SCORG™ Setup for CFD Simulation of Twin Screw Machines with ANSYS CFX®

SCORG™ is the CFD grid generation tool for rotary twin screw machines. The tool includes additional modules for designing and editing rotor profiles, executing a basic thermodynamic calculation based on quasi 1D chamber models and generating the deforming working chamber grids for selected commercial CFD solvers.

For more information on the product please visit the website: www.pdmanalysis.co.uk or refer to documentation help.

This guide lists the steps for setting up a CFD simulation for Twin Screw Compressor with SCORG™ and ANSYS CFX Solver. The user is expected to be familiar with screw machines, CFD and ANSYS CFX® in order to be able to use these procedures. It is highly recommended that books on that topic are studied[1][2]

The setup steps here are demonstrated for Linux & Windows 7, x64 bit OS. Refer SCORG™ Installation Guide for system and hardware requirements.

Table of Contents

[1] N. Stosic, I.K. Smith, A. Kovacevic Screw Compressor Mathematical Modelling and Performance Calculation, Springer, UK 2005, ISBN-10 3-540-24275-9
[2] A. Kovacevic. N. Stosic, I.K. Smith, Screw Compressor Three Dimensional Computational Fluid Dynamics and Fluid Solid Interaction, Springer, 2006, ISBN 3-540-36302-5

1 Introduction

Screw Compressors are rotary positive displacement machines. Although the working principle of these machines is simple, the geometry of rotors which are in the form of multi -lobe helical screws meshing with each other, is making analysis by use of Computational Fluid Dynamics (CFD) challenging. The process starts when the lobes are engaged at one end, which creates continuous increase of the volume between the rotors and the casing which reduces pressure in the suction domain and draws the working fluid in. Further rotation of the rotors makes this volume between the rotors and the casing enclosed when the compression of fluid begins. This increases the pressure within the chamber. Further rotation exposes the pressurized fluid to the outlet port and the fluid is delivered (Stosic, et al., 2005). Similar process is occurring in other helical screw machines such as pumps, vacuum pumps, gear pumps, expanders, extruders and motors. The CFD is equally challenging in such machines due to sliding and stretching

The main objectives of CFD simulations of a screw compressor are to:

a. Obtain the pressure field inside the rotor chamber and in the suction and discharge domains. Example shown in *Figure 1-1*.
b. Obtain the velocity fields in critical regions of the computational domain.
c. Obtain temperature fields in critical regions of the computational domain.
d. Obtain integral parameters of the machine such as power, mass flow rate, discharge temperature, torques on the rotor shafts, etc.
e. Obtain the loads and temperatures on boundaries with solid parts of the machine for further structural and thermal analysis.

