Parallel execution with Automated Changes

PAC for SHETRAN

Easy Reference Manual v.1.0

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Dedicated to my loving mother - Nirmal Prabha,
who dedicated her life for others

The Development Team

The PAC v1.0.tesla development team consists of three names - Pallav and Sangam from AIT, Thailand and Steve from Newcastle University, UK. Their brief info and contribution are as follows.

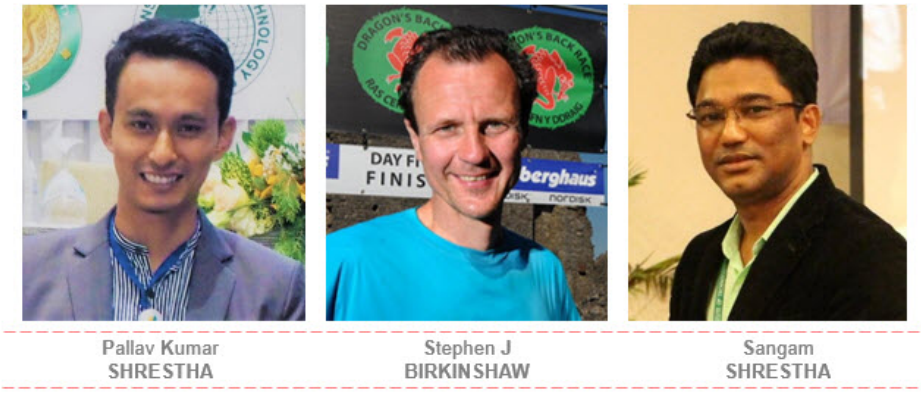


Figure 1: PAC development team

Pallav – Pallav K Shrestha, MSc

- Lead - concept, methodology, software programming, validation, pre-release tests, review and edits
- Pallav is currently Water Resources Specialist and Programmer working under Sangam at Water Engineering and Management program, AIT. Apart from work he likes to workout and is into music.

Steve – Stephen J Birkinshaw, PhD

- Lead - supervision; Supporting - methodology, review

- Steve is a Senior Researcher in the Department of Civil Engineering and Geosciences of Newcastle University. His involvement with SHETRAN dates back to 1993 and is Pallav's SHETRAN guru.
- Did you know? There's one more thing that Steve has massive experience in - Running (>40 years)! Steve is hailed by many as a running legend. Get to know him and his running habits in his book *There is no map in hell* (https://www.v-publishing.co.uk/books/categories/biographies/there-is-no-map-in-hell.html)

Sangam – Sangam Shrestha, PhD

- Lead - resources; Supporting - supervision, review
- Sangam is the Program Chair and Associate Professor at the Water Engineering and Management Program in AIT. With a broad knowledge in the field of water resources management, Sangam is highly respected for supporting young researchers and innovation.
- Did you know? Sangam's research article entitled *Assessment of surface water quality using multivariate statistical techniques: A case study of the Fuji river basin, Japan* featured in *Environmental Modelling & Software* (EMS) in 2007 has almost 1k citations till date (Google scholar, https://scholar.google.co.th/citations?user=cukxp2sAAAAJ&hl=en&oi=ao) and is one of the most cited papers of EMS.

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1

PAC in a nutshell

This chapter gives an *under 5 minutes introduction* to PAC, ideal for scanning the suitability of PAC for your research situation.

Estimated read-time: *5 minutes*

1.1 In 4-sentences

SHETRAN is a widely used hydrological model for analyses involving land use change, climate change, sediment transport, and nutrient transport among others. However, even a decent grid size in SHETRAN entails massive runtimes that originate from its time intensive solution of physically based equations. We made PAC for you to run SHETRAN in parallel in *Linux OS,* and thus achieve medium to massive speedups depending on your hardware (beginning from multiprocessor laptops). PAC is ideal for saving time during sensitivity analysis, model calibration and multiple-scenario runs (say 100 rainfall realization forcing).

1.2 How much time does it actually save?

We tested PAC on four pre-existing models. Using from 1 to 30 processors at a time, the run time for completion of 30 runs each time were noted. The result is as illustrated in Figure 1.1 the details of which are discussed in Section 3.3.

There is no doubt that the speed up achieved with PAC is of tremendous utility. This holds true especially in cases with large computational grids where hours and hours of runtime can be reduced to minutes.

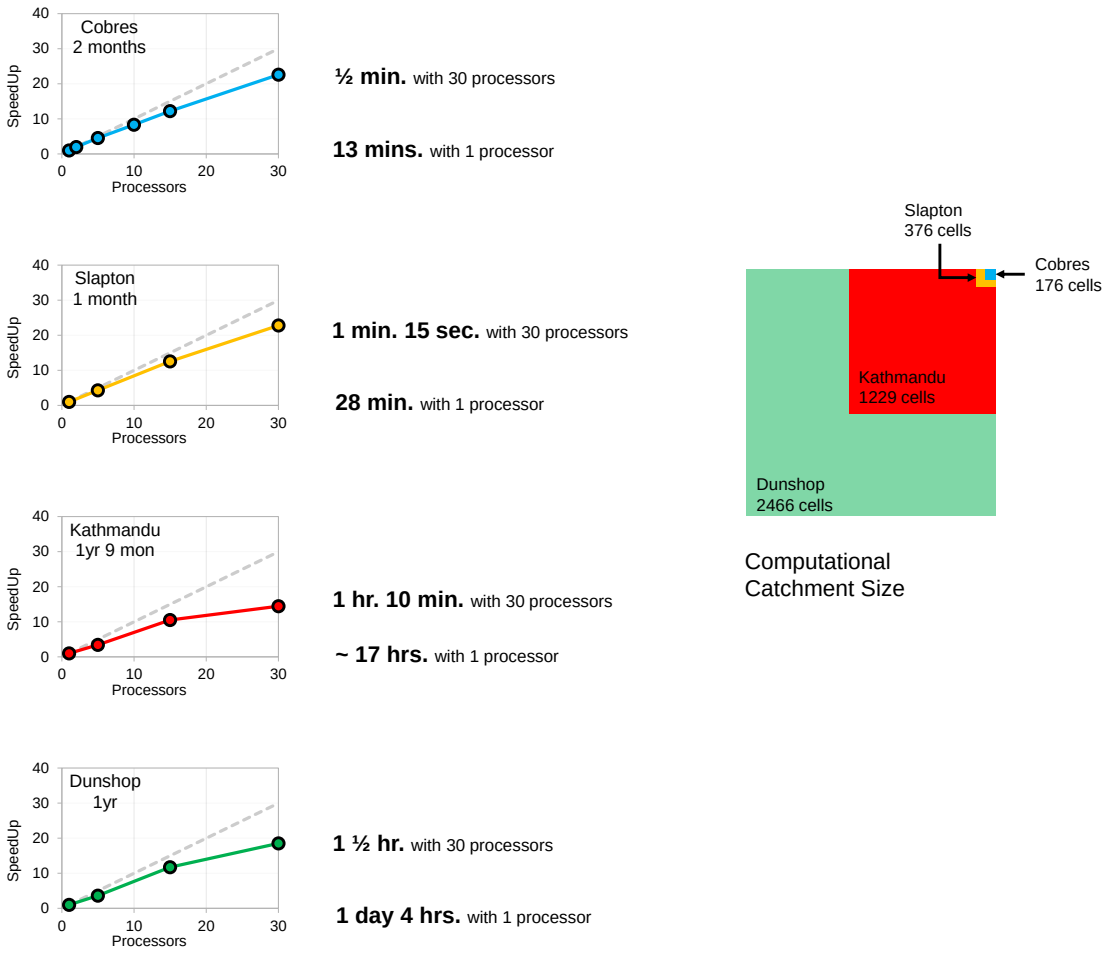


Figure 1.1: Runtime saved with PAC: Test results

1.3 What are the prerequisites?

- The current release of PAC (v1.0.tesla) is programmed in Linux bash and thus requires **Linux OS**. However, Windows users can also use it with a slightly indirect approach (Yes its possible! Go to sections 1.4 and Chapter 4 of this document for details).

- PAC runs SHETRAN model in parallel but is not made to develop the SHETRAN model itself[1] . You need **a running SHETRAN model**

[1]PAC for SHETRAN is similar to what SWAT Cup is for SWAT. Both of them enable tremendous augmentation for a pre-existing model. Refer to Section 6 for a comparison between PAC and SWAT Cup based on their function.

to augment its run time using PAC.

- Before it can work, PAC requires you to prepare some files and input information that require **working knowledge of SHETRAN**. Thus, learn SHETRAN before using PAC (Refer Section 6 of this document to get starter tips on SHETRAN).

1.4 I don't have Linux OS!

You don't have Linux or don't know about Linux. Worry not! You still can work your way around to use PAC. Its a slightly indirect approach and consists of following three basic steps -

1. Download and Install a virtualization software (approx. 130 MB) (E.g. Oracle VM VirtualBox)
2. Download our pre-cutomized virtual machine file (.vdi) from cloud (approx. 1 GB)
3. You are good to go. Enjoy using PAC!

The steps have been dealt in detail in Section 4 of this document.

2

How do I use PAC?

This Chapter takes you through a worked out example and also lets you know the dos and don'ts of PAC.

Estimated read time: *15 minutes*
Estimated tutorial time: *15 more minutes*

2.1 Attention!

Keep the following (mostly obvious) points in mind while using PAC -

1. *Always backup your data*, input output alike. All the output from PAC and other files and folders, except those pertaining to the program, are removed each time you run PAC. So if you are happy with a completed PAC run, make a copy of the new output first!

2. *Don't max out your CPU.* PAC shows total number of processors your machine has for you to involve for parallel processing. It is advised to use 1 or 2 processors less than the maximum allowed. In case you make up your mind to utilize all processors, be sure that you are going to leave your computer idle without any running programs.

2.2 I/O and formatting

PAC has very few input information collected from the user (which will be elaborated in the worked out example in the next section). Out of which only a handful of them need discretion during formatting as enlisted in the following table 2.1 below -

Table 2.1: Points to remember regarding I/O formatting in PAC

S.No.	I/O	Remarks
1	Model folder path	The path should be devoid of spaces
2	Path to the iteration files	The path should be devoid of spaces
3	Names of the iteration files	The file name should be devoid of spaces and should have **__i** type of append before the extension. Here **i** is the simulation number and [1 ≤ i ≤ total number of simulations] should hold true. E.g. If *input_basin_ocd.txt* is an input file selected for iteration in PAC then the first iteration file should be *input_basin_ocd_*1.*txt*

2.3 Example workout

The following is step-by-step example worked out based on a model (Cobres basin, 176 computational cells, 2-months run) provided with the PAC software. The model consists pre-setup input files for water flow and sediment transport components. In this example of PAC run, the Overland and Channel Flow module (OCD) input file for the model will be modified and iterated for 10 runs with 5 processors in parallel. It will also be illustrated how much run time is saved in this case as well as the water flow sensitivity from the OCD iterations.

Pre–PAC run notes

1. Download the PAC software package from the SHETRAN website in Newcastle University's web domain `http://research.ncl.ac.uk/shetran/` and unzip it. In this example the software folder has been added to the desktop (refer Figure 2.1).

2. Inside it, the folder *.../PAC–GUI/TestModel/Cobres_model* is the sample model that is going to be used. The folder should consist of a complete pre-existing SHETRAN model input files and the *shetran–linux* program as shown in Figure 2.2.

3. As mentioned earlier, this example (and the usage of PAC in general) requires iterations of input file for PAC run. The folder *.../PAC–GUI/Cobres_OCD_iterations* consists of 10 versions of the OCD input file having **_i** type of append before the extension (refer Figure 2.3). If you open the files, you will see that the input information of the files are identical except the value for (under) *CDRS*(refer Figure 2.4. Thus the parameter *CDRS* (the overland roughness coefficient) is being iterated over the 10 model runs for this example.

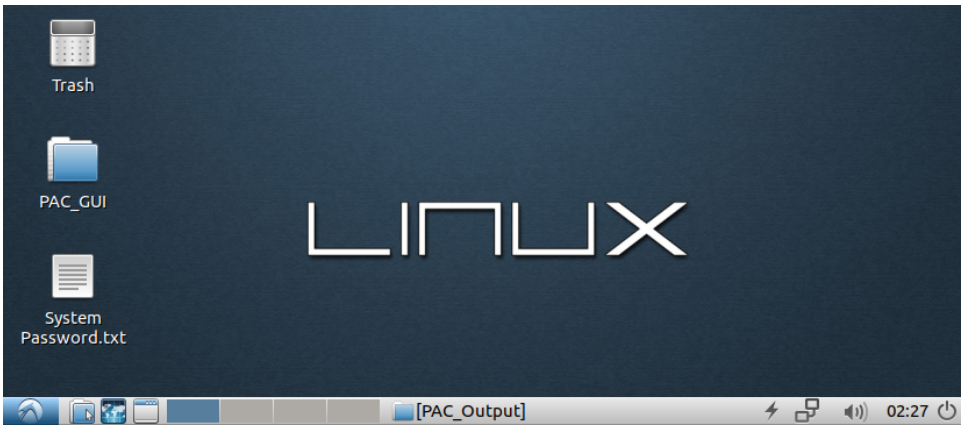


Figure 2.1: PAC-GUI folder

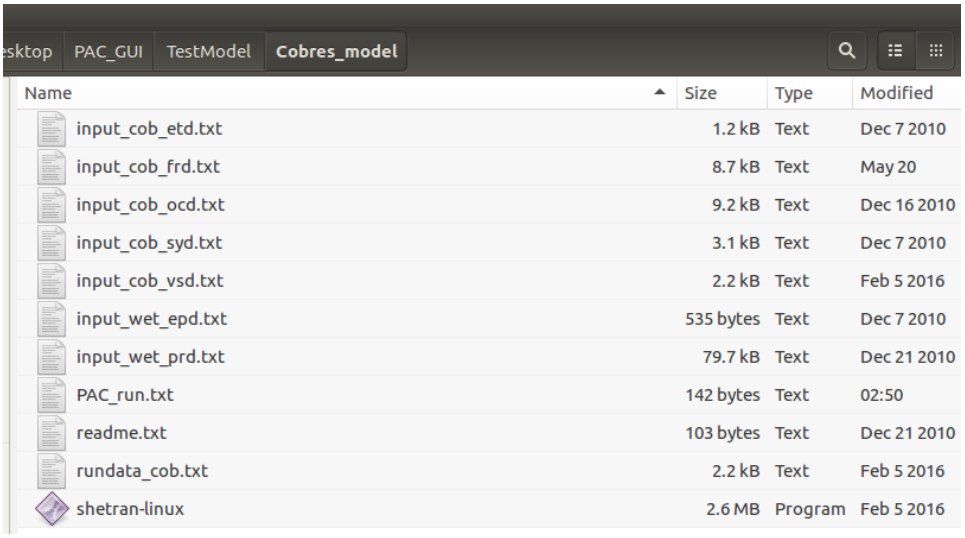


Figure 2.2: SHETRAN model folder for Cobres basin



Figure 2.3: OCD Iteration files for PAC run

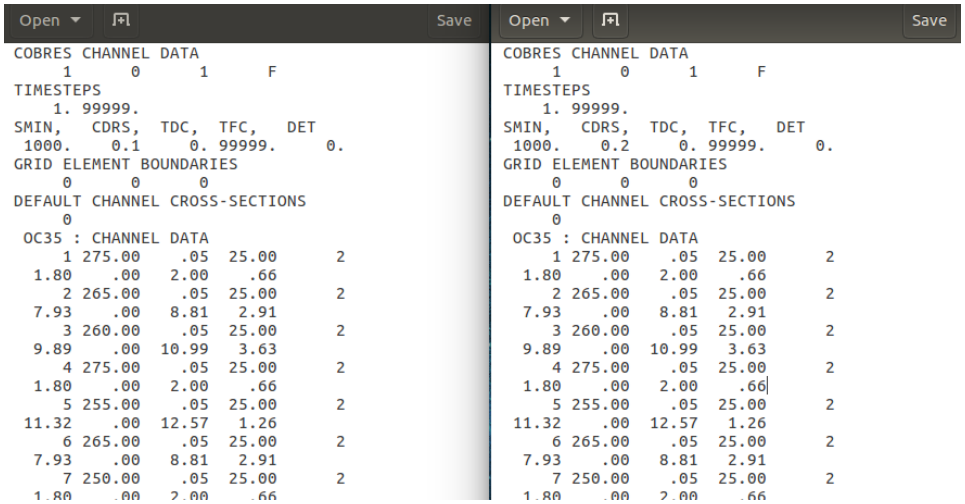


Figure 2.4: Comparing contents of OCD iteration files

PAC run steps

1. Enter the PAC–GUI folder and run the *SHETRAN–PAC* file (refer Figure 2.5). This can be done by double clicking it. In some systems a dialogue box is prompted asking for permission to execute the file (refer 2.6. If double clicking doesn't work, you can run it from the terminal/bash by typing *sudo ./SHETRAN–PAC*. In the later case, you might have to provide the root password. Additionally, if your OS doesn't already have some of the dependency packages, it will prompt for permission for installation which you can respond by typing *y (y for yes)*.

2. If everything goes fine, the loading screen should be visible as shown in Figure 2.7.

   That will follow up with a Warning dialog box (refer Figure 2.8) which basically reminds you to save your last PAC run output in case if you haven't. Press *Proceed*.

   The next dialog box (refer Figure 2.9) also is an informative one giving you a short information regarding PAC. Press *Next* to proceed.

