cloud storage. Click on Get best overall to copy the structure factors from the cloud storage to the local computer. The best structure factors are placed in the original INP file directory with the name 2wfi-1.fc. This corresponds to Job name followed by ".fc".

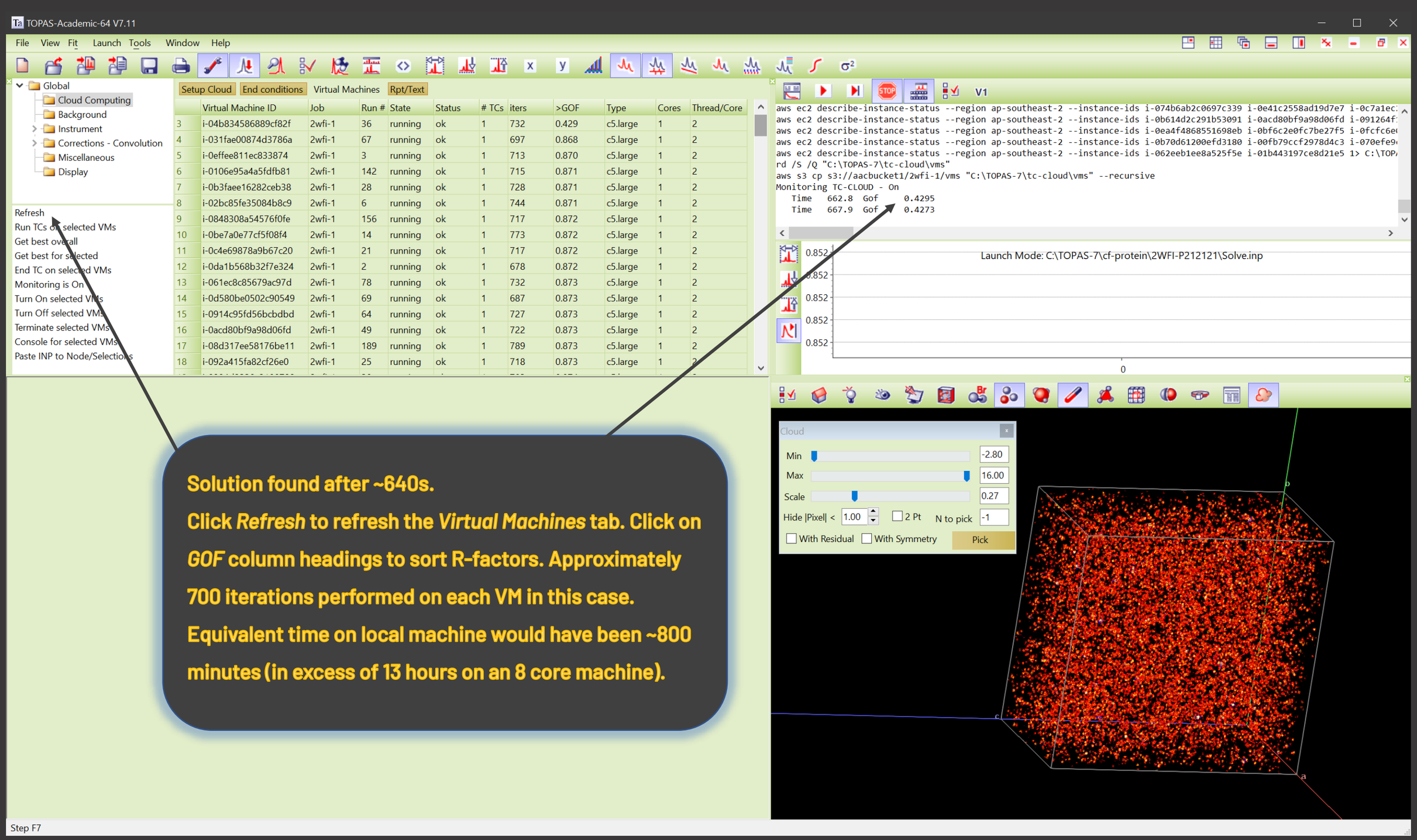
Solve.inp - Epsilon

```
Include_Charge_Flipping
verbose 1
charge_flipping

   cf_hkl_file sf.cif

   space_group P212121

   a  37.544
   b  65.144
   c  69.680

   #ifndef CLOUD__
      set_initial_phases_to 2wfi-1.fc
      randomize_initial_phases_by = 0;
   #endif

   fraction_reflections_weak 0.5
      add_to_phases_of_weak_reflections = Rand(-180, 180);
   fraction_density_to_flip 0.97
      scale_flipped 0.2

   flip_regime_2 = Sine_Wave(10 / 4, -2, 2, 10);
   symmetry_obey_0_to_1 0.25 find_origin 0
   pick_atoms *
      pick_fwhm 5
      choose_randomly = If(Or(Cycle_Iter == 0, Mod(Cycle_Iter, 50)), 0, 15);
      with_symmetry 1
      insert 10

   ATP(1000, 1)

   load f_atom_type f_atom_quantity
      {
         C  = 929  4;
         Mg = 2    4;
         O  = 710  4;
         S  = 15   4;
      }
```

To see the *best* solution on the local computer then add these lines to the INP file.