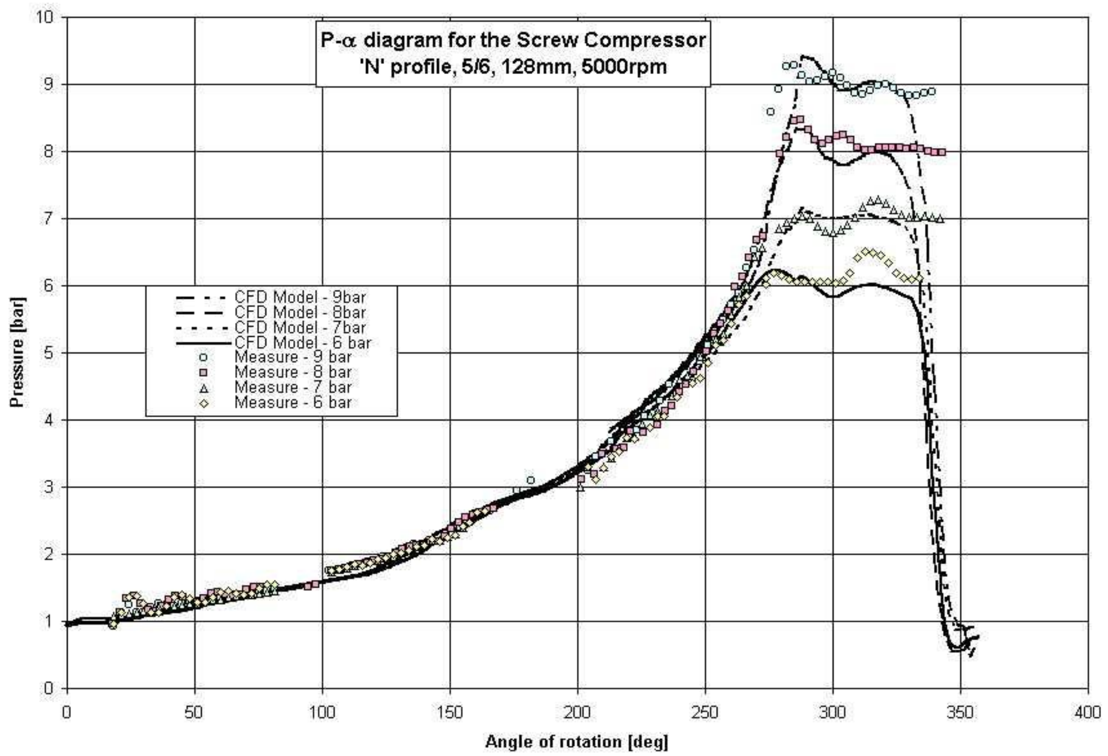
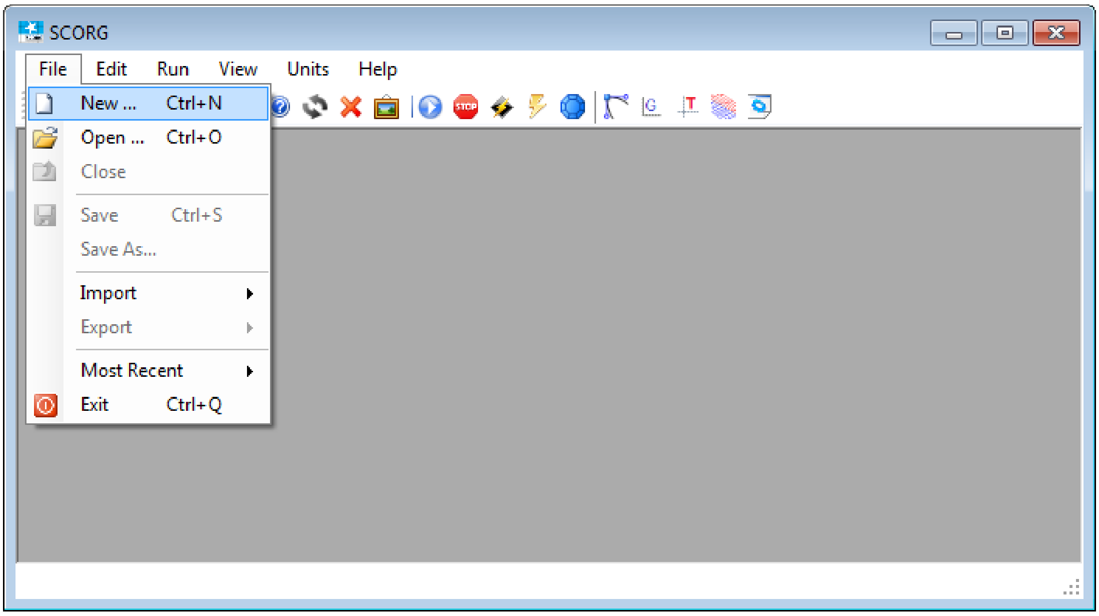


Figure 1-1 *Pressure Variation diagram of a Twin Screw Compressor* **(Kovacevic, et al., 2007)**