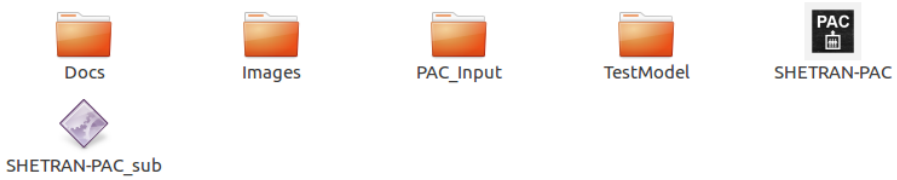


Figure 2.5: Contents of the PAC-GUI folder

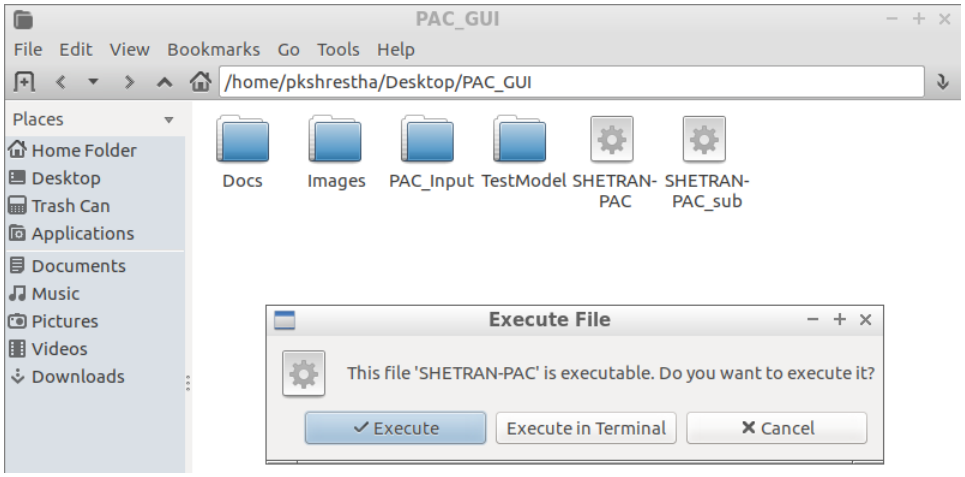


Figure 2.6: Prompt for executing permission

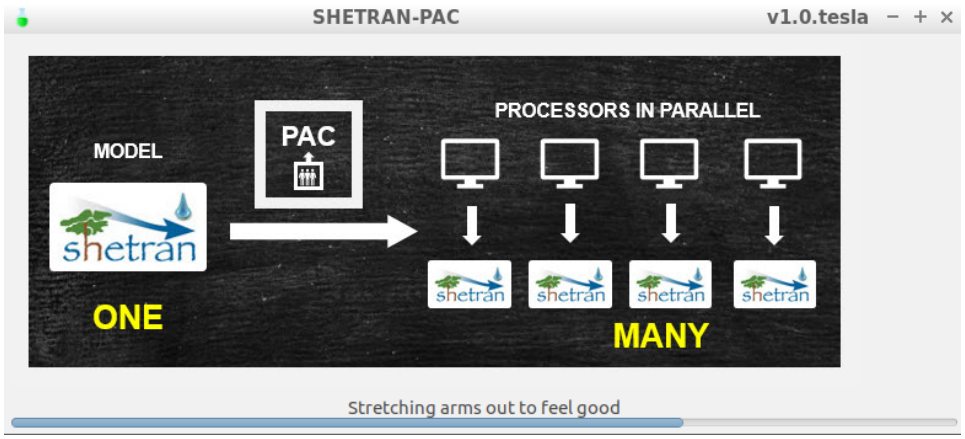


Figure 2.7: Loading screen of PAC

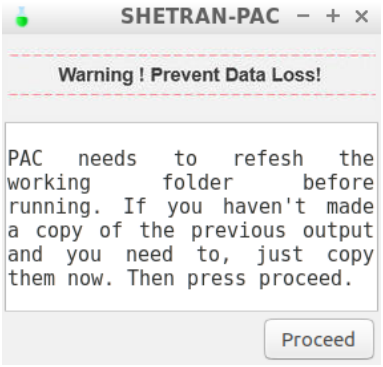


Figure 2.8: Warning screen regarding previous PAC run

3. The next screen (refer Figure 2.10) asks you to enter the number of processors to use in parallel. You can use the slider to chose between the range of 2 to max number of processors applicable. The number that you select here will be the number of model runs that are carried out in one shot (parallel). Thus, if you have 18 simulations and you allocate 6 processors to work in parallel, the your PAC run will be completed in (18/6 =) 3 waves of simulations. This is the same information depicted in the figure in the dialog box. The example shown in the Figure 2.10 employs 5 processors.

4. The next screen (refer Figure 2.10) asks you to select the model folder. Browse through inside the PAC folder and to select the model folder named *Cobres_model*. Its located inside *.../PAC_GUI/TestModel/*. Click *Next*.

5. This leads you to the last dialog box of the PAC's user input interface (refer Figure 2.11). It asks you to enter the total number of simulations to be run using PAC.

   You are also required to browse for the file path to the iteration input files. Browse for *Cobres_OCD_iterations* folder located at *.../PAC_GUI/TestModel/* (refer Figure 2.13).

   Finally select the SHETRAN input file that is to be iterated. As mentioned before, for this example we are going to iterate the OCD input file. Thus select *input_cob_ocd.txt* from the drop down list (refer Figure 2.14 and Figure 2.15). Press *Run PAC*.



Figure 2.9: PAC description screen

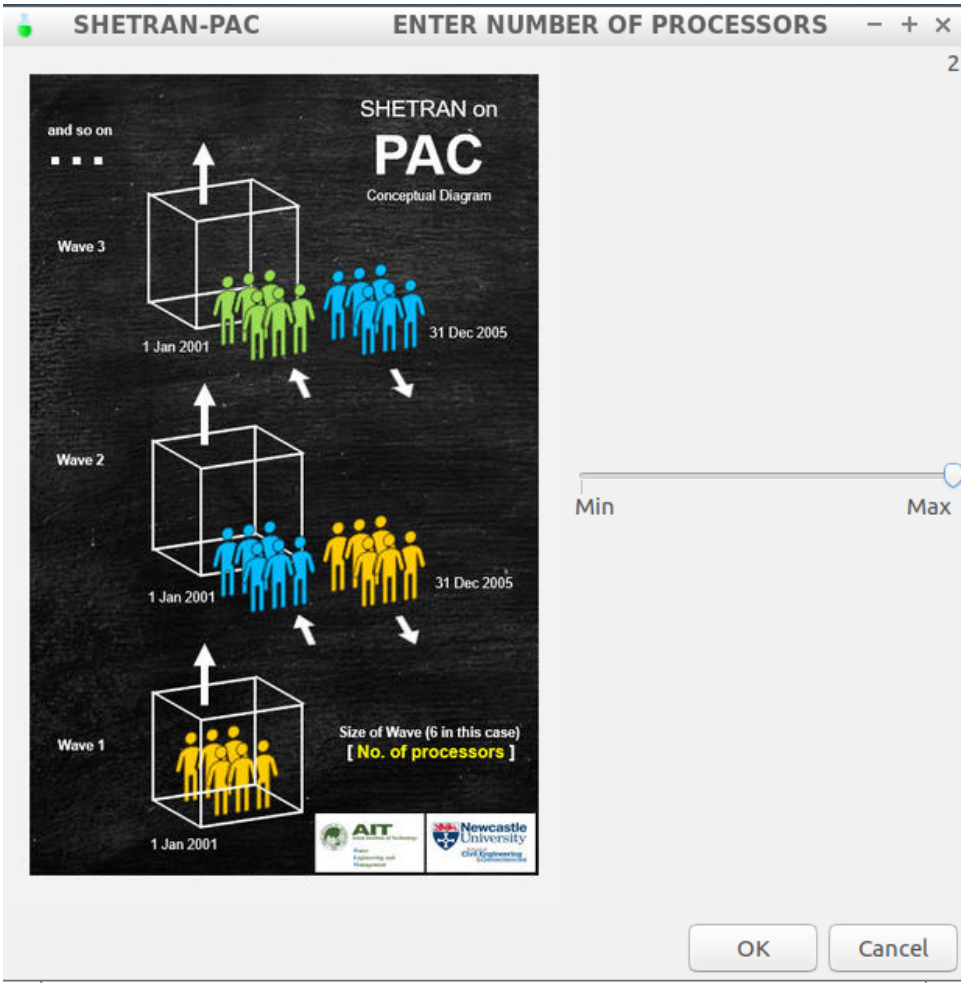


Figure 2.10: Assigning the number of processors in PAC

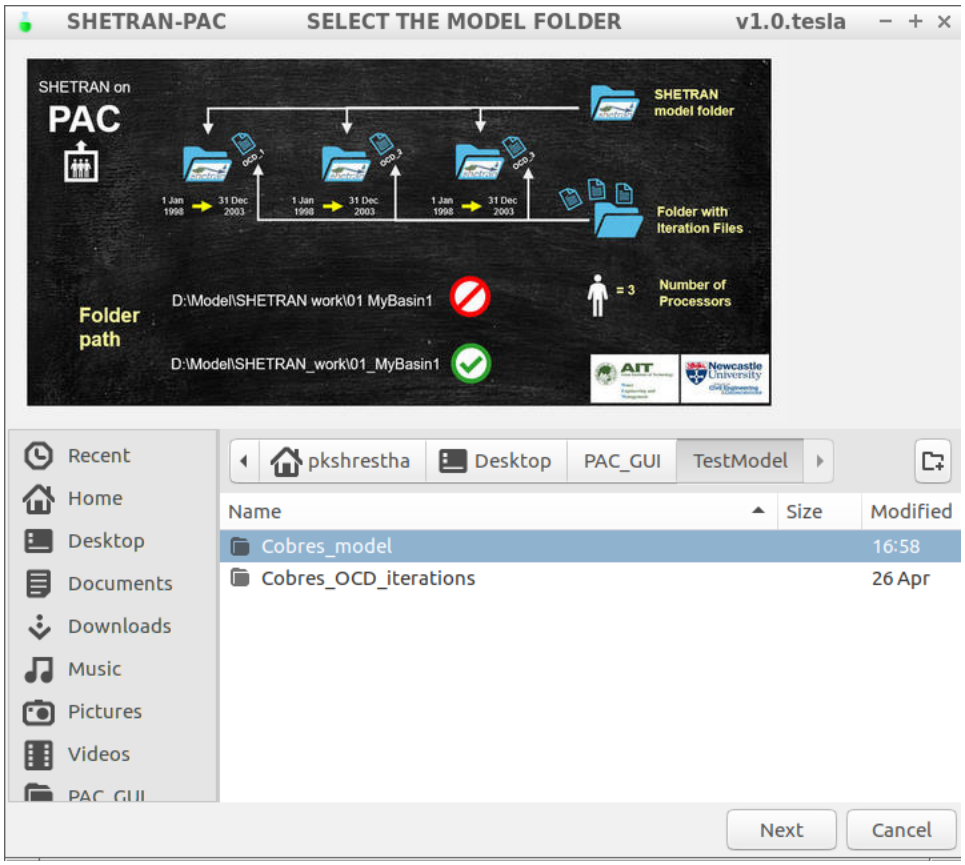


Figure 2.11: Browsing for the model folder

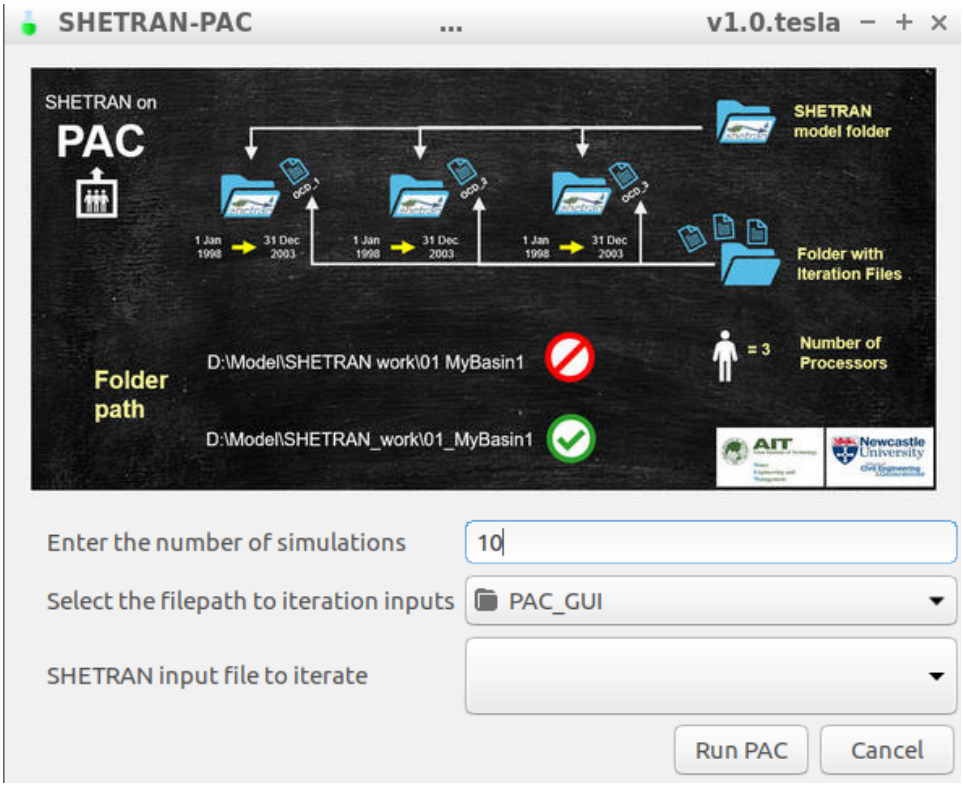


Figure 2.12: Entering the total number of model runs to be carried out in PAC

6. Next you should be getting a terminal with multiple tabs as shown in 2.16. The number of tabs formed depends upon the number of processors that you had entered earlier on. If everything goes well, all the terminals would show SHETRAN running without any starting errors [1] from PAC.

   An error free PAC run should give you the message *All simulations under Process... completed* in each terminal tab (refer Figure 2.17). The run time is displayed at end of simulations at each of the tab. The largest run time out of the tabs is the run time of the PAC run.

   Congratulations! You have completed your first PAC run successfully!.

[1] In case you get any starting errors here, check out section 2.4 which discusses on the most common errors while using PAC