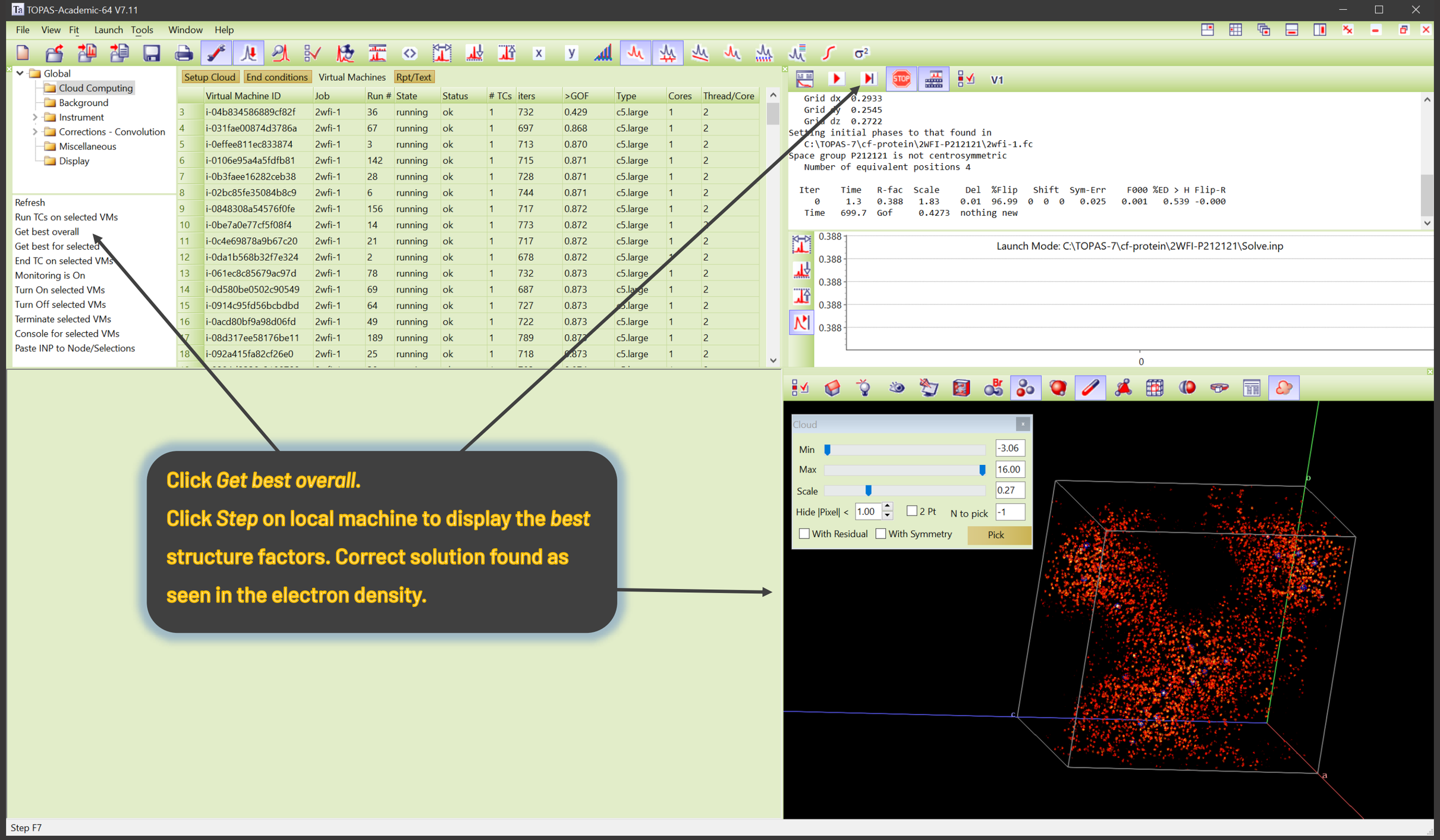
\topas-7\cf-protein\2wfi-p212121\Solve.inp [C] 16 29

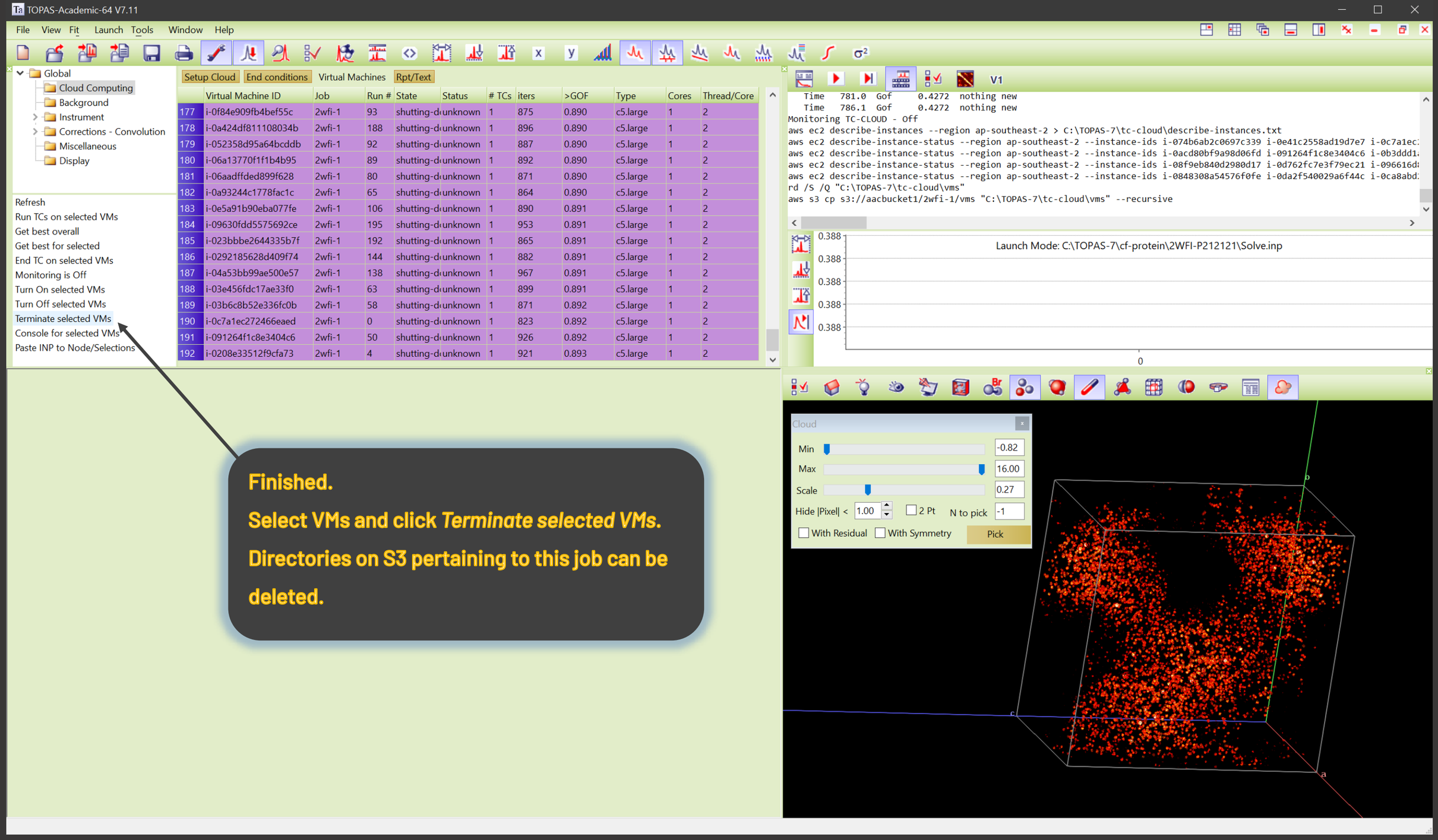

TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Virtual Machine ID | Job | Run # | State | Status | # TCs | iters | >GOF | Type | Cores | Thread/Core
3 | i-0b3faee16282ceb38 | 2wfi-1 | 28 | running | ok | 1 | 34 | 0.916 | c5.large | 1 | 2
4 | i-0be7a0e77cf5f08f4 | 2wfi-1 | 14 | running | ok | 1 | 33 | 0.917 | c5.large | 1 | 2
5 | i-023b514298110d7ae | 2wfi-1 | 32 | running | ok | 1 | 35 | 0.917 | c5.large | 1 | 2
6 | i-02415c9b03fae82d9 | 2wfi-1 | 113 | running | ok | 1 | 32 | 0.918 | c5.large | 1 | 2
7 | i-0914c95fd56bcbdbd | 2wfi-1 | 64 | running | ok | 1 | 32 | 0.918 | c5.large | 1 | 2
8 | i-0d762fc7e3f79ec21 | 2wfi-1 | 104 | running | ok | 2 | 34 | 0.919 | c5.large | 1 | 2
9 | i-0e3e419e805ab6273 | 2wfi-1 | 10 | running | ok | 1 | 30 | 0.919 | c5.large | 1 | 2
