

Getting Started

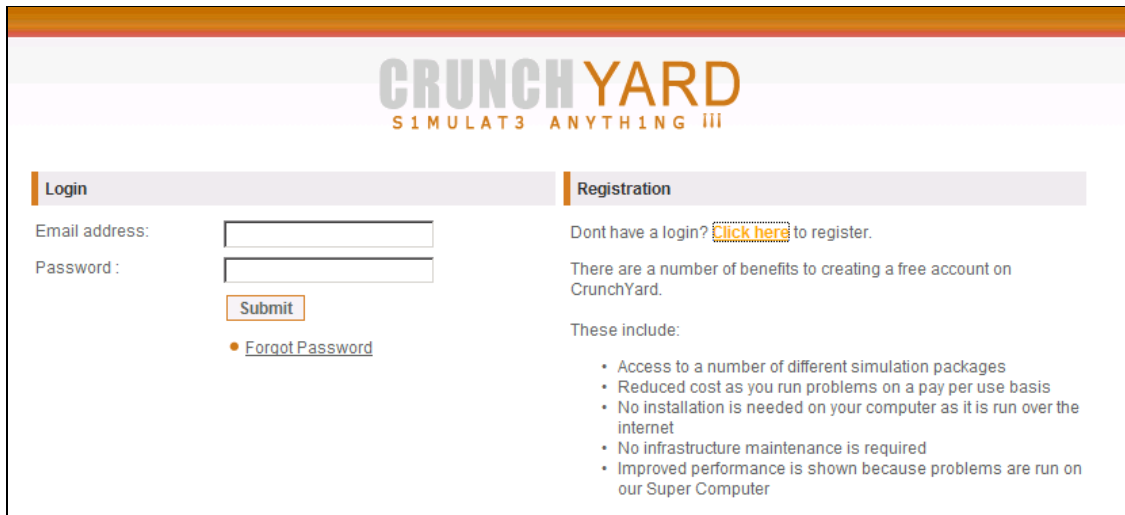
This guide aims to help you get going on the CrunchYard website www.crunchyard.com by explaining the basic functionality of the website. The guide will explain the requirements for the various packages, how to purchase credits, submit files for simulations and view the progress of simulations and the results etc.

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2. Registration and Login

To create an account you will be required to complete the registration section. The registration link is located on the main landing page of CrunchYard i.e. www.crunchyard.com . Once you have registered you will be able to login to your account. Registration is FREE.



The screenshot shows the CrunchYard website interface. At the top, the logo reads "CRUNCH YARD" with the tagline "SIMULAT3 ANYTHING III" below it. The page is divided into two main sections: "Login" and "Registration".

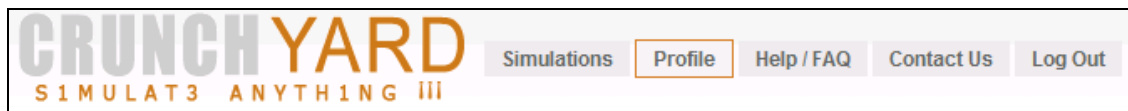
Login Section:

- Email address:
- Password:
-
- [Forgot Password](#)

Registration Section:

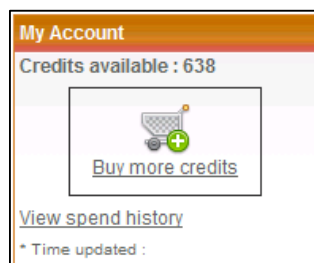
- Text: "Dont have a login? [Click here](#) to register."
- Text: "There are a number of benefits to creating a free account on CrunchYard."
- Text: "These include:"
- List of benefits:
 - Access to a number of different simulation packages
 - Reduced cost as you run problems on a pay per use basis
 - No installation is needed on your computer as it is run over the internet
 - No infrastructure maintenance is required
 - Improved performance is shown because problems are run on our Super Computer

You can change your password at any stage. To do this you will need to navigate to the "Profile" section after you have logged in.



3. Purchasing Credits

Simulations are charged on a per hour per CPU basis. The form of payment is handled through credits that can be purchased upfront using a credit card. Please note that there might be slight fluctuations in the purchase price due to exchange rates. To purchase credits, click on the shopping cart in your profile.



Buy credits

Credits required? :

* This gets calculated based per hour x 10 nodes x \$1
* \$1 = R7.50

Card holder name and surname: *

Type of Card *

Card Number *

Expiry Date *

3 Digit Code*

* Required

4. Submitting Files for Simulation

Once you have created a file to be simulated and have sufficient credits, you are ready to upload files for simulation. In the first section of the “Simulations” tab:










- 1) Select the application you want to use.
- 2) Fill in the required fields (Each application is explained in detail in later sections in this document)
- 3) Upload the file.