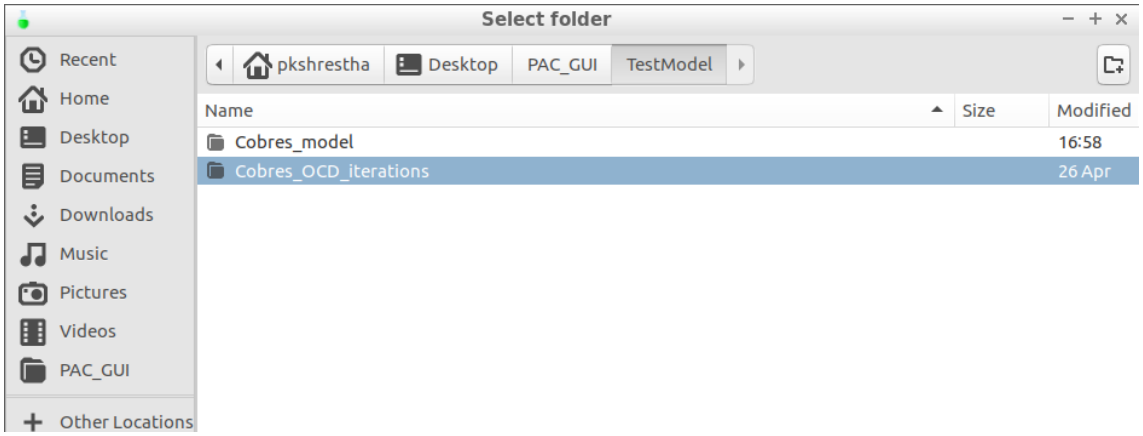


Figure 2.13: Browsing for the folder containing iteration files

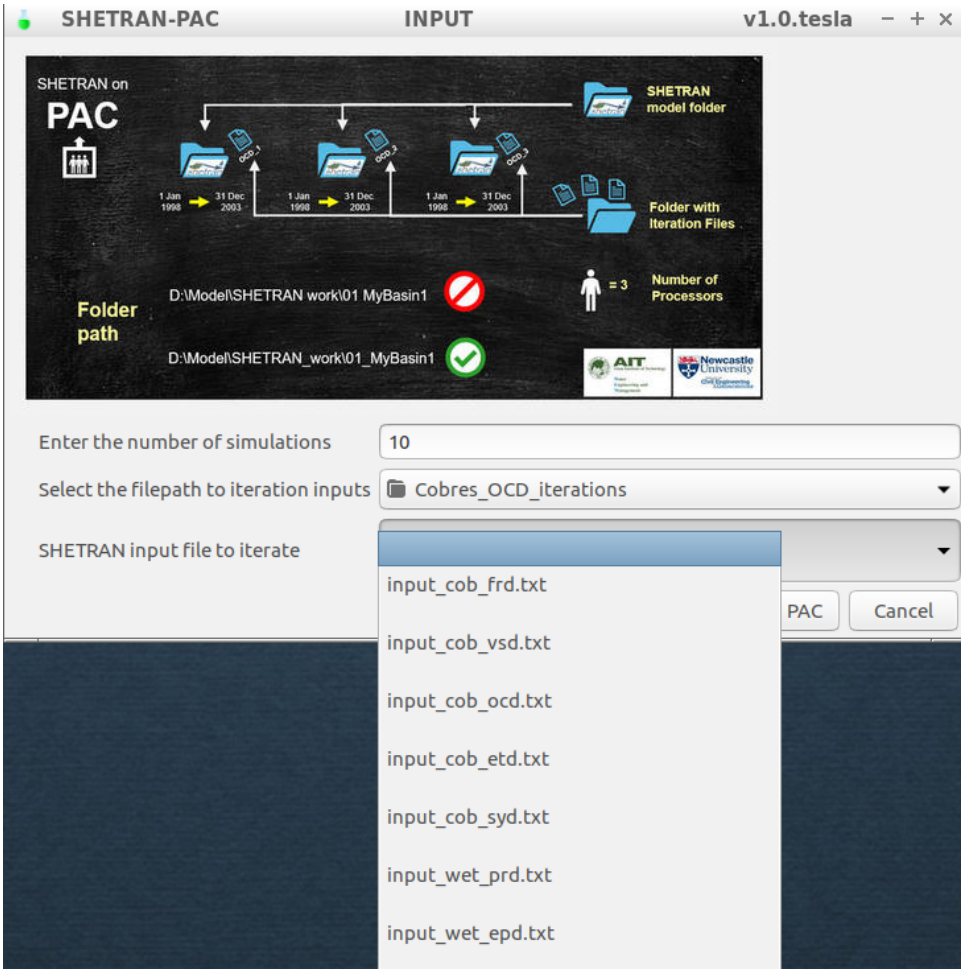


Figure 2.14: Selecting the model input file from the drop-down menu

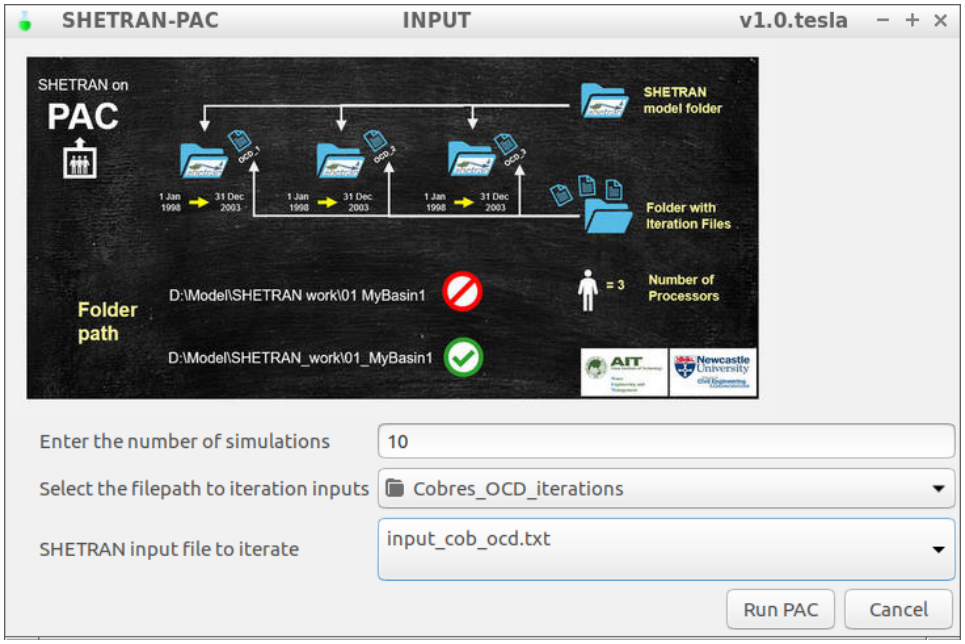


Figure 2.15: Selecting the OCD input file for PAC iterations

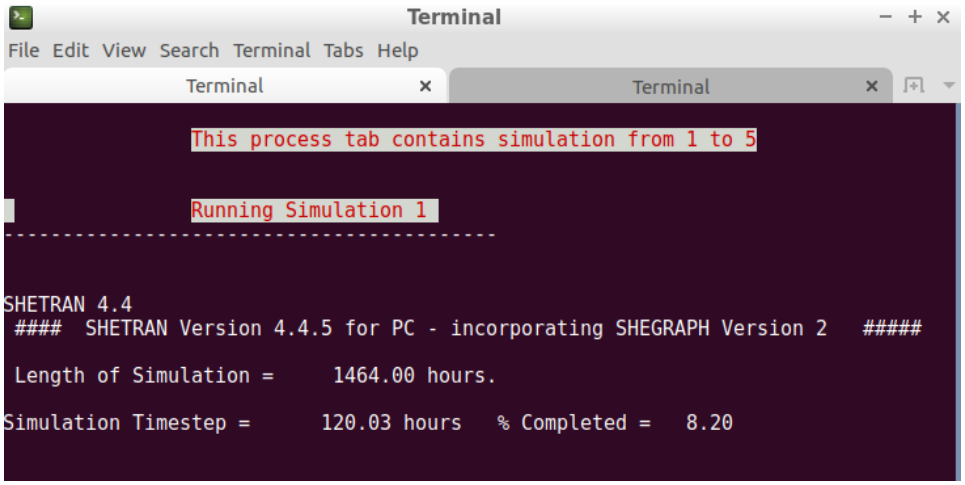


Figure 2.16: Multiple tabs running SHETRAN in parallel under PAC

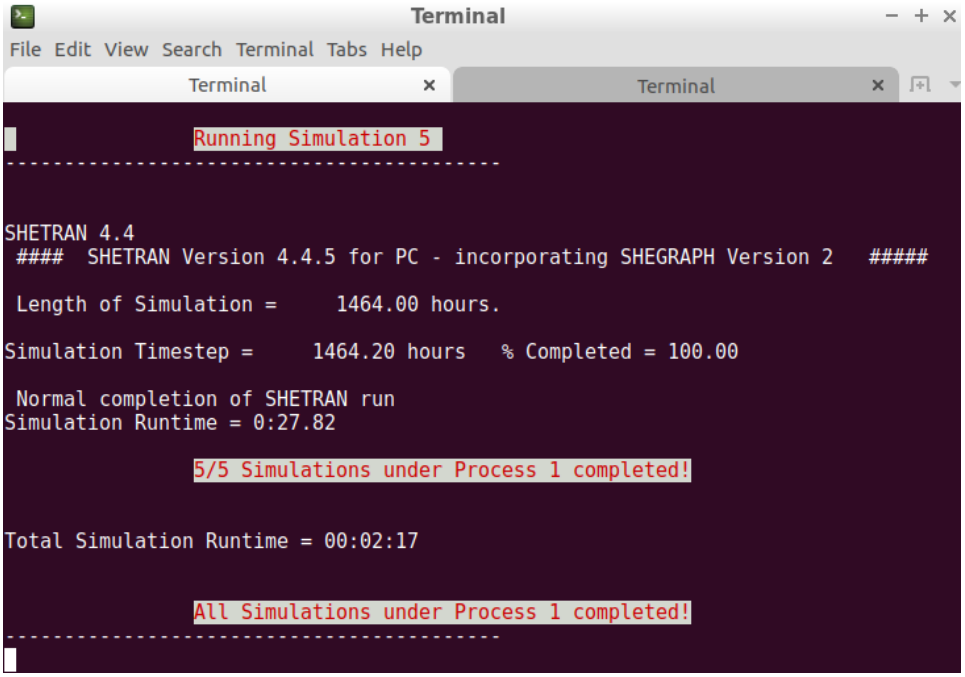


Figure 2.17: Successful run of SHETRAN simulations assigned to a processor under PAC

Post PAC run notes

1. After the PAC run, go inside the PAC folder and you will realize that there are two additional folders produced (refer Figure 2.18) – *PAC_Output* and *PAC_Processes*. *PAC_Output* is the folder that consists of the model outputs of each run while *PAC_Processes* is an intermediate processing folder for PAC.

   If you go inside the *PAC_Output* folder you will see those 10 model run output folders (refer Figure 2.20). Each of the folder would contain all the model outputs from SHETRAN run (refer Figure 2.21) and also includes an additional file named *output_dump.txt* which stores all of the model output messages for later reference (refer Figure **??**). This is especially useful if some of the simulation shows errors and you want to refer to the error output messages.

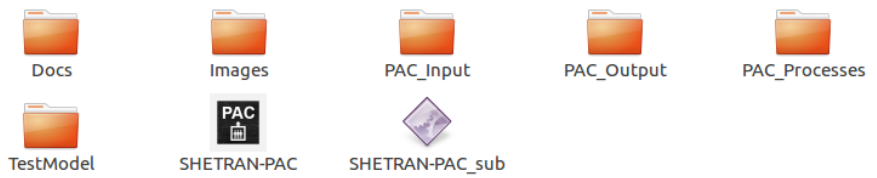


Figure 2.18: PAC GUI folder after PAC run

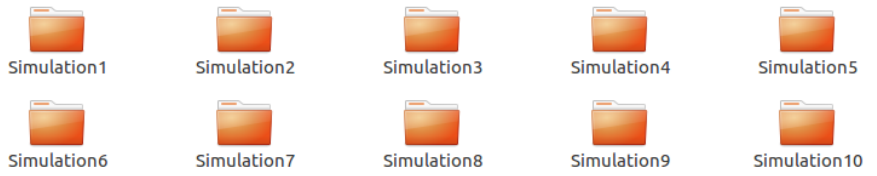


Figure 2.19: Folder-wise SHETRAN run outputs

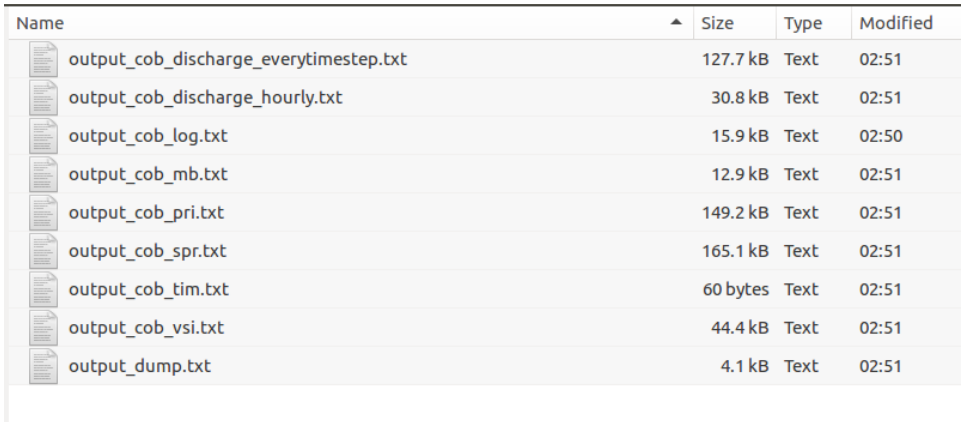


Figure 2.20: SHETRAN run output files under PAC

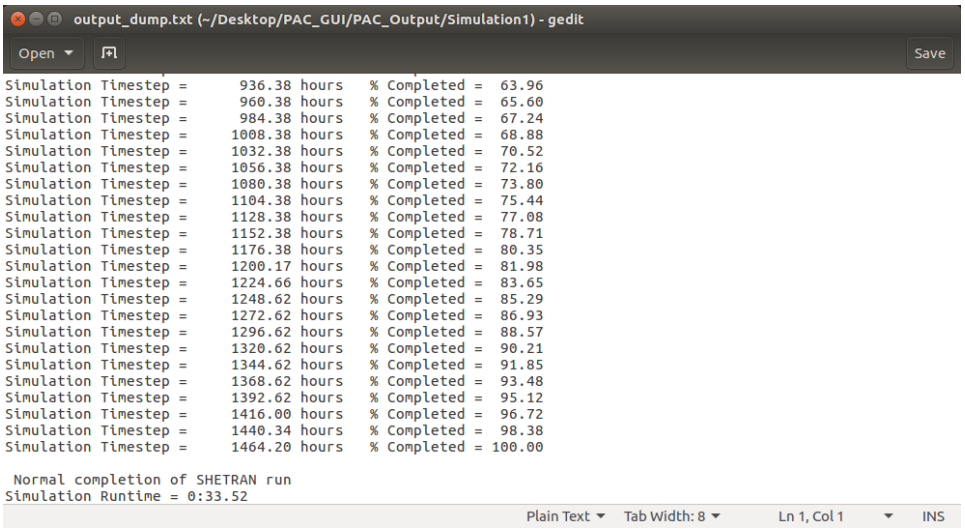


Figure 2.21: Content and usage of output_dump.txt

2. For a comparison, you can run the Cobres model without PAC from the terminal/ bash by typing *sudo ./shetran-linux –f rundata_cob.txt*. Then you can multiply this run time by number of simulations (10 in this case) and compare that with the run time that you had achieved with PAC run.

   In a normal desktop PC with i7 processor, the normal run time without PAC was found to be 4 minutes while with PAC the runs were completed in 1 minute 16 seconds. Thus employing 5 processors and PAC, the simulations were completed 3.1x faster. Three minutes might seem negligible in terms of time saved. But when the process involves hundreds/thousands of simulations or the computational size of the model is much larger, PAC contributes to save hours or even days of run time.

3. As mentioned before, the 10 iterations included in this example were for observing the sensitivity of the model's water flow to the parameter CDRS. The plots of hydrographs are shown in Figure 2.22. It is seen that water flow in the basin is sensitive to CDRS especially during high magnitude events. Both shape and size of the event hydrograph are altered to a great extent during those events. The same is reflected from the statistics calculated for the 10 flow outputs (refer Table 2.2). This shows that CDRS is an important model parameter in calibrating the Cobres basin model's water flow component.

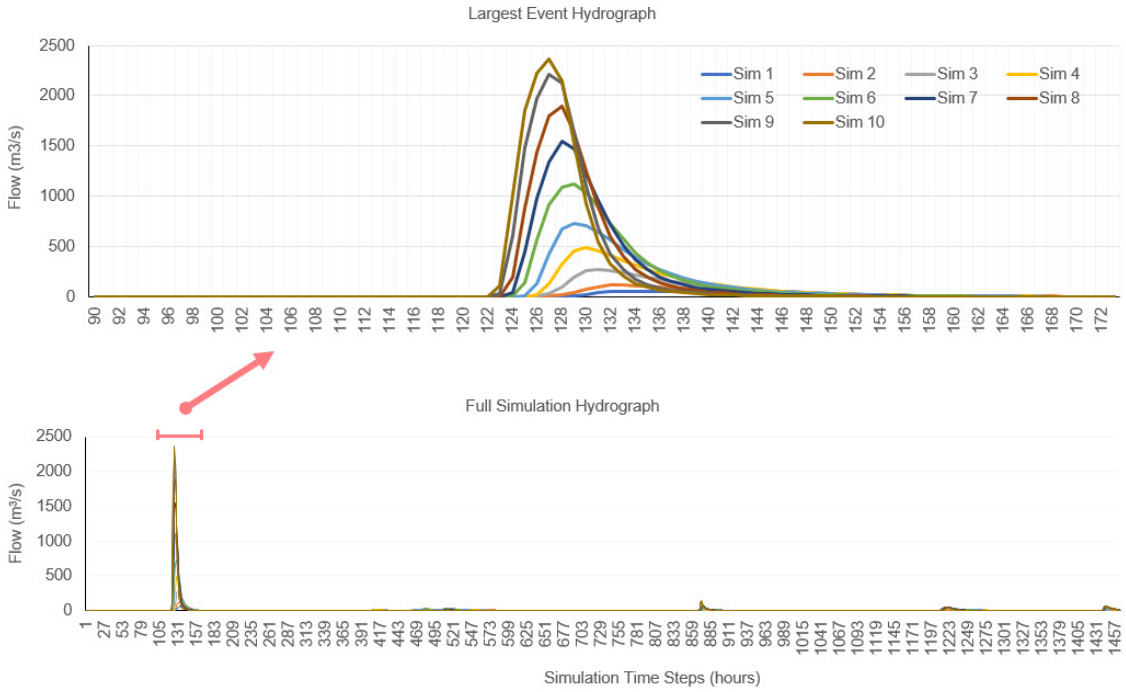


Figure 2.22: Sensitivity of Water flow to CDRS in Cobres basin

Table 2.2: Sensitivity of Water flow to CDRS in Cobres basin

Simulation	CDRS	Standard Deviation of flow (m^3/s)	Mean of flow (m^3/s)
1	0.1	5.7	3.9
2	0.2	10.0	4.8
3	0.5	19.8	6.2
4	1	31.7	7.2
5	2	46.2	8.1
6	5	68.3	9.2
7	10	86.6	9.9
8	20	102.5	10.4
9	50	118.3	10.9
10	100	126.0	11.1

2.4 Common errors

Following are the most common errors that developers made themselves during pre-release testing (and foresee the same to be the encountered by most users) -

1. The terminal shows an error locating the file and shows some incomplete file path as reference. The obvious reason would be ***spaces* present in your file path**. Make sure that your paths don't have spaces.

2. The terminal shows an error that your file could not be found and gives a trimmed or truncated filename (e.g. input_model_.tx ^r). In that case, the most probable source of error could be ***spaces* after the filenames in the *rundata* file.** Make sure that there are no trailing spaces.

3. The terminal shows an error that your file could not be found and refers to a proper filename. In such cases, you can do few checks. First, make sure the SHETRAN input **filenames** in the rundata correspond to those given in the model folder - **spelling and case**. Secondly, check whether you have all the files you have specified in the *rundata* in the model folder. Further, re-confirm the model folder that you had selected from the PAC GUI. Lastly, sometimes its the folder permission issues that throws such errors. If that is the case, changing folder of PAC and/ or the model and other input field would help.

4. Lastly, check whether your SHETRAN model runs or not. Trying to run hundred simulations with PAC using a ***faulty model*** doesn't make it right. Thus, errors pertaining to SHETRAN (e.g. input file formatting, violation of flow criteria, convergence of solution, etc.) should be fixed before augmenting your model with PAC.

3

Pre-release Tests

This chapter gives you full information regarding the PAC pre-release tests.

Estimated read time: *15 minutes*

3.1 Linux distros compatibility

The current release of PAC (version 1.0.tesla) is compatible through most Ubuntu-based Linux distributions (refer Table 3.1). Ubuntu and Linux Mint are among the most popular Linux distros out there and PAC runs flawlessly on both of them. Unfortunately for now, PAC is not compatible for other popular Linux systems like Red Hat or RedHat-based systems (like Fedora, CentOS) and OpenSUSE. Drastic improvement in OS compatibility is among the top agenda for the developers in the next release of PAC.

The compatibility tests for PAC have been carried out on almost a dozen of popular Linux distros (distributions) as shown in Table 3.1. The screenshots of PAC tests being successfully carried out have been added for readers' reference (Figure 3.1 through Figure 3.5).