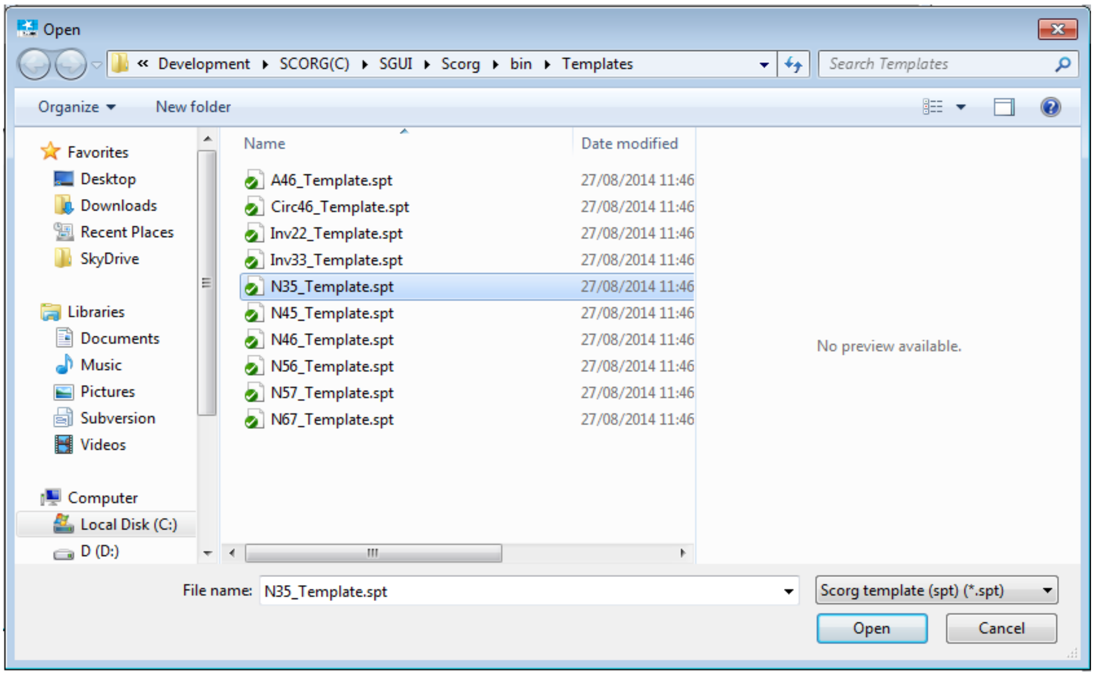
This Tutorial will provide a step by step guide for the procedure to setup and execute a typical twin screw compressor, pump or motor simulation. An example of a dry air compressor with 3/5 lobe combination, L/D ratio of 1.7 and wrap angle 285 deg has been considered.

2 SCORG™ Project

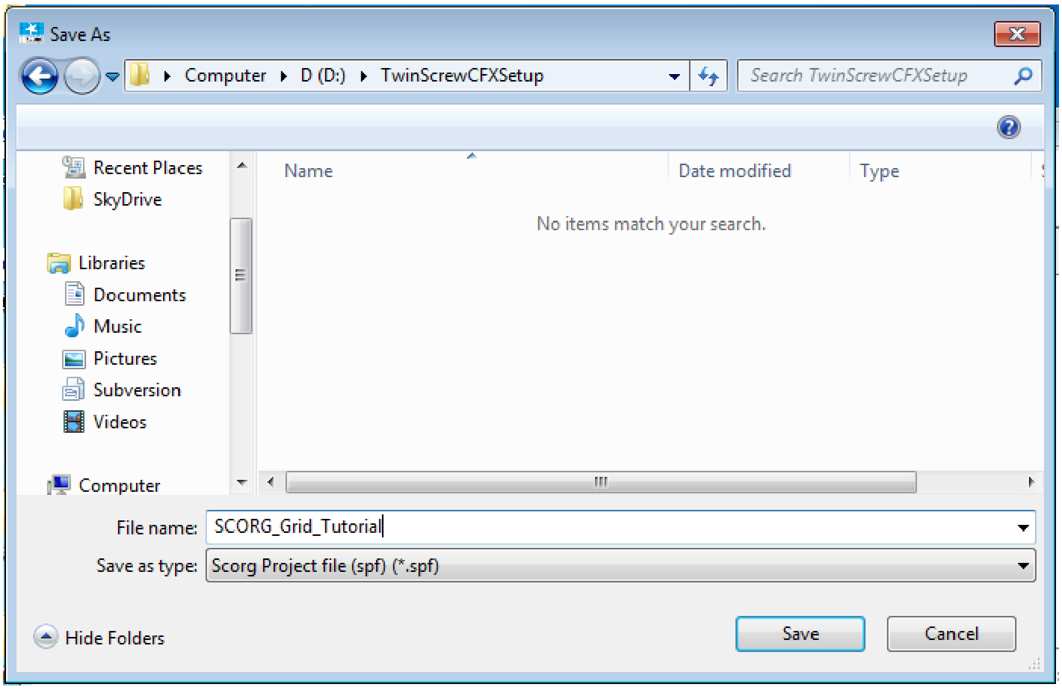
- Launch SCORG™ on the Desktop.
- Select File → New