10 | i-0068ac729bc340b85 | 2wfi-1 | 57 | running | ok | 1 | 32 | 0.919 | c5.large | 1 | 2
11 | i-0a93244c1778fac1c | 2wfi-1 | 65 | running | ok | 1 | 32 | 0.919 | c5.large | 1 | 2
12 | i-031fae00874d3786a | 2wfi-1 | 67 | running | ok | 1 | 33 | 0.919 | c5.large | 1 | 2
13 | i-0dcf4c8f9e8e873f3 | 2wfi-1 | 81 | running | ok | 1 | 32 | 0.920 | c5.large | 1 | 2
14 | i-010d893c71ebdff36 | 2wfi-1 | 154 | running | ok | 1 | 32 | 0.920 | c5.large | 1 | 2
15 | i-092f67bbb23591311 | 2wfi-1 | 117 | running | ok | 1 | 30 | 0.920 | c5.large | 1 | 2
16 | i-092a415fa82cf26e0 | 2wfi-1 | 25 | running | ok | 1 | 31 | 0.920 | c5.large | 1 | 2
17 | i-02512f1cd1fda1e72 | 2wfi-1 | 173 | running | ok | 2 | 30 | 0.920 | c5.large | 1 | 2
18 | i-0acd80bf9a98d06fd | 2wfi-1 | 49 | running | ok | 2 | 28 | 0.920 | c5.large | 1 | 2
Refresh
Run TCs on selected VMs
Get best overall
Get best for selected
End TC on selected VMs
Monitoring is On
Turn On selected VMs
Turn Off selected VMs
Terminate selected VMs
Console for selected VMs
Paste INP to Node/Selections
STOP
V1
Grid dy 0.2545
Grid dz 0.2722
Setting initial phases to that found in
C:\TOPAS-7\cf-protein\2WFI-P212121\2wfi-1.fc
Space group P212121 is not centrosymmetric
Number of equivalent positions 4
Iter Time R-fac Scale Del %Flip Shift Sym-Err F000 %ED > H Flip-R
0 1.3 0.852 3.09 0.04 96.99 0 0 0 0.046 0.003 1.964 -0.000
Time 402.8 Gof 0.8714 nothing new
Time 408.1 Gof 0.8714 nothing new
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
0.852
0.852
0.852
0.852
0.852
0
Cloud
Min -2.80
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick
Click Step to run the INP file locally. This displays the best so far which in this case is a non-solution where the R-factor is 0.852. The Job on the VMs continue to execute whilst working on the local computer.