Table 3.1: PAC compatibility test results on Linux Distributions

Linux Base	Linux Distribution	Does PAC work?
Debian	Ubuntu 16.04.2 x64	Yes
Ubuntu, Debian	Linux Mint 18.1 x64	Yes
Ubuntu, Debian	Lubuntu 16.04 x64	Yes
Ubuntu, Debian	Kubuntu 16.04.2 x64	Yes
Ubuntu, Debian	Zorin 12.1 x64	Yes
Ubuntu, Debian	Xubuntu 16.04 x64	No
Ubuntu, Debian	Linux Lite 3.4 x64	No
SUSE Linux	OpenSUSE 42.2 x64	No
Fedora, RedHat	Cent OS 7 x64	No
RedHat	Fedora 25.1.3 x64	No
Arch Linux	Manjaro 17.0.2 x64	No

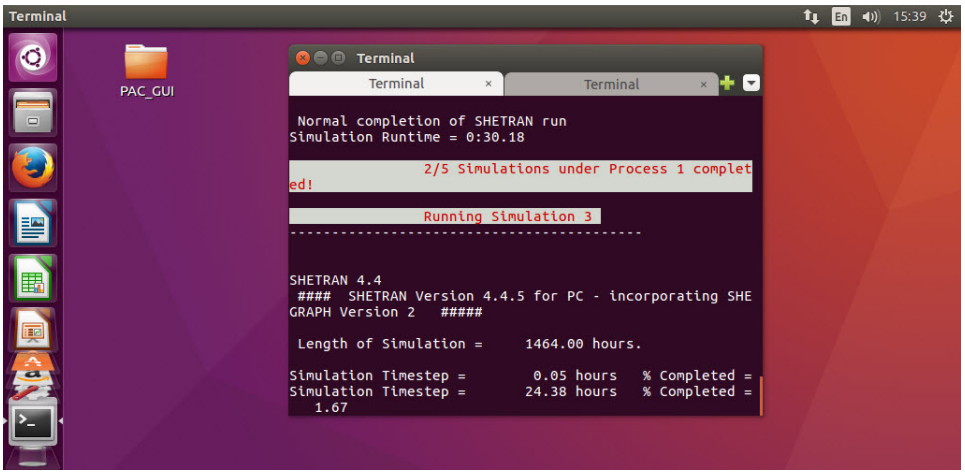


Figure 3.1: Successful PAC run in Ubuntu

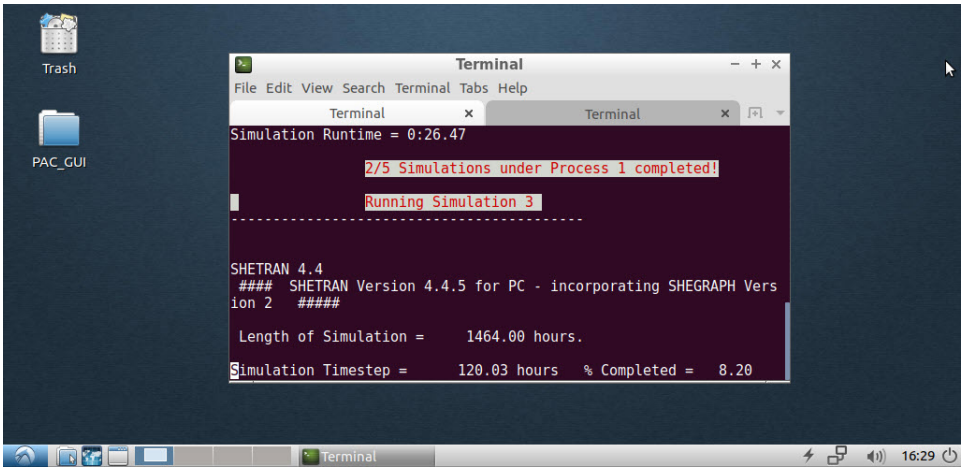


Figure 3.2: Successful PAC run in Lubuntu

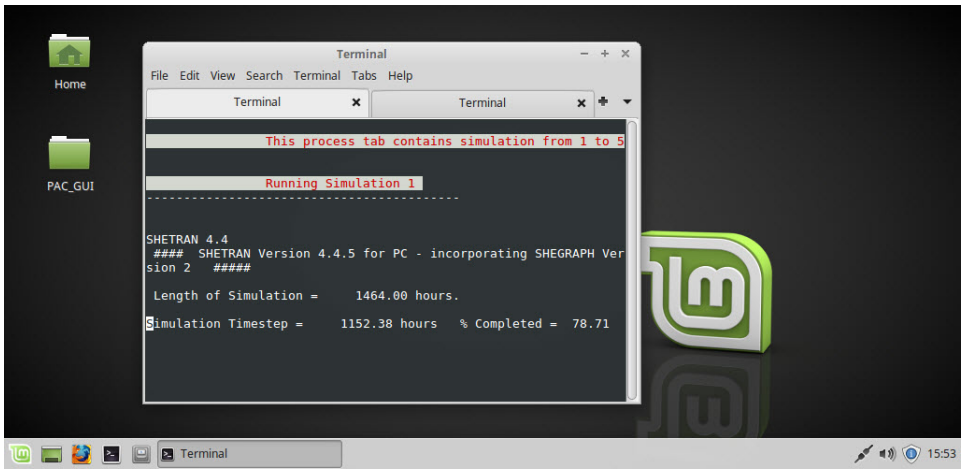


Figure 3.3: Successful PAC run in Linux Mint

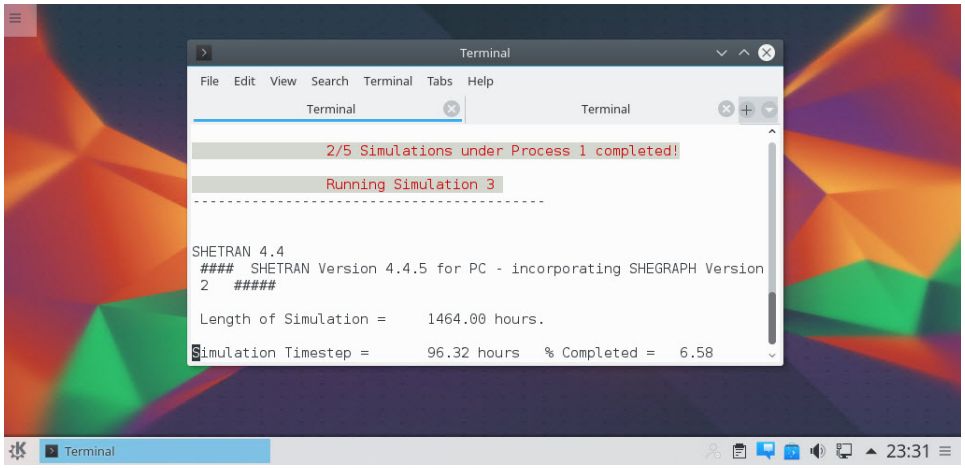


Figure 3.4: Successful PAC run in Kubuntu

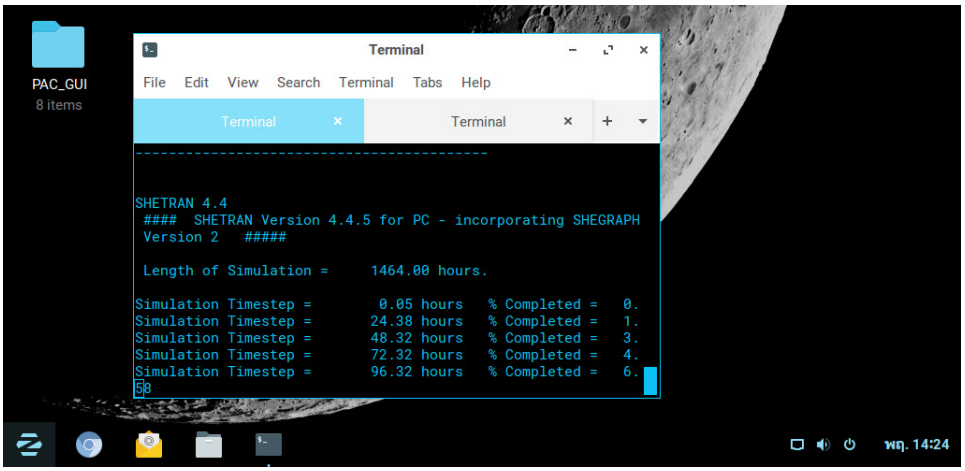


Figure 3.5: Successful PAC run in Zorin

3.2 Test Models

Four models with varying complexities were used for pre-release testing of PAC (refer Figure 3.6). The models (except Kathmandu[1]) are included in the SHETRAN download package bundle.

The models differ in terms of geographical location (Nepal, UK, Argentina), geographical size of the catchment (refer Figures 3.8), computational size (refer Figures 3.7) and model components incorporated. Thus a range of complexities were incorporated in the pre-release testing of PAC as shown in Table 3.2 and Figures 3.8 and 3.7.

Table 3.2: Pre-release Test models for PAC

Characteristics	Dunshop	Kathmandu	Slapton	Cobres
Geographical Location	UK	Nepal	UK	Argentina
Geographical Size	25 km^2	602 km^2	1 km^2	704 km^2
Computational Size				
Grid size	100 m	700 m	50 m	2000 m
Computational cells	2466	1229	376	176
Additional modules enabled (apart from water flow)	-	GW abstractions, Observation wells output	Contaminant transport (CMD file), Full set meteorology input (MED file)	Sediment transport (SYD file)

[1]Shrestha PK, Shakya NM, Pandey VP, Birkinshaw, SJ and Shrestha S (2017). Model-based Estimation of Land Subsidence in Kathmandu Valley, Nepal. *Geomatics, Natural Hazard and Risk* http://dx.doi.org/10.1080/19475705.2017.1289985

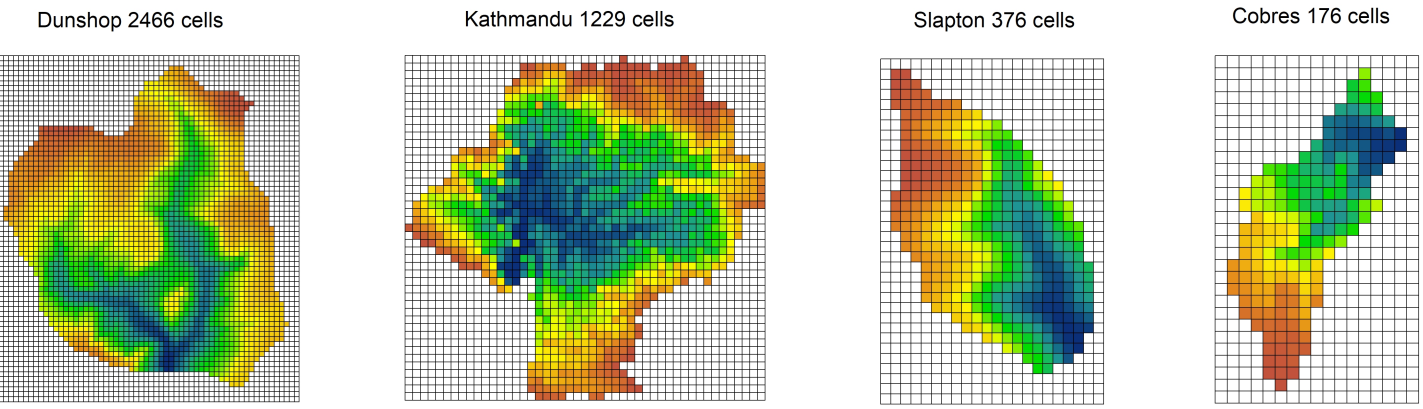


Figure 3.6: PAC pre-release test models - SHETRAN model grids

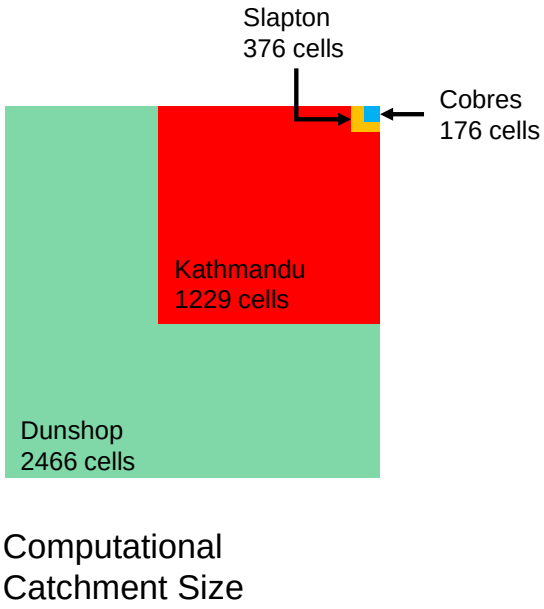


Figure 3.7: PAC pre-release test models - Computational size comparison

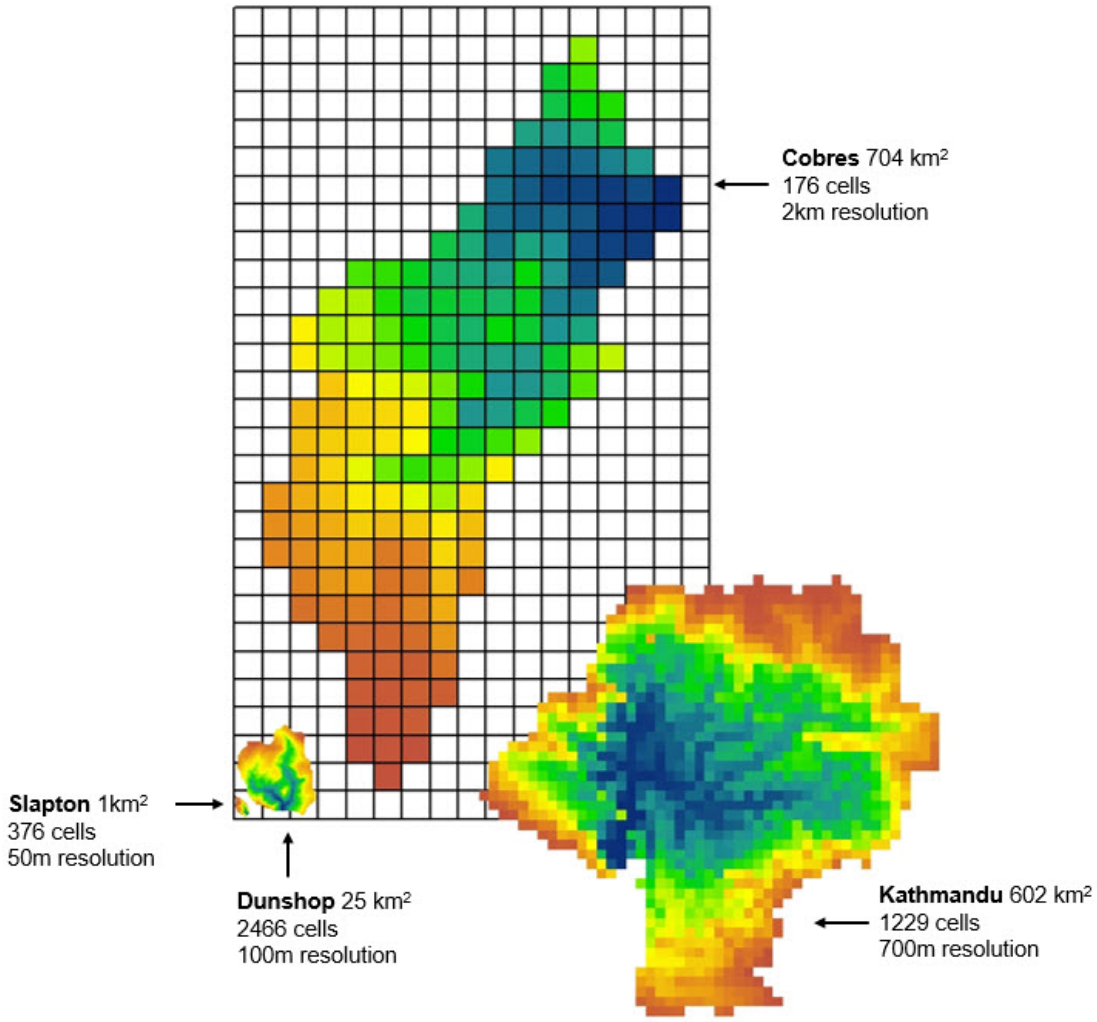


Figure 3.8: PAC pre-release test models - Geographical size comparison

3.3 Speed Up and Performance

The speed up performance of PAC on the previously mentioned models are as shown in Figure 3.9. The corresponding time of the model runs are depicted in Figure 3.10 which was also discussed in brief in Section 1.2. Thus we conclude that there is a tremendous relief in the time resource demand from SHETRAN when augmented with PAC on a resourceful machine.