You can browse for the file created using the Browse button and then upload the file. Once uploaded, you will see your package file displayed under “View History” Please note that packages uploaded may not exceed 16 characters and may not start with a dot (.)

Sample simulation files can be found under the HELP/FAQ section. The OpenFOAM example will require you to select 4 CPUs.

5. Viewing Progress & Results

Once the simulation has been submitted on the system you will be able to view its progress. Wait for a few minutes for the “Simulation Progress” section to update. Your uploaded simulation will show as “Being Processed”, for example test22.393.master.cluster1 below. To view the various status options, move your mouse over the information icon next to the “Status” header.

File Name	Status 
jan20_test1.395.master.cluster1	Being Processed  
refresh11.394.master.cluster1	Being Processed  
test22.393.master.cluster1	Being Processed  
mpitest16_49cpu.392.master.cluster1	Paid 
long_pre.391.master.cluster1	Paid 

* Time updated : 10:58:30 AM

[View History](#)

You will be able to view the text output from a simulation by clicking on the process file name. A text file, with the extension .pro, gives you a screenshot of the current progress and can be downloaded and viewed as shown below. This file is updated approximately every minute.

```

test21.313.master.cluster1[1].pro
RUNFEKO  Version 6.23 from 2009-08-10 (FEKO Suite 5.5)
          Copyright (c) 1999-2009 EM Software & Systems-S.A. (Pty) Ltd

NOTE: Running PREFEKO since file "Test10.fek" not found

PREFEKO  Version 34.48-92 from 2009-09-15 (FEKO Suite 5.5)
          Copyright (c) 1999-2009 EM Software & Systems-S.A. (Pty) Ltd

Creating file Test10.fek. please be patient ...
File Test10.fek has been created:
 12544 metallic triangles in free space










FEKO.CSV Version 55.371      from 2009-09-07 (FEKO Suite 5.5)
          Copyright (c) 1999-2009 EM Software & Systems-S.A. (Pty) Ltd

NOTE: This version supports a maximum number of 100 CPUs
Memory: Limited to 973.311 MByte, reason 160
        (for parallel runs memory limit is per process)

File:      Test10
----> Process 16 of 98 active on node41          (PID: 32484)
----> Process 24 of 98 active on node37          (PID: 32395)
----> Process 26 of 98 active on node36          (PID: 32390)
----> Process 47 of 98 active on node26          (PID: 31431)
----> Process 95 of 98 active on node2           (PID: 15224)
----> Process 30 of 98 active on node34          (PID: 30496)
----> Process 29 of 98 active on node35          (PID: 30544)
----> Process 27 of 98 active on node36          (PID: 32391)
----> Process 56 of 98 active on node21          (PID: 868)
----> Process 59 of 98 active on node20          (PID: 18913)

```

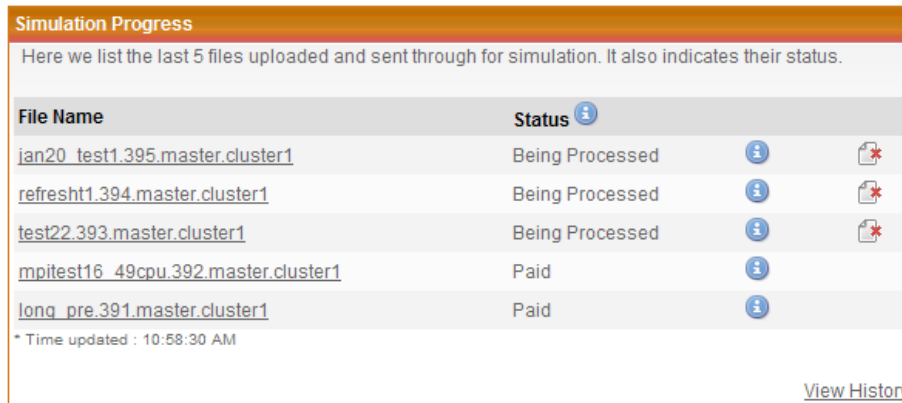
Once the simulation is complete the results will appear on your profile and your credits will be updated. This might take a couple of minutes to appear. You will then be able to download the output file by clicking on the name of the simulation you want to download. For example clicking on test20.output.pkg will download the results for the package names test20. To delete the results from your profile click on the icon displaying the red cross next to the output you want to delete.