Step F7

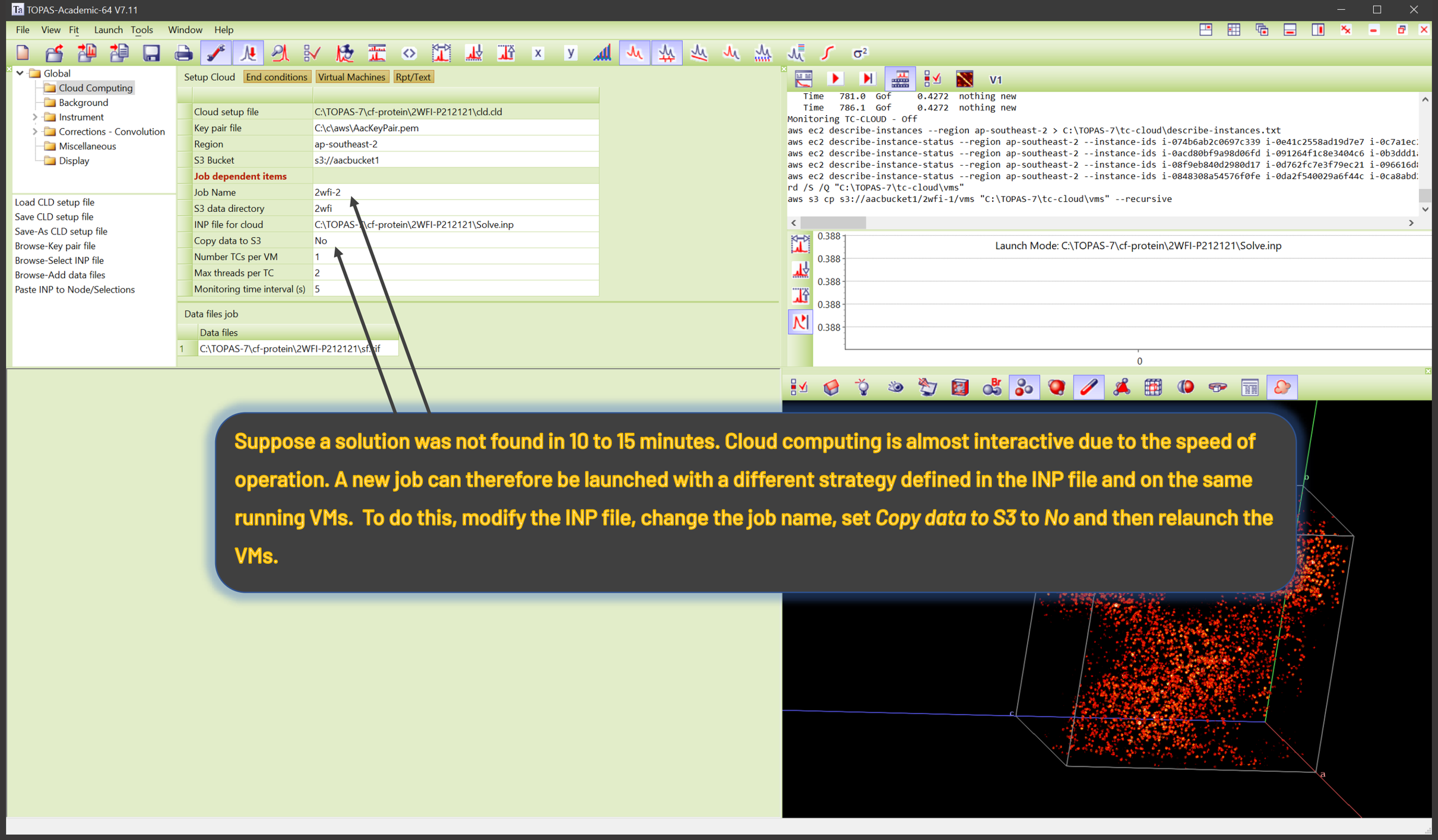


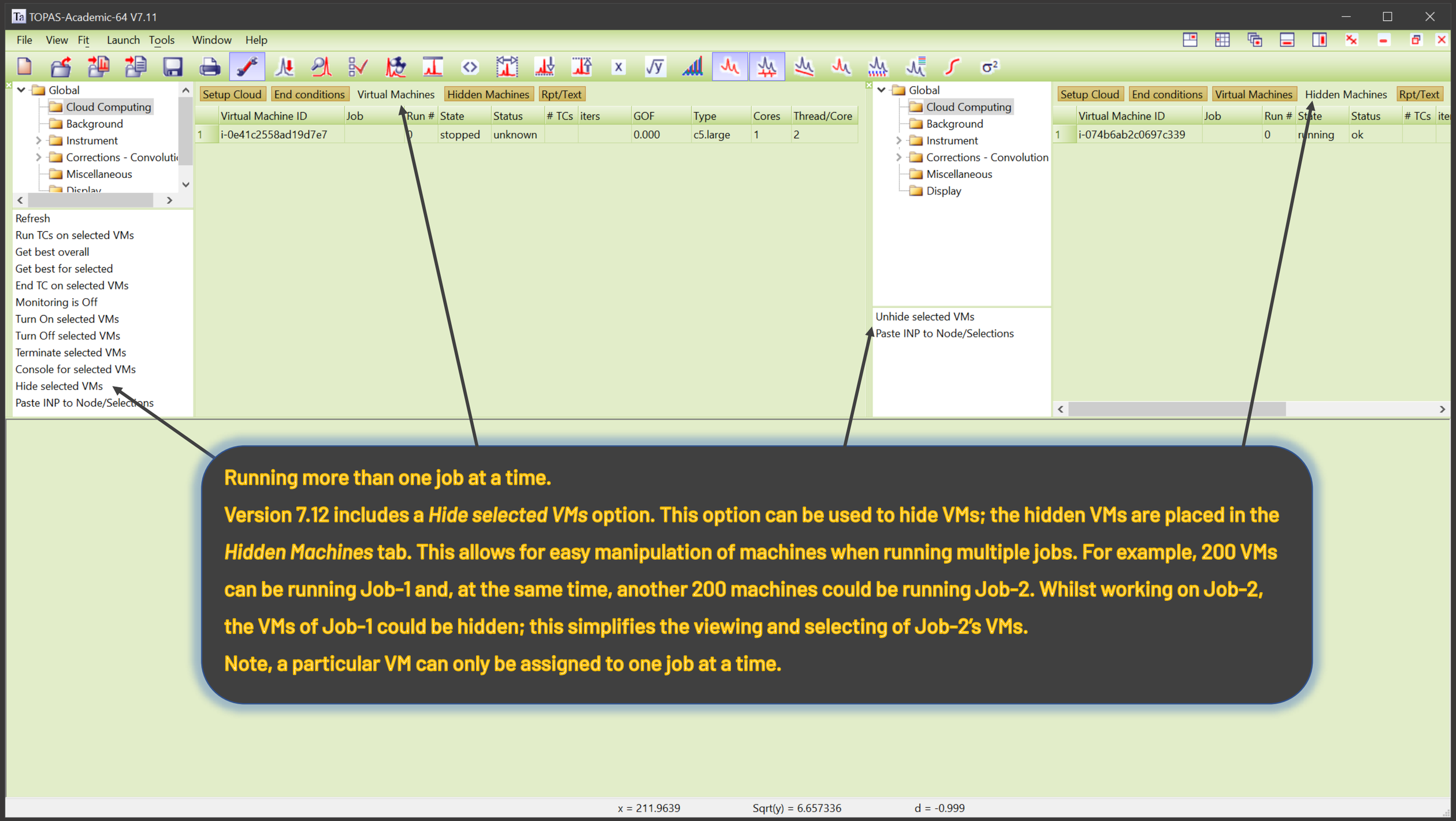
Solution found after ~640s.

Click *Refresh* to refresh the *Virtual Machines* tab. Click on *GOF* column headings to sort R-factors. Approximately 700 iterations performed on each VM in this case. Equivalent time on local machine would have been ~800 minutes (in excess of 13 hours on an 8 core machine).


TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Virtual Machine ID | Job | Run # | State | Status | # TCs | iters | >GOF | Type | Cores | Thread/Core
3 | i-04b834586889cf82f | 2wfi-1 | 36 | running | ok | 1 | 732 | 0.429 | c5.large | 1 | 2
4 | i-031fae00874d3786a | 2wfi-1 | 67 | running | ok | 1 | 697 | 0.868 | c5.large | 1 | 2
5 | i-0effee811ec833874 | 2wfi-1 | 3 | running | ok | 1 | 713 | 0.870 | c5.large | 1 | 2
6 | i-0106e95a4a5fdfb81 | 2wfi-1 | 142 | running | ok | 1 | 715 | 0.871 | c5.large | 1 | 2
7 | i-0b3faee16282ceb38 | 2wfi-1 | 28 | running | ok | 1 | 728 | 0.871 | c5.large | 1 | 2
8 | i-02bc85fe35084b8c9 | 2wfi-1 | 6 | running | ok | 1 | 744 | 0.871 | c5.large | 1 | 2
9 | i-0848308a54576f0fe | 2wfi-1 | 156 | running | ok | 1 | 717 | 0.872 | c5.large | 1 | 2
10 | i-0be7a0e77cf5f08f4 | 2wfi-1 | 14 | running | ok | 1 | 773 | 0.872 | c5.large | 1 | 2
11 | i-0c4e69878a9b67c20 | 2wfi-1 | 21 | running | ok | 1 | 717 | 0.872 | c5.large | 1 | 2
12 | i-0da1b568b32f7e324 | 2wfi-1 | 2 | running | ok | 1 | 678 | 0.872 | c5.large | 1 | 2
13 | i-061ec8c85679ac97d | 2wfi-1 | 78 | running | ok | 1 | 732 | 0.873 | c5.large | 1 | 2
14 | i-0d580be0502c90549 | 2wfi-1 | 69 | running | ok | 1 | 687 | 0.873 | c5.large | 1 | 2
15 | i-0914c95fd56bcbdbd | 2wfi-1 | 64 | running | ok | 1 | 727 | 0.873 | c5.large | 1 | 2
16 | i-0acd80bf9a98d06fd | 2wfi-1 | 49 | running | ok | 1 | 722 | 0.873 | c5.large | 1 | 2