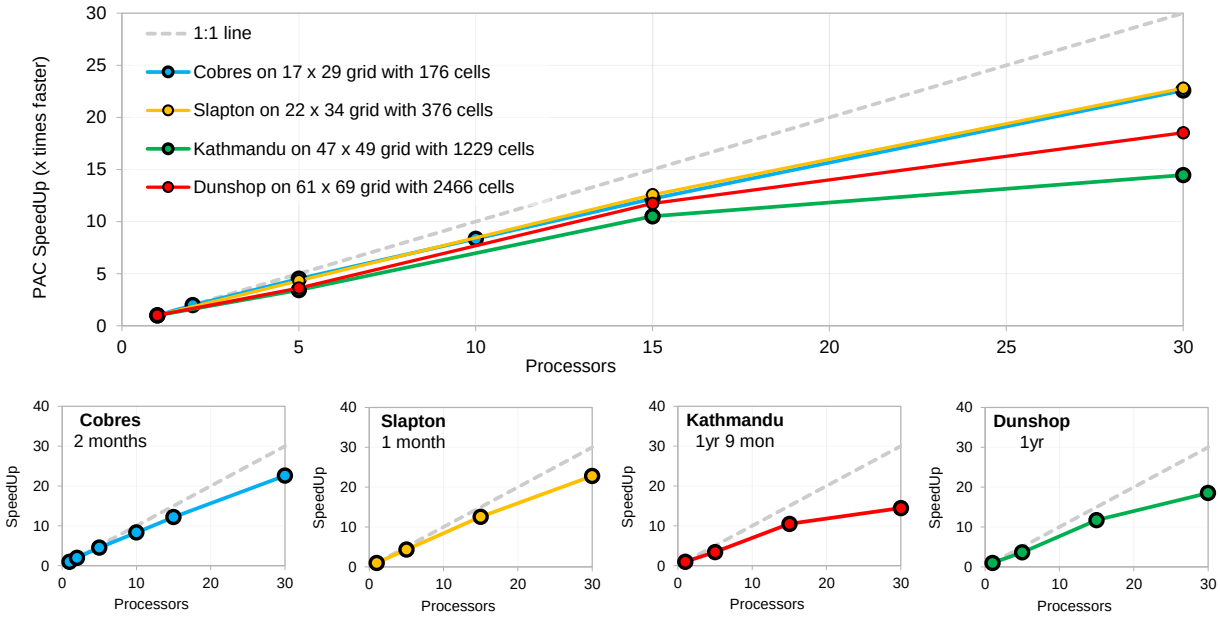


Figure 3.9: PAC speed up performance on models of various complexities

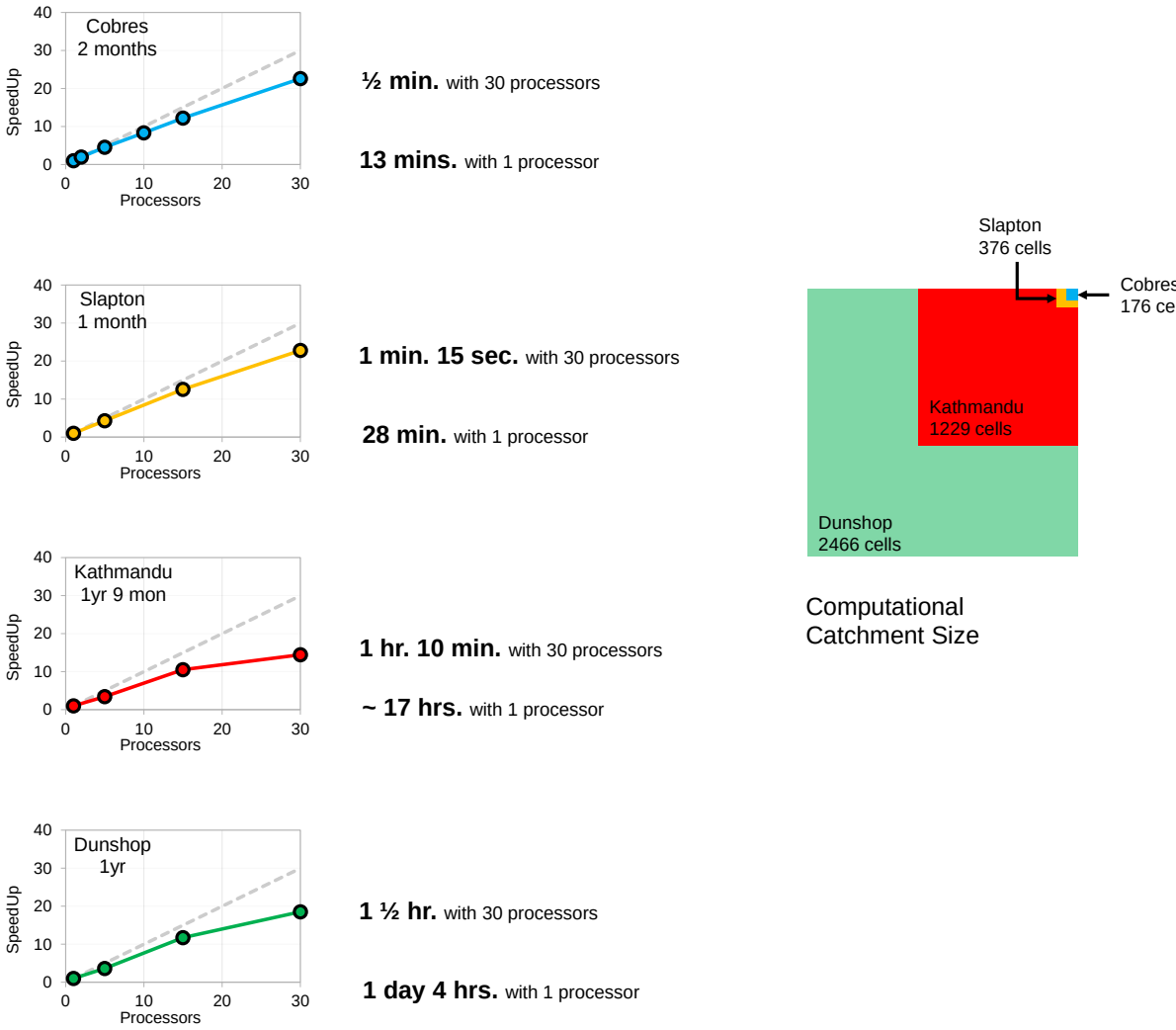


Figure 3.10: Runtime saved with PAC: Test results

4

Windows work around for PAC

Welcome Windows users. This section will show you the detailed work around for using PAC in PCs with Windows OS.

Estimated read time: *10 minutes*
Estimated tutorial time: *30 more minutes* [excluding download time]

Step 1: Download Virtualization Software.

- We shall use the Oracle VM VirtualBox among other options.
- Google *Oracle VM VirtualBox* and go to the website (https://www.virtualbox.org/).
- On the main page, click **download** option (Figure 4.1) and then **windows host** in the next page (Figure 4.2).
- Your download should begin. Open the downloaded installer file and install VirtualBox.
- Open VirtualBox and your screen should have a similar windows as shown in Figure 4.3



Figure 4.1: Download VirtualBox - click on *Downloads*



Figure 4.2: Download VirtualBox - click *Windows hosts*

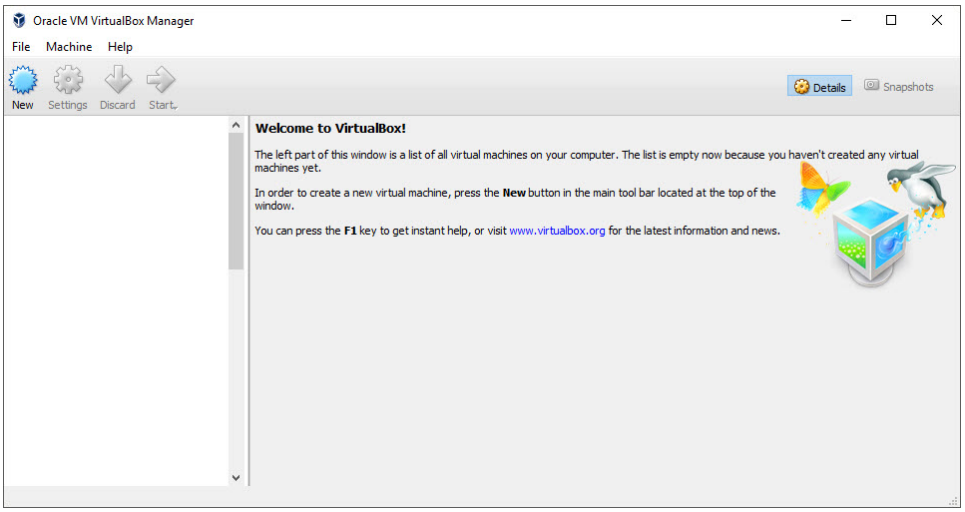


Figure 4.3: VirtualBox StartScreen

Step 2: Download our pre-customized Virtual Machine file (.vdi) from cloud

- Use this link for download from cloud -

  https://mega.nz/#!ISB33J4S!HsV5JJsDyOwrgV3w5hrlWvYjXd4Z5NGd87tGnBor070

  Note that the login information to this OS are -

  - username: *pkshrestha*
  - password: *pacsac*

- After clicking the above URL, it should prompt you in your browser page as shown in Figure 4.4.

- Although the file size is large (around 1 GB), with good internet speed the download should be completed in under 30 minutes.

- The Linux OS being provided is Lubuntu. We chose Lubuntu for two reasons. First, it is very lightweight yet powerful enough for the current purpose. Secondly, Lubuntu has one of the fastest OS startup and shutdown time[1] among the Linux distros tested.

[1] startup time $<$ 30 seconds, shutdown in $<$ 5 seconds

- Open VirtualBox if you haven't already, and click the *new* button in the menu. Give a name for the Virtual OS that includes the word *Linux*. (Figure 4.5). Also adjust the RAM you want to dedicate to this OS (Figure 4.6). You can always change this later so don't worry.
- In the next window (Hard Disk), use the third option of selecting an existing virtual hard disk file (Figure 4.7) and browse for the file that you had previously downloaded from cloud (Figure 4.8).
- If everything goes straight, you should see a Virtual OS added to your list as shown in Figure 4.9. Congratulations on successfully importing our pre-cutomized LinuxOS!

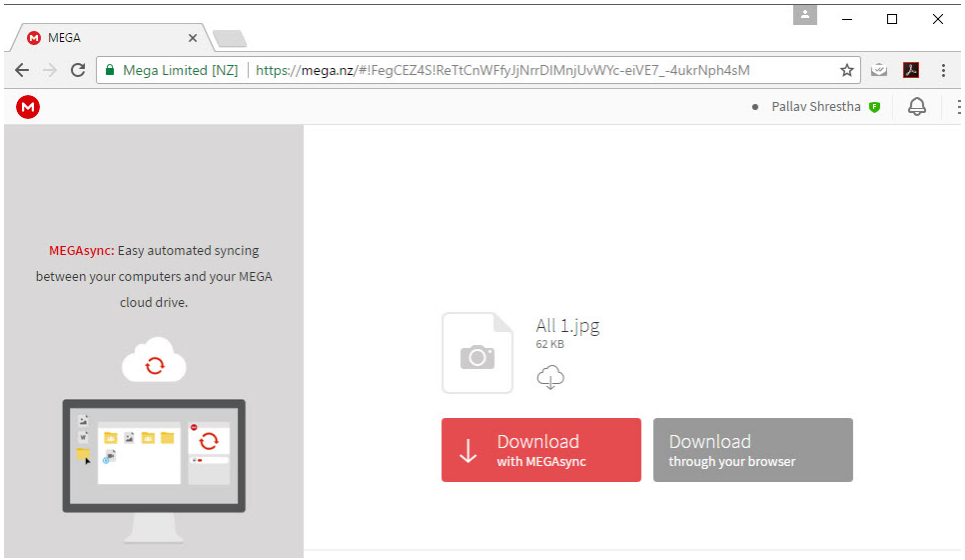


Figure 4.4: Downloading pre-customized .vdi file - click on the *grey Download* tab

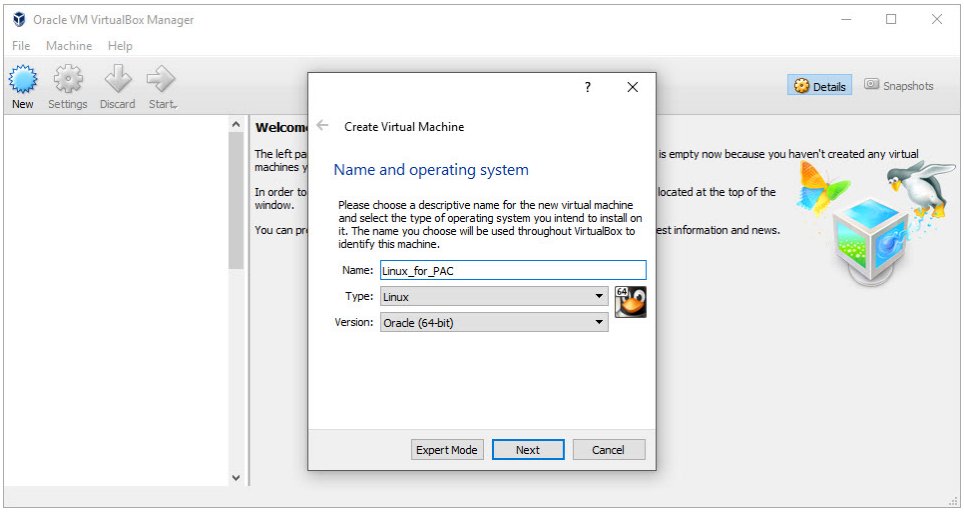


Figure 4.5: Importing .vdi file in VirtualBox - click on the *New* button and write a name containing the word *Linux*

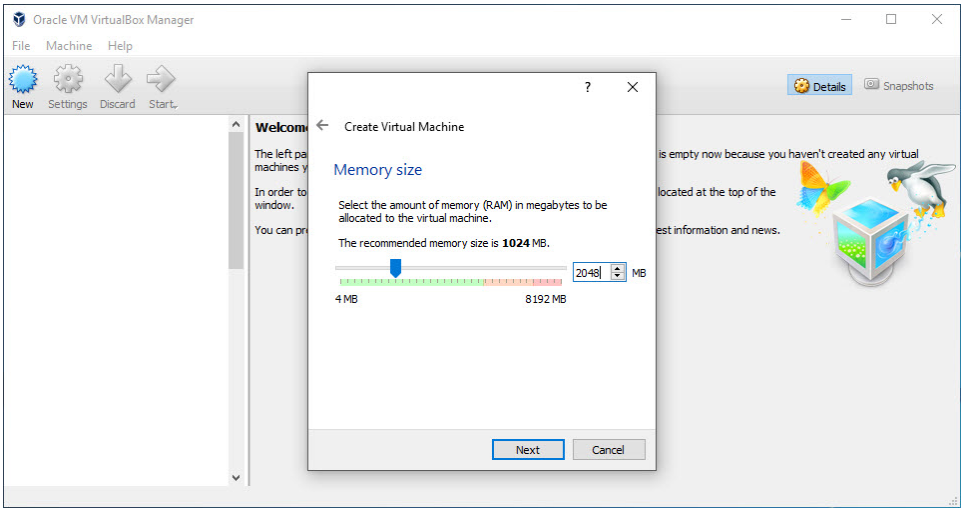


Figure 4.6: Adjust the amount of RAM you want to dedicate to this Virtual OS

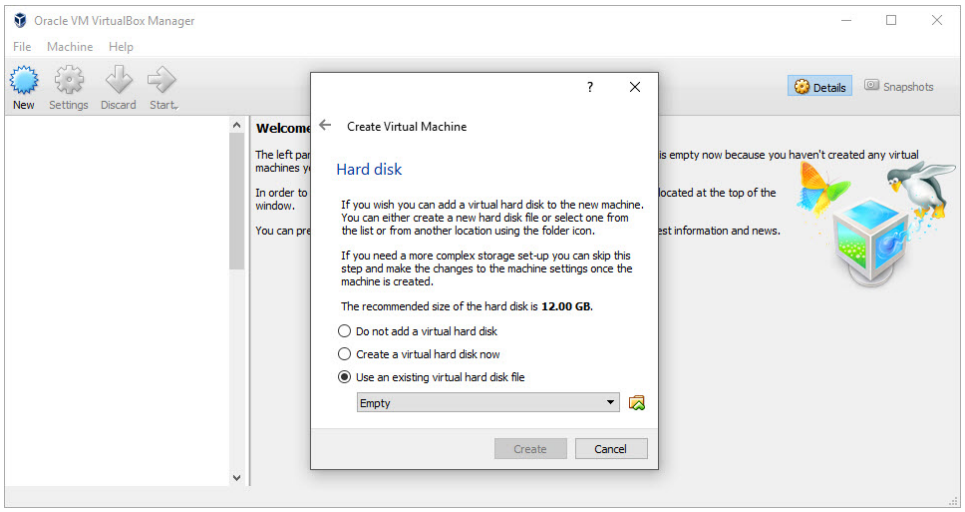


Figure 4.7: Select the .vdi file using the third option

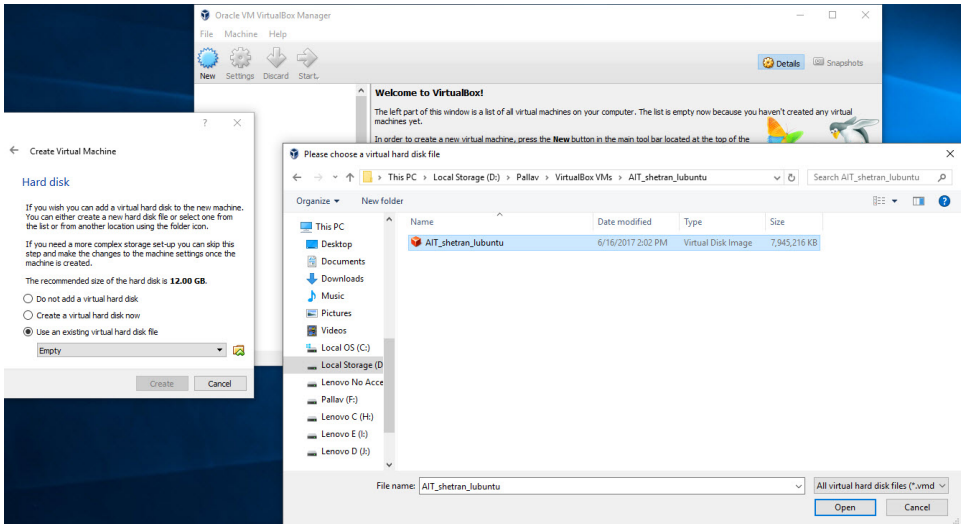


Figure 4.8: Browse for the downloaded .vdi file and select it

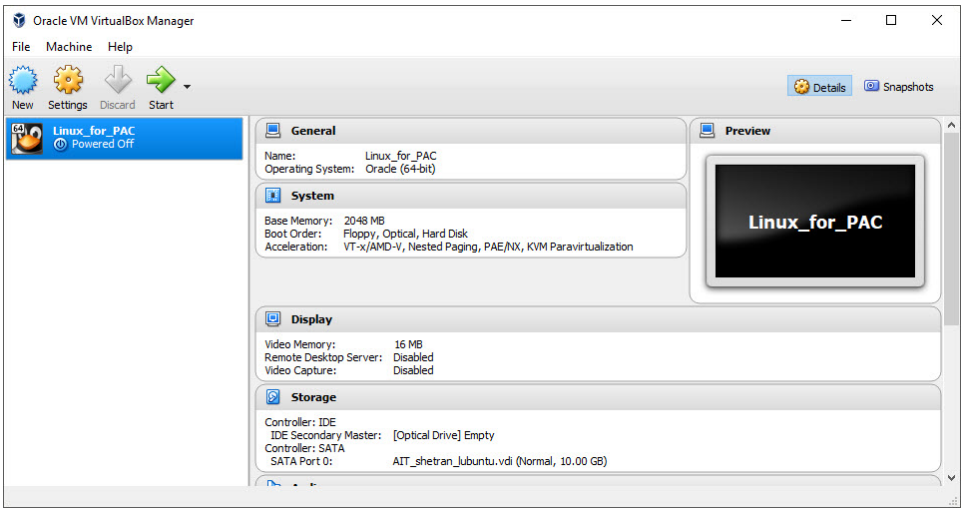


Figure 4.9: Congratulations, you have successfully imported the .vdi file

Step (additional): There are some additional steps that we recommend you to do for the VirtualBox to work properly:

- From the same website, download the **Extension Pack** for VirtualBox as shown in Figure 4.10. A successful installation should give you a message as shown in Figure 4.11.

- Now you will make few changes in the setttings of the newly added OS. Selecting the OS, click on the *settings* button on the menu. From the General tab, change the *shared clipboard* and *drag n drop* to *bidirectional (Figure 4.12)*. From the *system* tab, change the RAM (if necessary) and increase the number of processors to at least 2 (Figure 4.13). Lastly, in the *USB* tab, select 2.0 option (Figure 4.14). This is a backup plan. In case the *shared clipboard* and *drag n drop* doesn't work between the host (Windows) and guest (Linux), you can transfer files using a USB.

- Now please proceed forward to complete **Step 3**. After that you can come back here to finish this last additional step. In the Virtual OS, mount the Guest Addition CD image as shown in Figure 4.15. A new icon will appear in the desktop. Right click on it and select *Open in Terminal* (Figure 4.16). Now a DOS like dialog box (aka Terminal in Linux) will appear. Type **./autorun.sh** and press enter (Figure 4.17). Enter the Virtual OS password (pacsac) if prompted (Figure 4.18). After the process is finished press enter again (Figure 4.19). Guest

Additions installation is finished! Now eject the CD image as shown in Figure 4.20 and reboot the Virtual OS (Figure 4.21).