Simulation Results			
Output files ready for download. Please download and delete.			
File Name	Application	Status	
Horn4_2010.output.pkg	FEKO	1175 Kb	
Horn8_2010.output.pkg	FEKO	1175 Kb	
JUL292010_2.output.pkg	FEKO	1175 Kb	
damBreak.output.zip	OpenFoam	18 Kb	
dBN0V3.output.zip	OpenFoam	18 Kb	
NIN.output.zip	OpenFoam	18 Kb	
yaqi.output.zip	SNEC	915 Kb	
yaqi_3.output.zip	SNEC	915 Kb	
yaqiNOV3.output.zip	SNEC	915 Kb	

* Time updated :

6. Cancelling a Simulation

If for some reason the progress file shows the simulation is not going as expected or you would like to cancel the simulation, you may do so. Clicking the icon with the red cross, as shown below, will cancel the simulation. If your simulation should show an error please refer to the .log file in the results to see what the problem could be. If you receive an MPI error, resubmit the simulation.



The screenshot shows a table titled "Simulation Progress" with a header row containing "File Name" and "Status". Below the header, there are five rows of simulation data. Each row includes a file name, a status, an information icon, and a cancellation icon (a red cross over a document). The first three rows have a status of "Being Processed", while the last two have a status of "Paid".

File Name	Status	Info	Cancel
jan20_test1.395.master.cluster1	Being Processed		
refresh1.394.master.cluster1	Being Processed		
test22.393.master.cluster1	Being Processed		
mpitest16_49cpu.392.master.cluster1	Paid		
long_pre.391.master.cluster1	Paid		

* Time updated : 10:58:30 AM

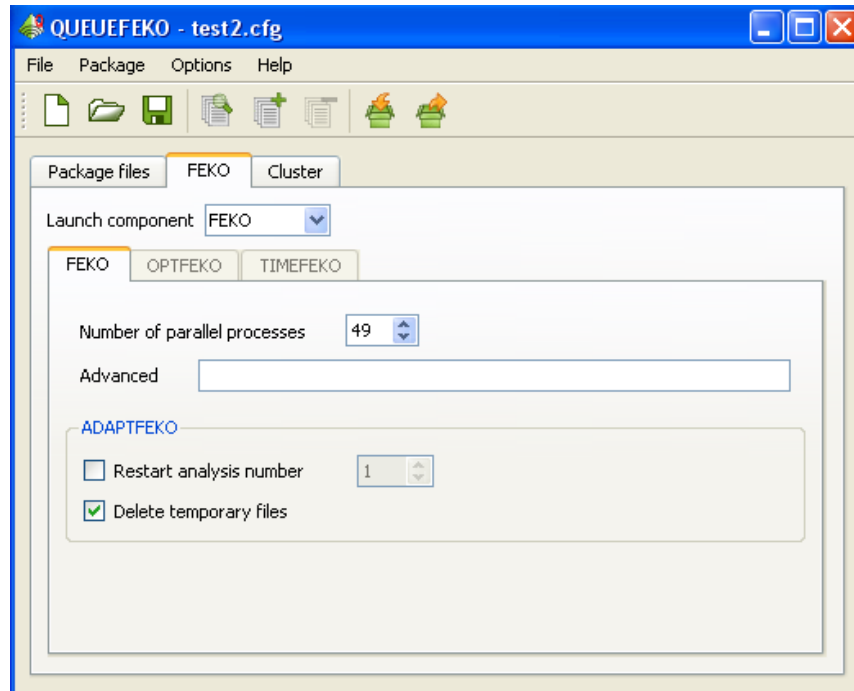
[View History](#)

7. FEKO

FEKO requires the user to first create a package file. This package file will then be uploaded to the cluster. This section looks at how to create an upload a FEKO package file and upload it.