17 | i-08d317ee58176be11 | 2wfi-1 | 189 | running | ok | 1 | 789 | 0.873 | c5.large | 1 | 2
18 | i-092a415fa82cf26e0 | 2wfi-1 | 25 | running | ok | 1 | 718 | 0.873 | c5.large | 1 | 2
Refresh
Run TCs on selected VMs
Get best overall
Get best for selected
End TC on selected VMs
Monitoring is On
Turn On selected VMs
Turn Off selected VMs
Terminate selected VMs
Console for selected VMs
Paste INP to Node/Selections
V1
Grid dx 0.2933
Grid dy 0.2545
Grid dz 0.2722
Setting initial phases to that found in
C:\TOPAS-7\cf-protein\2WFI-P212121\2wfi-1.fc
Space group P212121 is not centrosymmetric
Number of equivalent positions 4
Iter Time R-fac Scale Del %Flip Shift Sym-Err F000 %ED > H Flip-R
0 1.3 0.388 1.83 0.01 96.99 0 0 0 0.025 0.001 0.539 -0.000
Time 699.7 Gof 0.4273 nothing new
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
0.388
0.388
0.388
0.388
0.388
0
Cloud
Min -3.06
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick
Click Get best overall.
Click Step on local machine to display the best structure factors. Correct solution found as seen in the electron density.
Step F7


TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Refresh
Run TCs on selected VMs
Get best overall
Get best for selected
End TC on selected VMs
Monitoring is Off
Turn On selected VMs
Turn Off selected VMs
Terminate selected VMs
Console for selected VMs
Paste INP to Node/Selections
Virtual Machine ID | Job | Run # | State | Status | # TCs | iters | >GOF | Type | Cores | Thread/Core
177 i-0f84e909fb4bef55c 2wfi-1 93 shutting-d unknown 1 875 0.890 c5.large 1 2
178 i-0a424df811108034b 2wfi-1 188 shutting-d unknown 1 896 0.890 c5.large 1 2
179 i-052358d95a64bcddb 2wfi-1 92 shutting-d unknown 1 887 0.890 c5.large 1 2
180 i-06a13770f1f1b4b95 2wfi-1 89 shutting-d unknown 1 892 0.890 c5.large 1 2