- Well done, you have finished all the additional jobs.



Figure 4.10: Additional steps - download the extension pack by clicking on *all supported platforms*

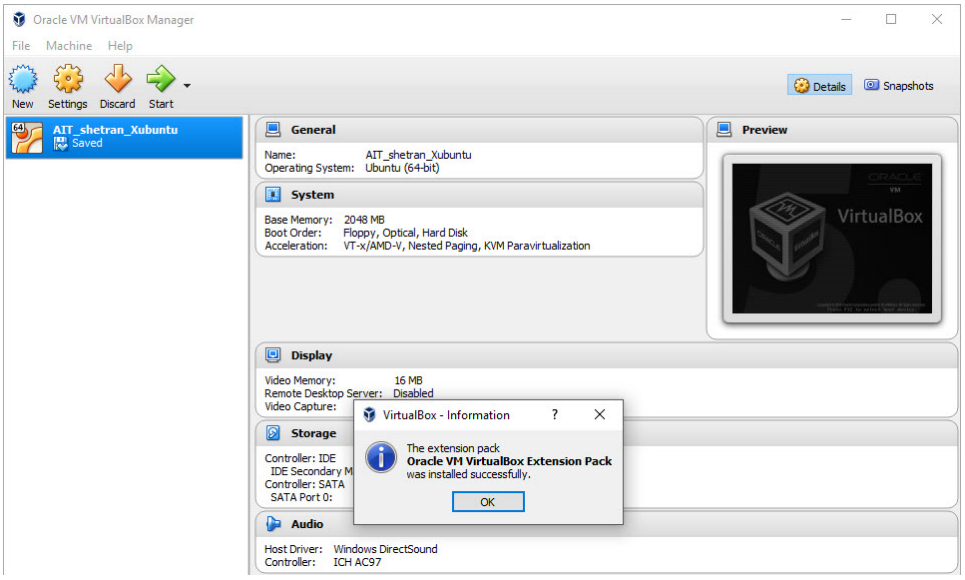


Figure 4.11: Additional steps - Extension pack installed!

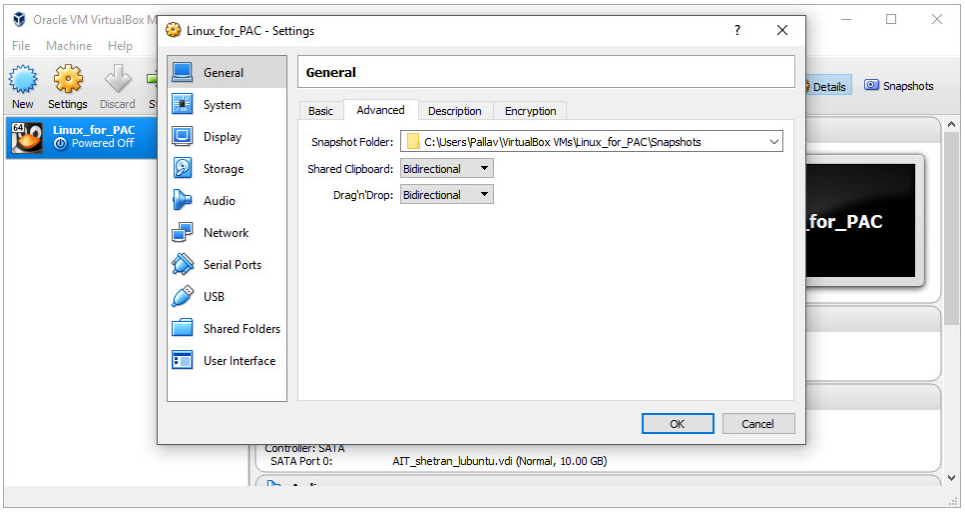


Figure 4.12: Changing settings - enabling *Shared Clipboard* and *Drag n Drop* between Windows and Linux

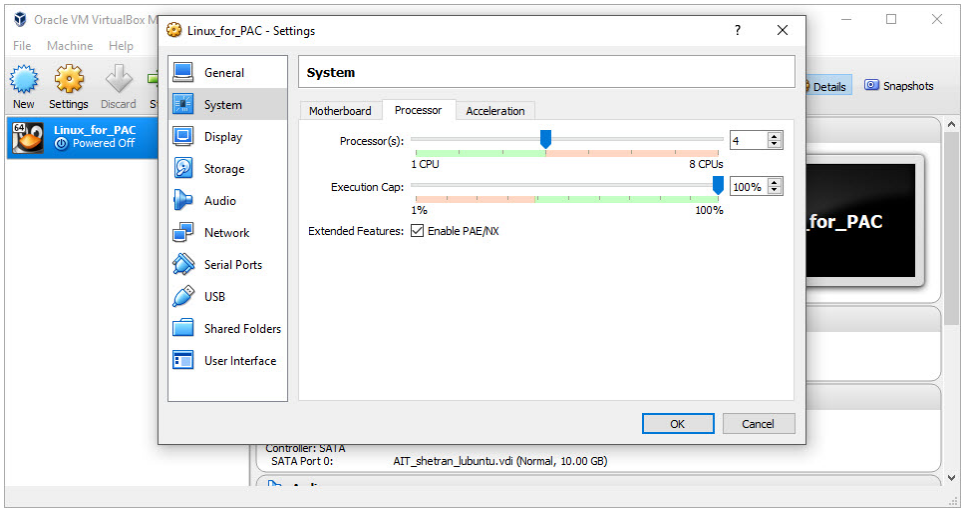


Figure 4.13: Changing settings - adjusting the number of processors dedicated to teh Virtual OS

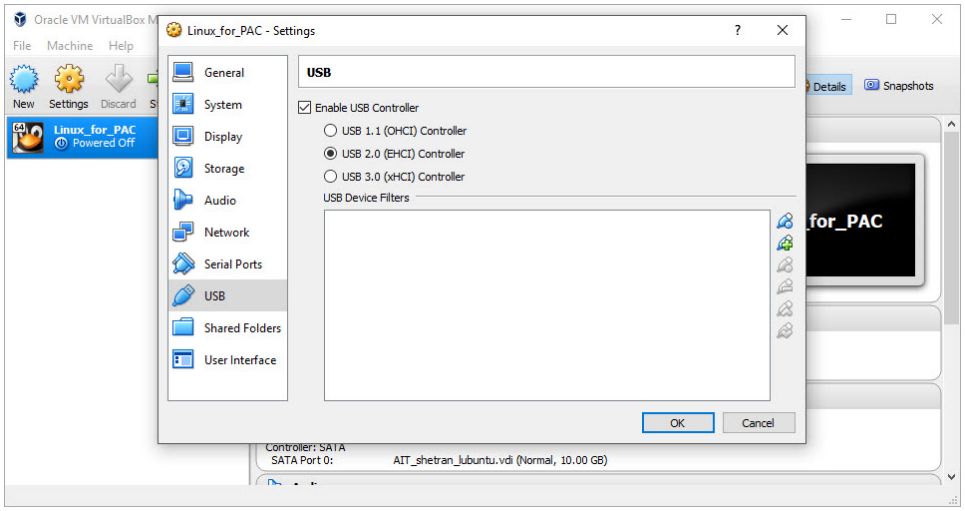


Figure 4.14: Changing settings - enabling USB

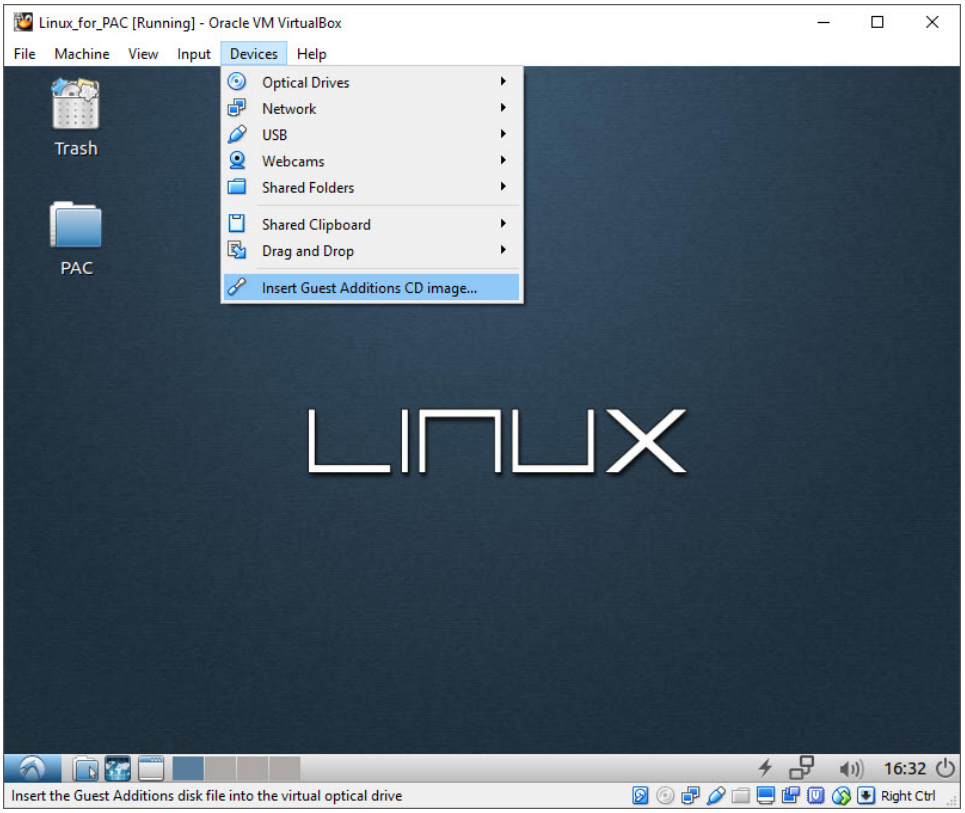


Figure 4.15: Installing Guest Additions - mounting the CD image

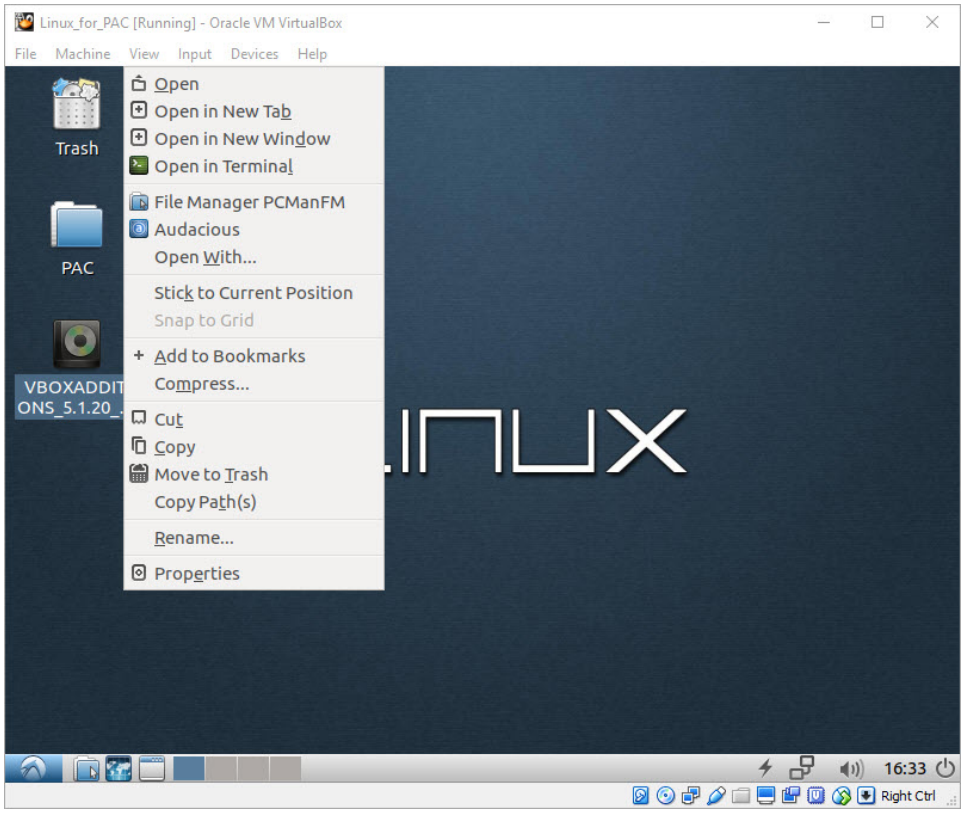


Figure 4.16: Installing Guest Additions - right click on the new icon and click *Open in Terminal*

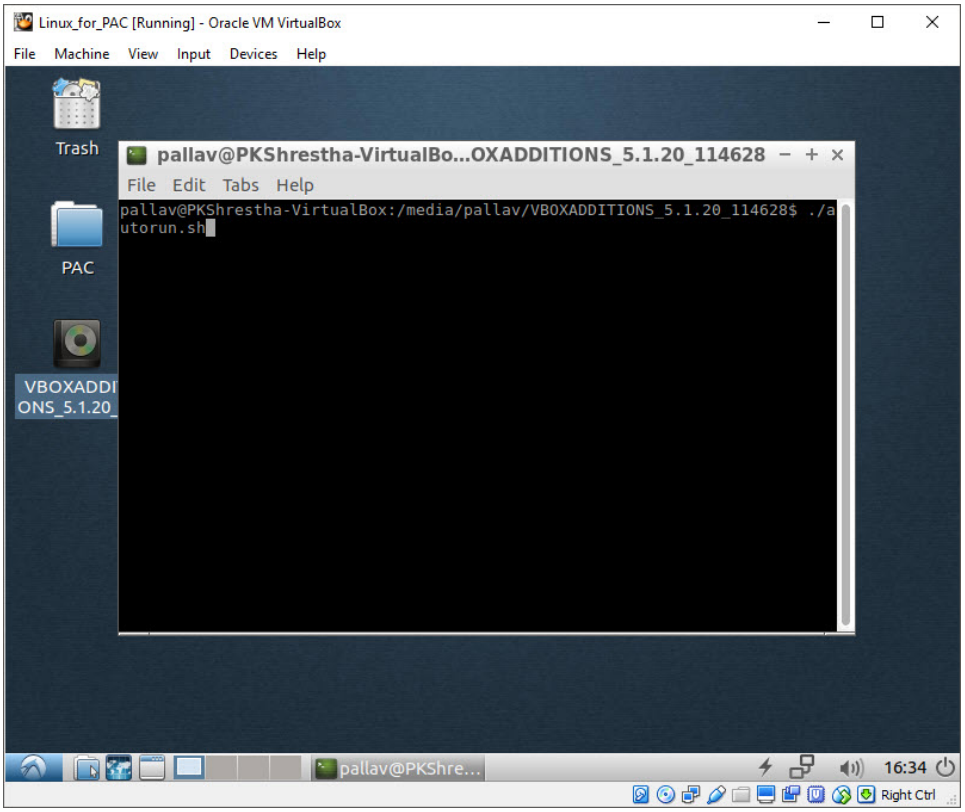


Figure 4.17: Installing Guest Additions - type *./autorun.sh*

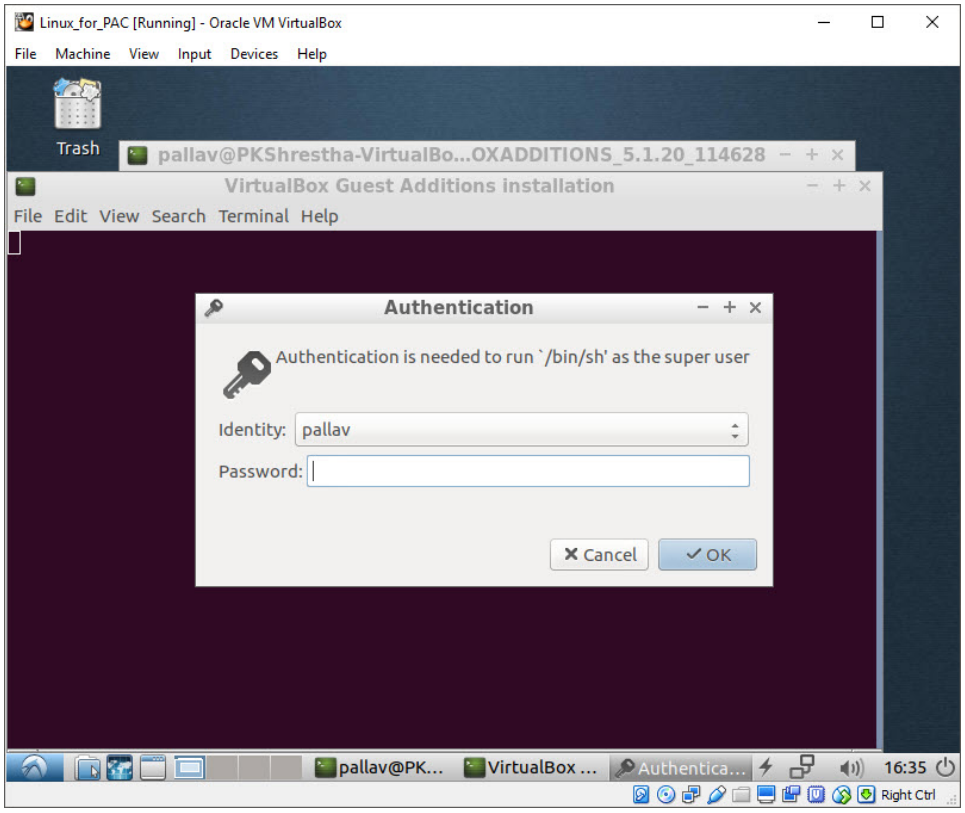


Figure 4.18: Installing Guest Additions - Enter the password of the OS if prompted