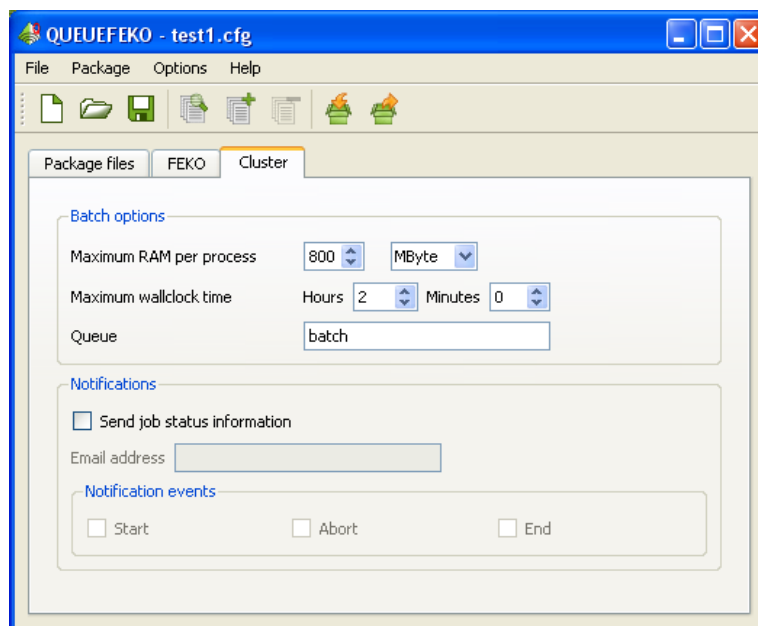
A component in FEKO, called QUEUEFEKO, is used to create packages to send to the cluster to be simulated. The full functionality for QUEUEFEKO can be found under "Help" in QUEUEFEKO.

Parameters that need to be specific for the CrunchYard cluster is shown here. As seen below, the number of parallel processes needs to be entered. Currently this is limited to a maximum of 49. This number represents the number of nodes used. Each node has 2 CPU cores.



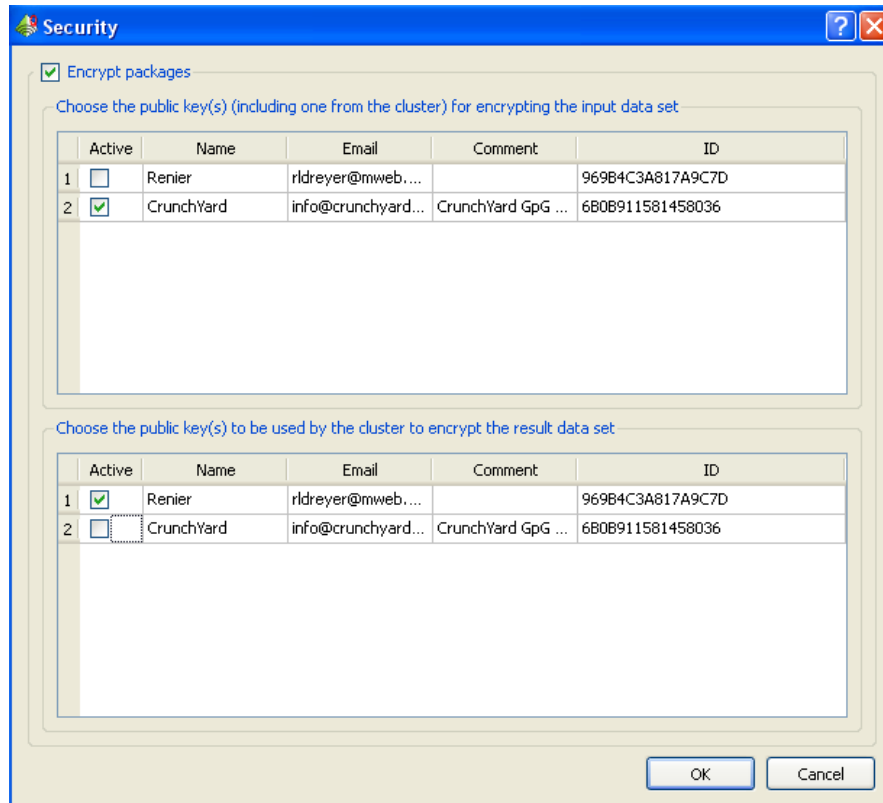
The cluster parameters that need to be set are as follows,

Maximum RAM per process: Set to 800 MBytes
 Maximum wallclock time: If simulation time exceeds this, it will be terminated.
 Queue: batch
 Send Job Status: E-mail updates are not currently enabled on the cluster.



Should you wish to encrypt your data before uploading it, you may do so. The CrunchYard Public key can be downloaded from the website under the Security info section. You will also find the security certificates from CrunchYard and EMSS. Once you have added the CrunchYard public key to your key ring and setup QUEUEFEKO with your encryption engine you can encrypt your data.

To encrypt the input data select the CrunchYard public key as shown below. You should choose your own public key to encrypt the output or results data.



Once the package file has been created you can upload it for simulation. After you have selected FEKO as your simulation package, you can browse for the .pkg file you have created with QUEUEFEKO and upload this for simulation.

FEKO is charged at **5 credits** per hour per CPU.
One credit is equivalent to US\$ 0.5

FEKO can be obtained from www.feko.info

Upload a Simulation

Please note that files with the same name cannot be uploaded at present. To list simulations names that was uploaded before click on the View History link.