181 i-06aadffded899f628 2wfi-1 80 shutting-d unknown 1 871 0.890 c5.large 1 2
182 i-0a93244c1778fac1c 2wfi-1 65 shutting-d unknown 1 864 0.890 c5.large 1 2
183 i-0e5a91b90eba077fe 2wfi-1 106 shutting-d unknown 1 890 0.891 c5.large 1 2
184 i-09630fdd5575692ce 2wfi-1 195 shutting-d unknown 1 953 0.891 c5.large 1 2
185 i-023bbbe2644335b7f 2wfi-1 192 shutting-d unknown 1 865 0.891 c5.large 1 2
186 i-0292185628d409f74 2wfi-1 144 shutting-d unknown 1 882 0.891 c5.large 1 2
187 i-04a53bb99ae500e57 2wfi-1 138 shutting-d unknown 1 967 0.891 c5.large 1 2
188 i-03e456fdc17ae33f0 2wfi-1 63 shutting-d unknown 1 899 0.891 c5.large 1 2
189 i-03b6c8b52e336fc0b 2wfi-1 58 shutting-d unknown 1 871 0.892 c5.large 1 2
190 i-0c7a1ec272466eaed 2wfi-1 0 shutting-d unknown 1 823 0.892 c5.large 1 2
191 i-091264f1c8e3404c6 2wfi-1 50 shutting-d unknown 1 926 0.892 c5.large 1 2
192 i-0208e33512f9cfa73 2wfi-1 4 shutting-d unknown 1 921 0.893 c5.large 1 2
Time 781.0 Gof 0.4272 nothing new
Time 786.1 Gof 0.4272 nothing new
Monitoring TC-CLOUD - Off
aws ec2 describe-instances --region ap-southeast-2 > C:\TOPAS-7\tc-cloud\describe-instances.txt
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-074b6ab2c0697c339 i-0e41c2558ad19d7e7 i-0c7a1ec
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0acd80bf9a98d06fd i-091264f1c8e3404c6 i-0b3ddd1
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-08f9eb840d2980d17 i-0d762fc7e3f79ec21 i-096616d
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0848308a54576f0fe i-0da2f540029a6f44c i-0ca8abd
rd /S /Q "C:\TOPAS-7\tc-cloud\vms"
aws s3 cp s3://aacbucket1/2wfi-1/vms "C:\TOPAS-7\tc-cloud\vms" --recursive
0.388
0.388
0.388
0.388
0.388
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
0
Cloud
Min -0.82
Max 16.00
Scale 0.27
Hide |Pixel| < 1.00
2 Pt
N to pick -1
With Residual
With Symmetry
Pick
Finished.