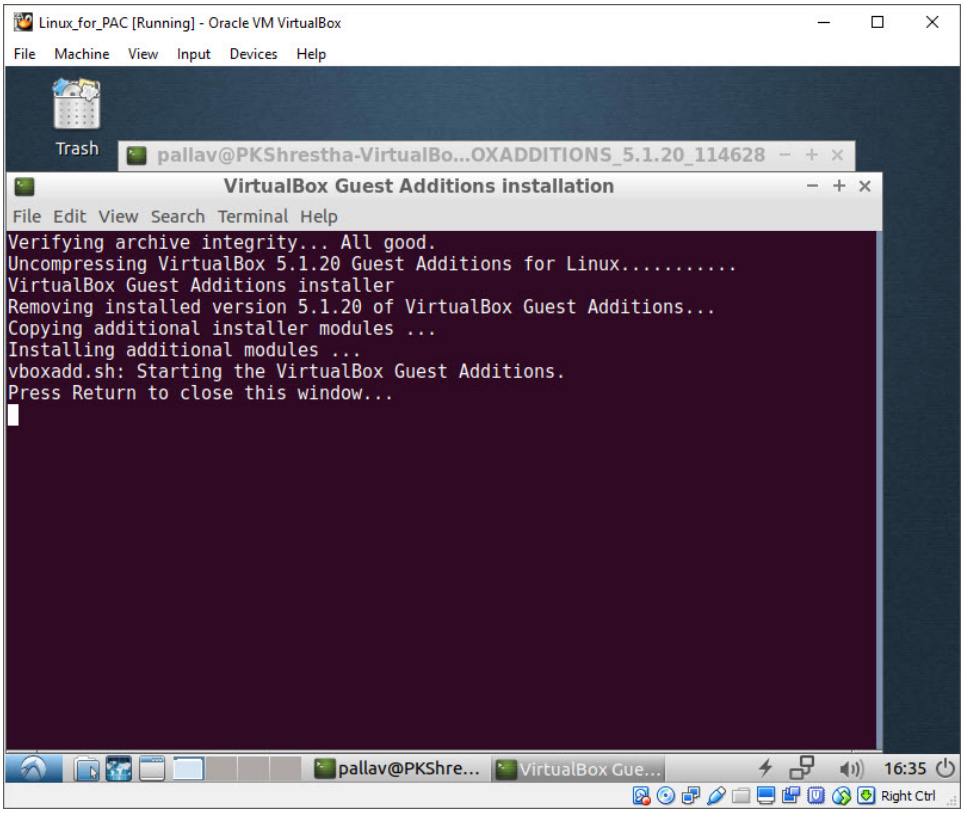


Figure 4.19: Installing Guest Additions - Press enter (Return) after process finishes

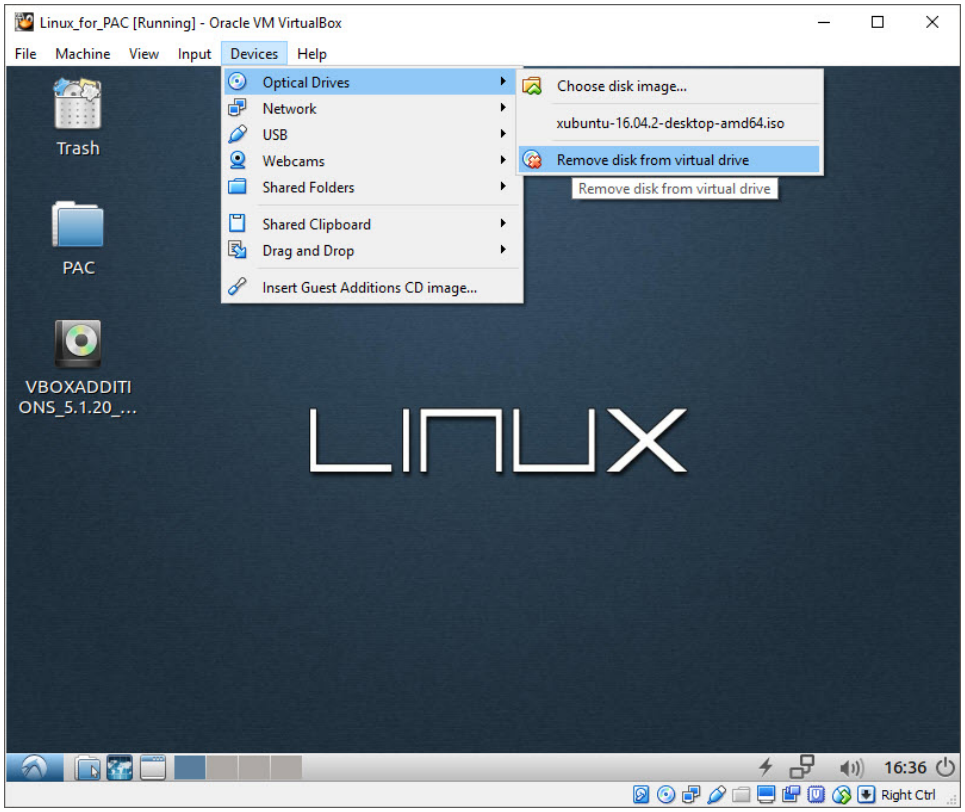


Figure 4.20: Eject the Guest Additions CD image

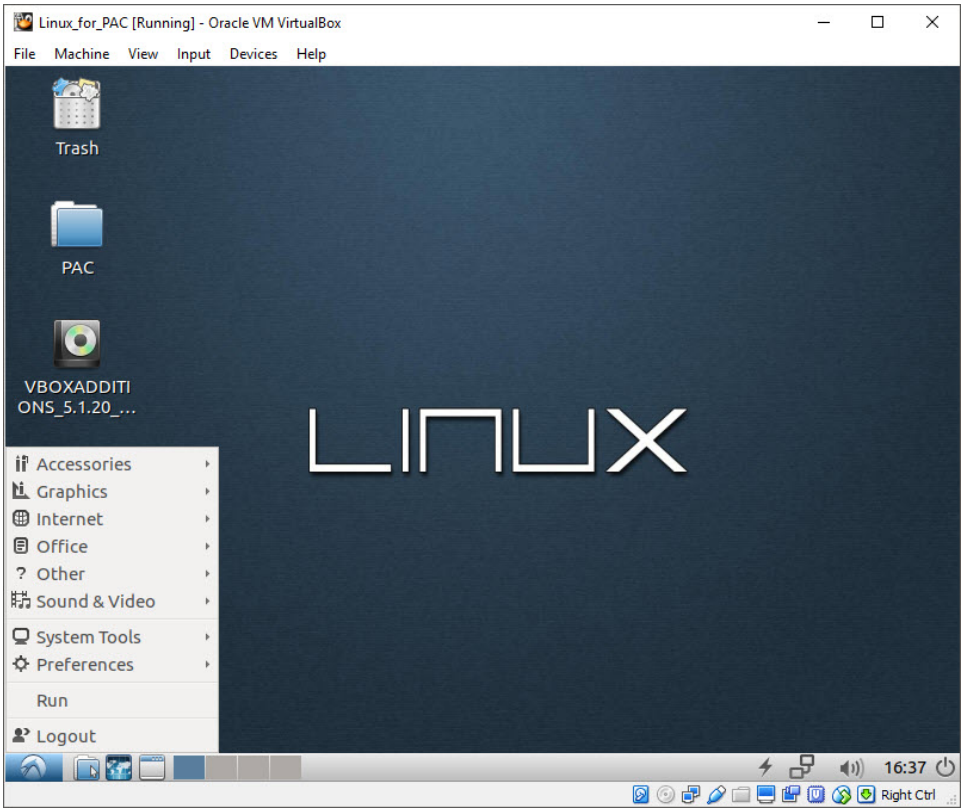


Figure 4.21: Almost done... Reboot the OS (startup menu is on bottom left)

Step 3: Enter the Virtual Linux OS and use PAC

- Selecting the newly added Virtual OS, press the Enter button in the menu. You should get a loading screen as shown in Figure 4.22. Congratulations, you now have a running Linux OS (*Guest*) inside of your Windows OS (*Host*). PAC is awaiting your orders in the desktop folder.

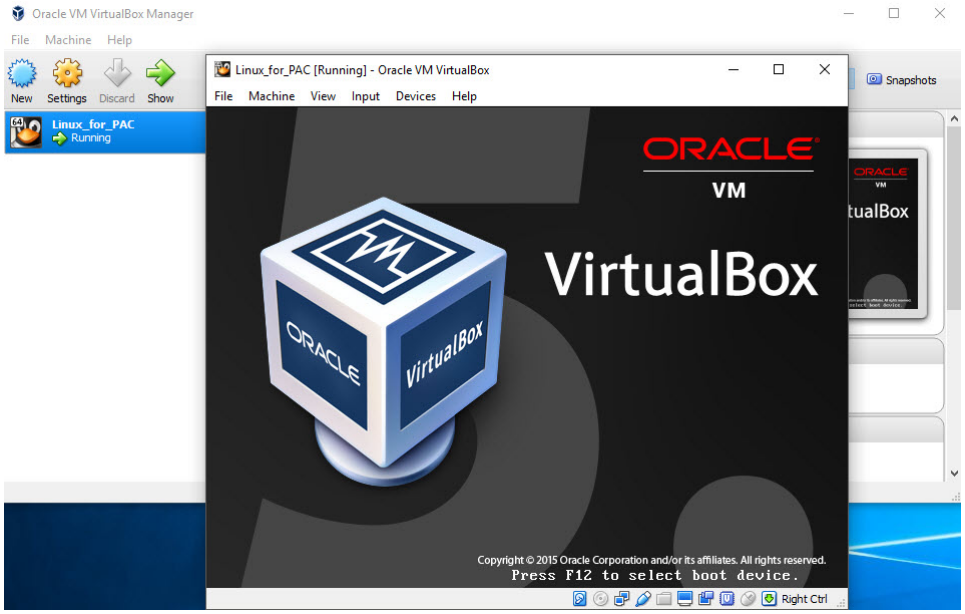


Figure 4.22: Loading Virtual Linux OS

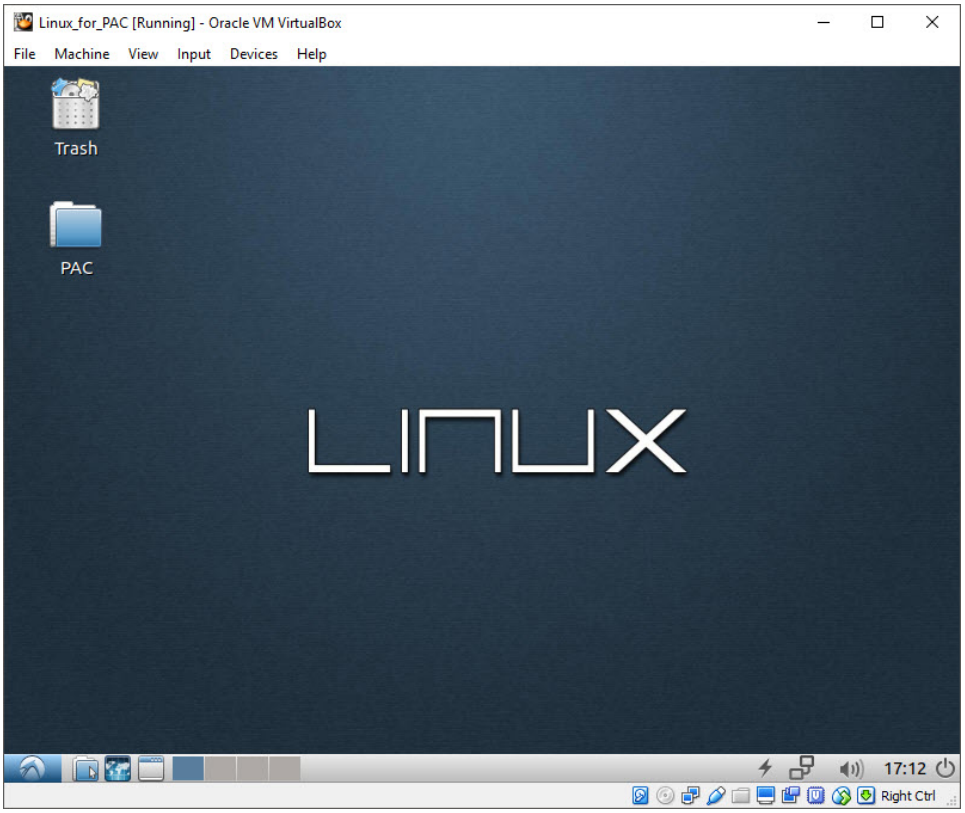


Figure 4.23: Virtual Linux OS ready!

5

PAC versus SWAT Cup

You are a SWAT or a SWAT Cup user. You want to know how different is PAC from SWAT Cup. Or you want to know which of the two is better suited for your modeling needs. You have come to the right place!

Estimated read time: *10 minutes*

5.1 Usage

The common thing about PAC and SWAT Cup is that they both use parallel processing to augment model run time. However, the two programs are quite contrasting in terms of functionality as discussed in the following couple of points -

- SWAT Cup was developed for optimization of SWAT model parameters. For this, it does parallel model runs changing model parameters' values based on input range of parameter values. But model inputs such as meteorology or land use can not be changed in SWAT Cup. PAC, on the other hand, doesn't come with optimization capabilities. However, PAC comes with greater flexibility and allows users to change model inputs in addition to model parameters. Thus, with PAC one can do scenario analysis (model input like rainfall, land use change).

  E.g. A simulation set from 1000 stochastics based rainfall realizations requires just a single PAC run. However, SWAT Cup is not able to do this. Instead, one will have to run the model itself (SWAT) 1000 times, each time changing the input rainfall manually.

- In SWAT Cup, user inputs the range of parameters. However, the value of the parameter within that range is not under user's control. On the contrary, in PAC, the value of the parameter is completely under user's control.

Table 5.1: Comparison of usage of PAC and SWAT Cup

Feature/ Run	**PAC**	**SWAT Cup**
Download site	https://www.researchgate.net/publication/...	http://www.neprashtechnology.ca/downloads/
License	Completely free	Free but parallel processing over 20 simulations requires license
Hydrological model	SHETRAN	SWAT
Pre-processing	SHETRAN-GUI/ Manual (PAC doesn't play role in Pre-processing)	ArcSWAT/Other Programs/ Manual (SWAT Cup doesn't play role in Pre-processing)
Model Setup	SHETRAN-GUI/ SHETRAN standard (PAC doesn't play role in Model setup)	ArcSWAT/Other Programs/ Manual (SWAT Cup doesn't play role in Model setup)
Model Optimization	N/A	Yes (SWAT Cup is auto optimization tool for SWAT)
User Defined Runs	Yes (PAC can be used for user defined runs)	N/A (SWAT Cup doesn't have this feature)
Sensitivity analysis	Manual input preparation. Automated simulation	Automatic input and simulation
Sim A: 10 Climate Models x 4 Climate Change Scenarios X 4 Land Use Scenarios = 160 runs	1 PAC run (automated, parallel runs)	SWAT Cup isn't able to do this. 160 SWAT runs required (manual, individual runs)
Sim B: 1000 stochastic rainfall realizations	1 PAC run (automated, parallel runs)	SWAT Cup isn't able to do this. 1000 SWAT runs required (manual, individual runs)
Sim C: Sim A x decadal land use change over 100 years = 1600 runs	10 PAC runs, one for each decade of model time frame (automated, parallel runs)	SWAT Cup can't do this. 1600 SWAT runs required (manual, individual runs)

E.g. For a range of 0 to 10 and 5 simulations, SWAT Cup (under SUFI-2) sub-divides the range into 0-2, 2-4, 4-6, 6-8, 8-10 and selects one value within each sub-range based on a randomization algorithm. However, PAC allows user to select the 5 parameter values for the 5 simulations. That can be (1,3,5,7,9) or (1,2,3,4,5) or (1.0,1.1,1.2,1.3,1.4) and so on.

Further comparison of usage between PAC and SWAT Cup is tabulated in Table 5.1.

5.2 Speed up

The speed up achieved using PAC and SWAT Cup in test runs are shown in Figure 5.1. It is seen that PAC is on par with SWAT Cup in terms of reducing run time. However, the amount of speed up obtained depends upon the computational resources available.

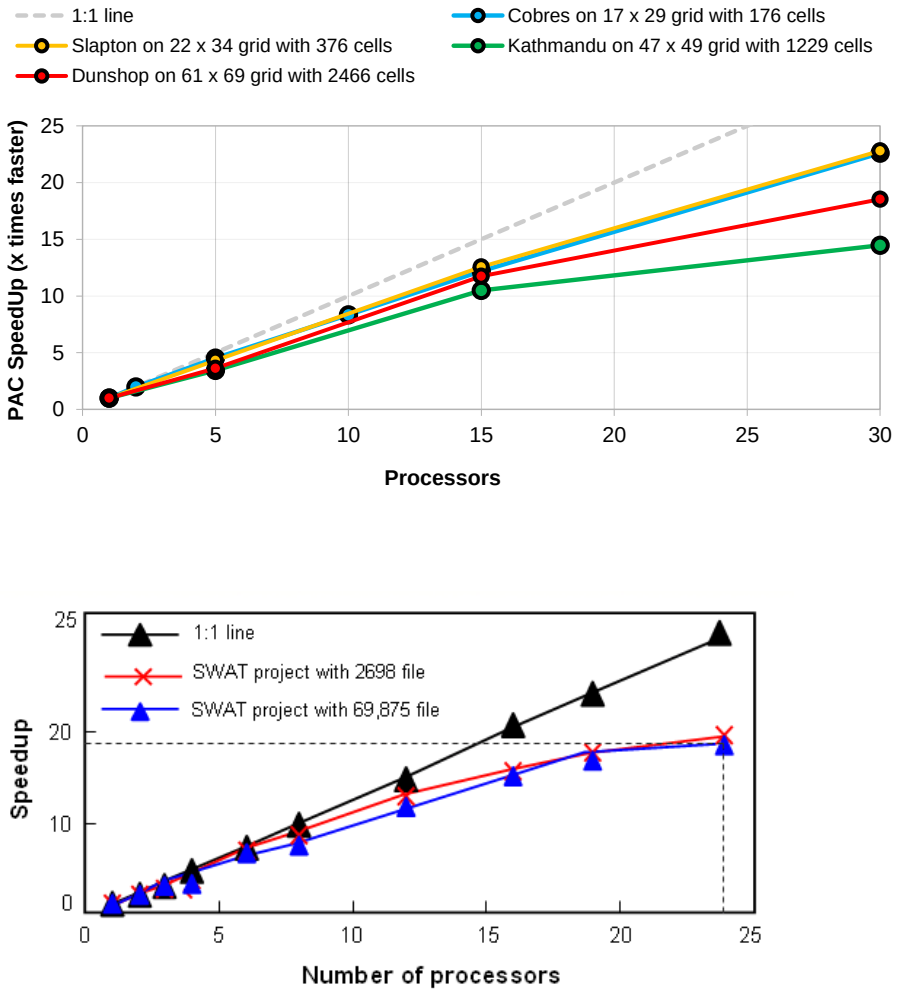


Figure 5.1: Comparison of speedup gained with PAC (top) to SWAT Cup (bottom). Source for SWAT Cup speedup graph: http://www.neprashtechnology.ca/products/

6

I want to learn SHETRAN - starter tips

Welcome modeling enthusiasts! This Chapter is the perfect place for you to gather information on SHETRAN and start exploring its modeling capabilities

Estimated read time: *45 – 60 minutes*
Estimated exploration (learning) time: *2 weeks*

6.1 What is SHETRAN?

SHETRAN is a model for water flow, solute and sediment transport in river catchments. Thus it can be used for hydrological analysis (water flow), water quality analysis (solute transport) and erosion analysis (sediment transport).