We do not keep a copy of the files for security reasons.

[View History](#)

Upload a file

Select Application :

Select your file :

* Please note that files cannot contain any . (dots) and a maximum of 16 characters allowed, excluding the file extension.

8. OpenFOAM

Once you have setup your OpenFOAM problem to be solved, you will be required to zip the files and folders. Please be sure to read the OpenFOAM documentation on how to select the number of parallel processes. This number needs to correlate to the number of CPU's chosen when uploading the .zip file.

Upload a Simulation

Please note that files with the same name cannot be uploaded at present. To list simulations names that was uploaded before click on the View History link.

We do not keep a copy of the files for security reasons.

[View History](#)

Upload a file

Select Application :

Name of file to be simulated : *

CPU Cores : *
Please specify even numbers

Memory to be used (max 800mb) : *

Maximum running time: *
Format hh:mm

Solver : *

Any extra arguments : *

Select your file :

* Please note that files cannot contain any . (dots) and a maximum of 16 characters allowed, excluding the file extension.

There are a number of parameters that need to be set. The name of the file should be the same as the .zip file name. (If the .zip file is called TEST.zip then the name of the file to be simulated is called TEST)

- The **CPU cores** needs to correlate to the number of number of parallel processes used when creating your OpenFOAM problem. There are a maximum of 98 cores that can be chosen
- It is best to set the **memory** to 800Mb, even if each node would use less. You can however not exceed 800Mb per CPU.
- Select the **maximum runtime**. If this time has been exceeded then the simulation will abort.
- There are a number of standard **solvers** in OpenFOAM. You will need to select the solver required for your simulation.
- For advanced users only, we have included a command line option that will allow you to add any **extra arguments**. Please refer to the OpenFOAM manual should you wish to use this option. In general it can be left blank.
- Your **source file** is the .zip file containing all the relevant folders and files for your OpenFOAM simulation that you have generated.

OpenFOAM is an open source package that can be downloaded free of charge from www.openfoam.com

CrunchYard does not charge for the use of the OpenFOAM software, but for the use of the computers only.

Computers using OpenFOAM are charged at **1 credit** per hour per CPU. One credit is equivalent to US\$ 0.5

9. SuperNEC

Running a SuperNEC simulation requires only a few basic parameters.

- Create the .nec file in SuperNEC
- Choose the number of CPU's to use (maximum of 49)
- Choose the maximum runtime before the simulation will be automatically aborted.
- Browse for the .nec file and upload.

SuperNEC usage is charged at **1 credit** per hour per CPU. One credit is equivalent to US\$ 0.5

SuperNEC can be downloaded from www.supernec.com

Upload a Simulation

Please note that files with the same name cannot be uploaded at present. To list simulations names that was uploaded before click on the View History link.

We do not keep a copy of the files for security reasons.

[View History](#)

Upload a file

Select Application :

CPU Cores : *

The maximum that can be specified is 49

Maximum running time: *

Format hh:mm

Select your file :

* Please note that files cannot contain any . (dots) and a maximum of 16 characters allowed, excluding the file extension.

10. CP2K

Running a CP2K simulation requires only a few basic parameters to be set.

- Zip all the files you created for the simulation into one file (.inp, POTENTIAL, BASIS etc)
- Choose the number of CPU's to use (maximum of 98)
- Choose the maximum runtime before the simulation will be automatically aborted.
- Browse for the .zip file you created and upload it.

CP2K usage is charged at **1 credit** per hour per CPU.

One credit is equivalent to US\$ 0.5

CP2K is a [freely available](#) (GPL) program, written in Fortran 95, to perform atomistic and molecular simulations of solid state, liquid, molecular and biological systems. It provides a general framework for different methods such as e.g. density functional theory (DFT) using a mixed Gaussian and plane waves approach (GPW), and classical pair and many-body potentials.

Upload a Simulation

Please note that files with the same name cannot be uploaded at present. To list simulations names that was uploaded before click on the View History link.

We do not keep a copy of the files for security reasons.

[View History](#)

Upload a file

Select Application :

Name of input file to be simulated (.inp) : *

CPU Cores : *
The maximum that can be specified is 98

Maximum running time: *
Format hh:mm

Select your file : *

* Please note that files cannot contain any . (dots) and a maximum of 16 characters allowed, excluding the file extension.

Should this guide not answer any of your questions, please refer to the FAQ section on the website. Alternatively please send an email to info@crunchyard.com

March 8, 2011
Renier Dreyer
(CEO of CrunchYard SA)