Select VMs and click Terminate selected VMs.
Directories on S3 pertaining to this job can be deleted.


TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Load CLD setup file
Save CLD setup file
Save-As CLD setup file
Browse-Key pair file
Browse-Select INP file
Browse-Add data files
Paste INP to Node/Selections
Setup Cloud
End conditions
Virtual Machines
Rpt/Text
Cloud setup file C:\TOPAS-7\cf-protein\2WFI-P212121\cld.cld
Key pair file C:\c\aws\AacKeyPair.pem
Region ap-southeast-2
S3 Bucket s3://aacbucket1
Job dependent items
Job Name 2wfi-2
S3 data directory 2wfi
INP file for cloud C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
Copy data to S3 No
Number TCs per VM 1
Max threads per TC 2
Monitoring time interval (s) 5
Data files job
Data files
1 C:\TOPAS-7\cf-protein\2WFI-P212121\sf.cif
Time 781.0 Gof 0.4272 nothing new
Time 786.1 Gof 0.4272 nothing new
Monitoring TC-CLOUD - Off
aws ec2 describe-instances --region ap-southeast-2 > C:\TOPAS-7\tc-cloud\describe-instances.txt
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-074b6ab2c0697c339 i-0e41c2558ad19d7e7 i-0c7a1ec
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0acd80bf9a98d06fd i-091264f1c8e3404c6 i-0b3ddd1
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-08f9eb840d2980d17 i-0d762fc7e3f79ec21 i-096616d
aws ec2 describe-instance-status --region ap-southeast-2 --instance-ids i-0848308a54576f0fe i-0da2f540029a6f44c i-0ca8abd
rd /S /Q "C:\TOPAS-7\tc-cloud\vms"
aws s3 cp s3://aacbucket1/2wfi-1/vms "C:\TOPAS-7\tc-cloud\vms" --recursive
Launch Mode: C:\TOPAS-7\cf-protein\2WFI-P212121\Solve.inp
0.388
0.388
0.388
0.388
0.388
0
Suppose a solution was not found in 10 to 15 minutes. Cloud computing is almost interactive due to the speed of operation. A new job can therefore be launched with a different strategy defined in the INP file and on the same running VMs. To do this, modify the INP file, change the job name, set Copy data to S3 to No and then relaunch the VMs.


TOPAS-Academic-64 V7.11
File View Fit Launch Tools Window Help
Global
Cloud Computing
Background
Instrument
Corrections - Convoluti
Miscellaneous
Display
Refresh
Run TCs on selected VMs
Get best overall
Get best for selected
End TC on selected VMs
Monitoring is Off
Turn On selected VMs
Turn Off selected VMs
Terminate selected VMs
Console for selected VMs
Hide selected VMs
Paste INP to Node/Selections
Setup Cloud
End conditions
Virtual Machines
Hidden Machines
Rpt/Text
Virtual Machine ID
Job
Run #
State
Status
TCs
iters
GOF
Type
Cores
Thread/Core
1
i-0e41c2558ad19d7e7
0
stopped
unknown
0.000
c5.large
1
2
Global
Cloud Computing
Background
Instrument
Corrections - Convolution
Miscellaneous
Display
Unhide selected VMs
Paste INP to Node/Selections
Setup Cloud
End conditions
Virtual Machines
Hidden Machines
Rpt/Text
Virtual Machine ID
Job
Run #
State
Status
TCs
1
i-074b6ab2c0697c339
0
running
ok
Running more than one job at a time.
Version 7.12 includes a Hide selected VMs option. This option can be used to hide VMs; the hidden VMs are placed in the Hidden Machines tab. This allows for easy manipulation of machines when running multiple jobs. For example, 200 VMs can be running Job-1 and, at the same time, another 200 machines could be running Job-2. Whilst working on Job-2, the VMs of Job-1 could be hidden; this simplifies the viewing and selecting of Job-2's VMs.
Note, a particular VM can only be assigned to one job at a time.
x = 211.9639
Sqrt(y) = 6.657336
d = -0.999