SHETRAN is a finite-difference model in which the physics-based governing partial differential equations for flow and transport are solved on a three-dimensional grid. Thus, SHETRAN is a PBSD model (physically-based, spatially-distributed). The plan area of the catchment in SHETRAN is usually in the range of one to a few thousand square kilometers and the horizontal depth of the subsurface is usually less than 100m.

The catchment is conceptualized as an ensemble of columns (refer Figure 6.1) and networks of stretches of channels, called river links. Each column is a stack of computational cells containing information of land cover/ vegetation type at the top and sequential depth of soil/s horizons underneath it. Each river link runs along the edge of a column. SHETRAN works out the

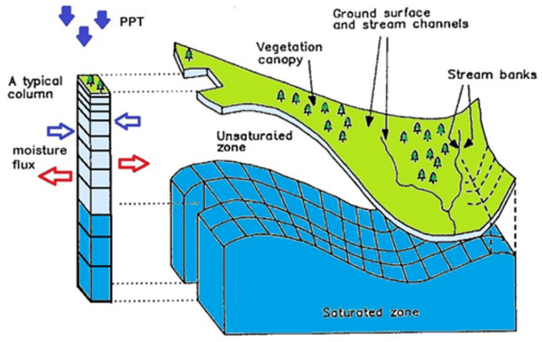


Figure 6.1: Conceptualization of catchment hydrology in SHETRAN (PPT - precipitation)

water balance in each column. The net outcome of hydrological processes at all the columns is the hydrological behavior of the catchment.

With its origins in Système Hydrologique Européen, SHE (DHI, the British Institute of Hydrology and SOGREAH), SHETRAN has been developed within the Water Resource Systems Research Laboratory, School of Civil Engineering and Geosciences, University of Newcastle upon Tyne. Steve (stephen.birkinshaw@newcastle.ac.uk) is the curator of the software as well as the software hosting site.

6.2 Is SHETRAN the right model for my research?

You will probably get the answer to this important question after carrying out following steps -

1. First, check whether SHETRAN includes the hydrological process/es that you want to model (refer Table 6.1)
2. Second, go thru the YouTube videos pertaining to SHETRAN setup and worked out examples in the Documents tab in the website. From this you should get clearer picture of what SHETRAN does.
3. Finally, check whether previous studies have used SHETRAN for a similar research task by scanning through to the list of SHETRAN publications in the Publications tab in the website.

Table 6.1: Components and Processes modelled by SHETRAN

Water flow	**Sediment Transport**	**Contaminant Transport**
Surface water flow on ground surface and in stream channels Soil-water and ground-water flow in unsaturated and saturated zones Includes systems of confined, unconfined, and perched aquifers	Soil erosion Multi-fraction transport on ground surface and in stream channels	Multiple, reactive solute transport on ground surface, stream channels and subsurface
• Canopy interception of rainfall • Evaporation and transpiration • Infiltration to subsurface • Surface runoff (overland, overbank, and in channels) • Snowpack development and snowmelt • Storage and 3D flow in variably saturated sub-surface • Combinations of confined, unconfined, and perched aquifers • Transfers between subsurface water and river water • Ground-water seepage discharge • Well abstraction • River augmentation and abstraction • Irrigation	• Erosion by raindrop and leaf drip impact and overland flow • Deposition and storage of sediments on ground surface • Total-load convection with overland flow • Overbank transport • Erosion of river beds and banks • Deposition on river bed • Down-channel advection • Infiltration of fine sediments into river bed	• 3D advection with water flow • Advection with sediments • Dispersion • Adsorption to soils, rocks, and sediments • Two-region mobile/immobile effects in soils and rocks • Radioactive decay and decay chains • Deposition from atmosphere • Point or distributed surface or subsurface sources • Erosion of contaminated soils • Deposition of contaminated sediments • Plant uptake and recycling (simple representation only) • Exchanges between river water and river bed

6.3 Newcastle University website

Visit the webpage below to start your SHETRAN journey. Its an "all-in-one" stop for SHETRAN resources including software, documentation and journal papers.

SHETRAN web page:

http://research.ncl.ac.uk/shetran/index.htm

This web page offers the following to its visitors -

- Background on SHETRAN
- SHETRAN applications Case studies
- SHETRAN documentation including user manual, theoretical documents and step-by-step worked out examples
- Publications on SHETRAN
- SHETRAN software
- Frequently asked questions

6.4 Downloading software

SHETRAN can be freely downloaded from a section that is dedicated to it in the Newcastle university website. The download page URL is -

http://research.ncl.ac.uk/shetran/Downloads.php

The download form asks for your name, email and plan of use (mainly for monitoring purpose). Filling out this form will take you to a download page with many information as shown in 6.2. However, in short, the page offers you two versions of SHETRAN -

- SHETRAN GUI (<3 mb)
- SHETRAN standard (<50 mb)

More details on the use of these two versions can be found in section 6.8. Over here we will further discuss on the contents of the download packages.

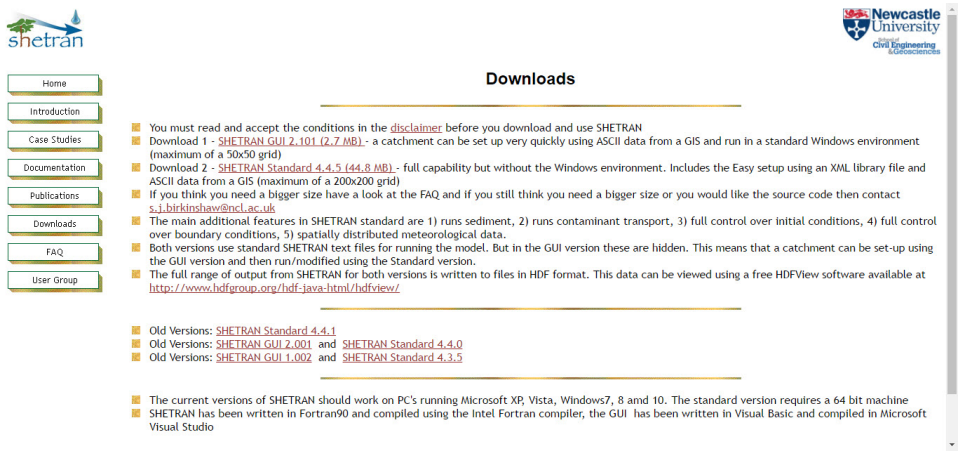


Figure 6.2: SHETRAN Download page after access

6.4.1 SHETRAN GUI download

The GUI version is only available for Windows OS and consists of a Windows installer. The installer sets up SHETRAN GUI in your machine. The installation also places files needed for step-by-step worked out example using the GUI. Take help from the documents named SHETRAN windows user guide and SHETRAN windows worked example and the YouTube video `https://youtu.be/7tvYoXxuje0` to get started with SHETRAN GUI!

6.4.2 SHETRAN standard download

This download consists of Windows and Linux versions of SHETRAN standard, easy setup system (this compensates lack of GUI in this version and helps in production of input files with proper formatting) and documentation. SHETRAN standard is a ready to use program without requiring any installation. Take help from the document named Shetran easy setup.pdf and the YouTube video `https://youtu.be/zYrDnVq5iD8` to get started with SHETRAN Standard!

6.5 Windows versus Linux

The SHETRAN standard version comes with Linux compatibility in addition to Windows OS. However, at the present release versions, there are few differences between the two -

1. The Windows version can be run by the usual "double click and then input in some dialog box that appears" method. However, for Linux version one has to run the program from the bash (similar to command

prompt in Windows). For that you need to go to the program location, open a bash there and type the following in bash-

» shetran-linux -f /path/to/rundata/file/rundata.txt

Where "rundata.txt" is the rundata file and the name of this file depends upon the given name.

2. Unlike the water flow output, the sediment and contaminant output are stored in .h5 (HDF5) file format in the Windows version. However, the Linux version is not capable of making this output at its current version. Due to this reason, the current Linux version made available is **not useful for sediment and contaminant modeling** and is useful for water flow only.

6.6 Documentation

The documents pertaining to SHETRAN can be accessed via the Documentation tab in the SHETRAN website. The documents consists of -

- Starter manuals and videos (as discussed in Sections 6.4.1 and 6.4.2)
- Theoretical documentation (under *general documentation*)
- User manuals (under *complete documentation*), and
- Additional documents to aid in understanding and pre–/post processing for SHETRAN.

6.7 Publications

The list of publications with SHETRAN application or the model related discussions can be accessed via the Publications tab in the SHETRAN website. The list consists of -

- Peer reviewed journal papers
- Conference proceedings
- Reports, and
- Book chapters

This list is valuable for literature review regarding SHETRAN and its applications and/or for decision making on the suitability of SHETRAN for your research!

6.8 Learning path for SHETRAN

Author's advice –

- **Looks hard, but its easy!** We strongly believe that exploring the SHETRAN website resources with continued enthusiasm, attentiveness and willpower for a couple of weeks is enough for a person from relevant background to get a knack of SHETRAN and enjoy playing with it.
- **Don't swallow it all.** Understanding SHETRAN by its entirety, including all the physically based equations, is achievable but a tough task. That should not be the aim, at least not at first. Instead it is advised to limit the focus to the SHETRAN components that you plan to incorporate in your research.
- **Don't turn a blind eye to the input.** One should evaluate and question the reliability and correctness of information put into the model (meteorological data, model concept, auxiliary components, etc.) in parallel to the model for improvement in simulations.

There are many ways to get acquainted with SHETRAN. If you are certain that SHETRAN is the right modelling system for you, this section prescribes a learning path that you may wish to follow, which is just one out of those many ways to learn SHETRAN.

Step 1: Explore the usage of SHETRAN and its output

Go though the following videos to get to know about SHETRAN program and the output that it offers -

1. <2 minute video on SHETRAN GUI usage – https://youtu.be/7tvYoXxuje0
2. 4 minute video on SHETRAN outputs – https://youtu.be/rXkQf84l0j0

Step 2: Install SHETRAN GUI and try out its video tutorial

Install SHETRAN GUI from the following link and try some hands-on worked out examples on SHETRAN GUI following the links below -

1. Download SHETRAN from the following link. Unzip the downloaded file. There are many things over there. For now just install the SHETRAN GUI.
   http://research.ncl.ac.uk/shetran/Downloads.php

2. Refer to the Video 1 mentioned in Step 1 above. Together with the PDF file from the following link, complete the Gais Gill worked out example –
http://research.ncl.ac.uk/shetran/Shetran%20windows%20worked%20example.pdf

Once you complete Step 2, you will understand what SHETRAN *needs* (input) and *gives* (output) from the GUI version

Step 3: Prepare your model in SHETRAN GUI: Get your first model run!

After completing the worked out example in Step 2, you are now ready to do replicate the process for your catchment. However, you need to prepare the model inputs for your catchment. In case of Gais Gill catchment you had used pre-existing set of inputs. The input required for SHETRAN GUI are - DEM, Mask, PRD (rainfall) and EPD (potential evapotranspiration) data.

1. The meteorological inputs (prd and epd) can be made by preparing files corresponding to format of files used for Gais Gill example.

2. For the DEM and Mask, follow the link below for the PDF that contains steps on creating them using ArcGIS and free ASTER data –
http://research.ncl.ac.uk/shetran/Create%20dem%20and%20mask.pdf

   If you already have your own DEM and catchment mask at intended model resolution and formatting, then you can skip this step.

Step 4: Play with model parameters in SHETRAN GUI: First sensitivity analysis

After you are able to run your catchment's SHETRAN model, try changing the vegetation, soil and river network parameters from the corresponding menu tabs in the GUI. You can find reference on how to do this in Sections 2,3 and 4 respectively of the PDF (link 2) of Step 2. The following document can be referred to in regards to the range of the vegetation and the soil parameters –
http://research.ncl.ac.uk/shetran/Shetran%20windows%20Userguide.pdf

Step 5: Acquire SHETRAN Standard and try out its video tutorial

Once you get hold of your model in SHETRAN GUI, its time for you to level up and try SHETRAN standard. As you may have noticed, SHETRAN GUI has grid size limit of 50x50 and has only single rainfall and potential evapotraspiration for the whole catchment. In SHETRAN standard, you can increase the grid size up to 200x200 and input spatially varying meteorological input. Apart from that you will be able to control virtually all the input instructions to SHETRAN.

1. From the previously downloaded SHETRAN package (in Step 2), copy the SHETRAN standard to your working folder. SHETRAN standard is a ready-to-run program and there is no installation process involved.

2. Refer to the following video which takes you through the Aire at Kildwick.
   https://youtu.be/zYrDnVq5iD8

   Together with the PDF file from the following link, complete the Aire at Kildwick worked out example –
   http://research.ncl.ac.uk/shetran/Shetran-easy%20setup.pdf

   There is no need to worry if you don't get 100% of this tutorial. Your understanding of SHETRAN will grow as you spend more and more time with it.

Step 6: Get your model up and running in SHETRAN standard

Now that you know how to use SHETRAN Standard, its time to get your model upgraded to SHETRAN standard. Prepare the files needed for SHETRAN Standard referring to the details for Step 5 and the input files for Aire-at-Kildwick.

1. An easier approach to make the input files for SHETRAN standard would be to just keep everything simple at first. In fact you might want to use some of the information (like vegetation, soil) from Aire at Kildwick for your input files. Once SHETRAN standard makes the standard input files for you, further adjustment can be made.

2. As mentioned above, once you run SHETRAN standard using the same approach as Aire at Kildwick, you will notice that it will prepare the standard SHETRAN input files for you. Check out the following video to understand what some of these files are about –
   https://youtu.be/ptimgTkRz0I

Step 7: Build up your understanding about the input system of SHETRAN

Once you have a running model in SHETRAN standard, you would have achieved a major milestone in the process of learning SHETRAN. However, even more significant is the next thing that you would learn - the SHETRAN input system.

1. The best way to understand the input files, the formatting and their meaning is to go through the input files of your catchment and refer to the SHETRAN user guide. The user guide has description about each of the input parameters and the corresponding formatting. The direct link to the user guide PDF is as follows – http://research.ncl.ac.uk/shetran/SHETRAN%20V4%20User%20Guide.pdf

   The users are advised to first cover formatting of the principal input files i.e. **rundata** file and the **frame module (frd)** file. After that, it is advised to explore the evapotranpiration/interception module (etd), sub-surface flow (vsd) and overland/ channel flow (ocd) files. Finally depending upon the modelling purpose the additional modules viz. sediment yield (syd), snowmelt (smd), contaminant migration (cmd) can be further explored/ added.

Step 8: Envisage and input complexities into the model as required

Your model is running in SHETRAN standard format but you still need to add more elements to it? SHETRAN has a long list of processes that it can simulate (refer to Table 6.1 of Section 6.2).

Let's say you have to change the landuse of the basin at some point of the simulation for a landuse change analysis. For that you need to run a model till a point of time, change the landuse, the model run dates, the meteorological data file's start date. You will also need initial condition so that there will be moisture continuum in the catchment. For this you can utilize the *vsi* file. You have the user guide document for reference. If anything new comes up, look up for it in the document. With the use guide and the knowledge of input system (Step 7), you should be able to make necessary modifications for incorporation of any additional model component.

Step 9: Increase model complexities but avoid unproductive complexities

Check model sensitivity to the input and the system prepared. Check whether adding more meteorological station improves the model. Or test if

finer model resolution helps which gives finer DEM and landuse information to the model. One can also add more number of soil layers for an instance. Check whether these help. If they do help keep it. If not (i.e. *unproductive complexities*) revert back as keeping them would charge more modelling effort including the run time.

Step 10: Locate the major model parameters and calibrate your model

Since the response produced by SHETRAN is based on solution of physically based equations, theoretically we are not suppose to change its parameters and just go with the field based experimental values. But these values don't represent the actual spatial heterogeneity of reality. The values would always be a bit under-/overestimation than the best fit value. Thus some fine turing is always necessary. Moreover, field based values may not be available in all cases and we have to go by the recommended parameter values. Thus, model parameterization and calibration are necessary in SHETRAN, the extent of which is dependent on the physical properties data at hand.

Although the sensitivity of model parameters differ from region to region, the major model parameters (based on previous studies) include –

1. Actual/potential evapotranspiration for each vegetation type (etd)
2. Aquifer depth (vsd)
3. Aquifer conductivity (vsd)
4. Strickler overland flow coefficient (ocd)
5. Strickler flow coefficient for river channels (ocd)

However, do take note that the above parameters work together with the spatial variability (of landuse, soil type, rainfall) which also need to be checked as mentioned in the beginning of this section.

When you don't have field values to work with, the startup values of the parameters can be taken from the Data Requirement document, specifically from the following two sections –

- Appendix A – library of soil parameters (for vsd)
- Appendix B - library of vegetation parameters (for ocd and etd)

Steve (co-developer of PAC and co-author of this manual) has documented few but very useful points for model calibration based on his 25 years of

experience with hydrological models. Users are advised to refer to it during model development and calibration. Follow the direct link below to access the document –
http://research.ncl.ac.uk/shetran/Producing%20a%20good%20hydrological%20simulation.pdf

6.9 SHETRAN errors

What do the errors mean?

The SHETRAN error codes are four digit numbers, where the first digit is the module identifier and the remaining three are used to identify the specific error thrown from the module. The module identifiers are as follows –
0 Library (AL);
1 Water (WAT) or Frame (FR);
2 Sediment (SY);
3 Contaminant (CM)

The details on each error can be found inside .../Shetran-standard-v4.4.5x64/standard version/program/helpmessages of the downloaded SHETRAN package.

More clues on the errors

Check the end of the pri output file to get some more clues for error tracing and solution.

Are there any discussion forums?

An effective way to solve errors is referring to pre-existing posts on the errors at discussion forums. For SHETRAN, currently, there are three options –

1. SHETRAN Google Group –
   https://groups.google.com/forum/#!forum/shetran
2. SHETRAN Facebook Group (closed group) –
   https://www.facebook.com/groups/1568152969884440/
3. SHETRAN's contact person –
   s.j.birkinshaw@ncl.ac.uk (Dr. Steve Birkinshaw)