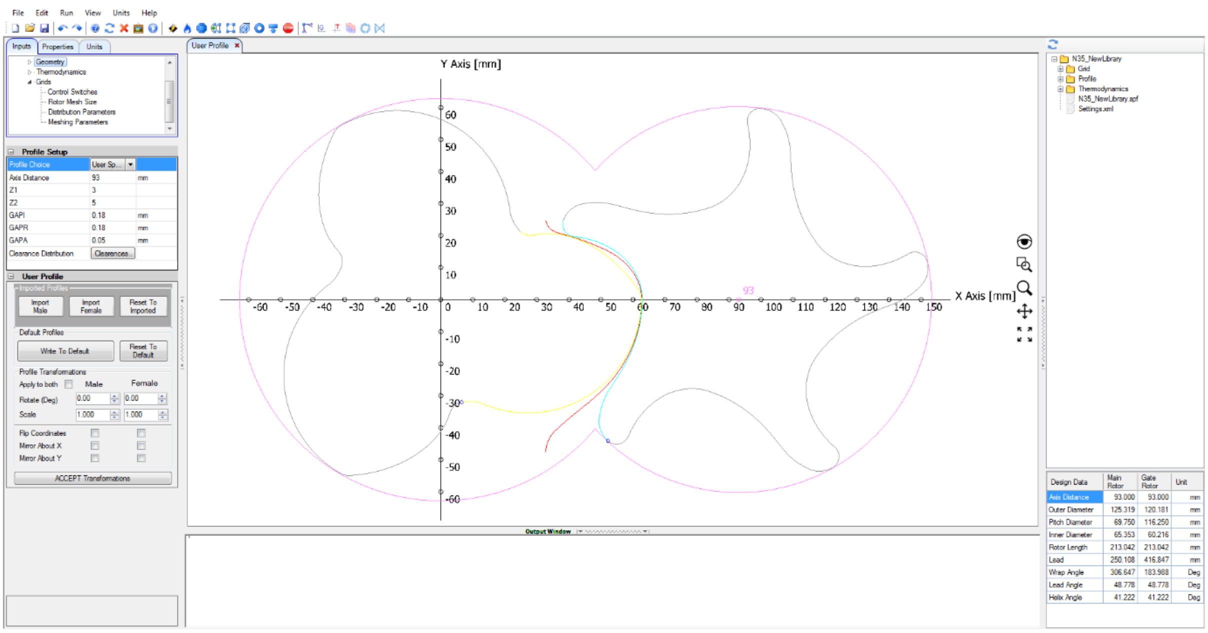
- Select N35_Template.spt → Open



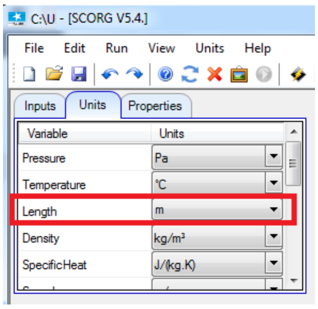
- Save the project in a new folder named TwinScrewCFXSetup → SCORG_Grid_Tutorial.spf



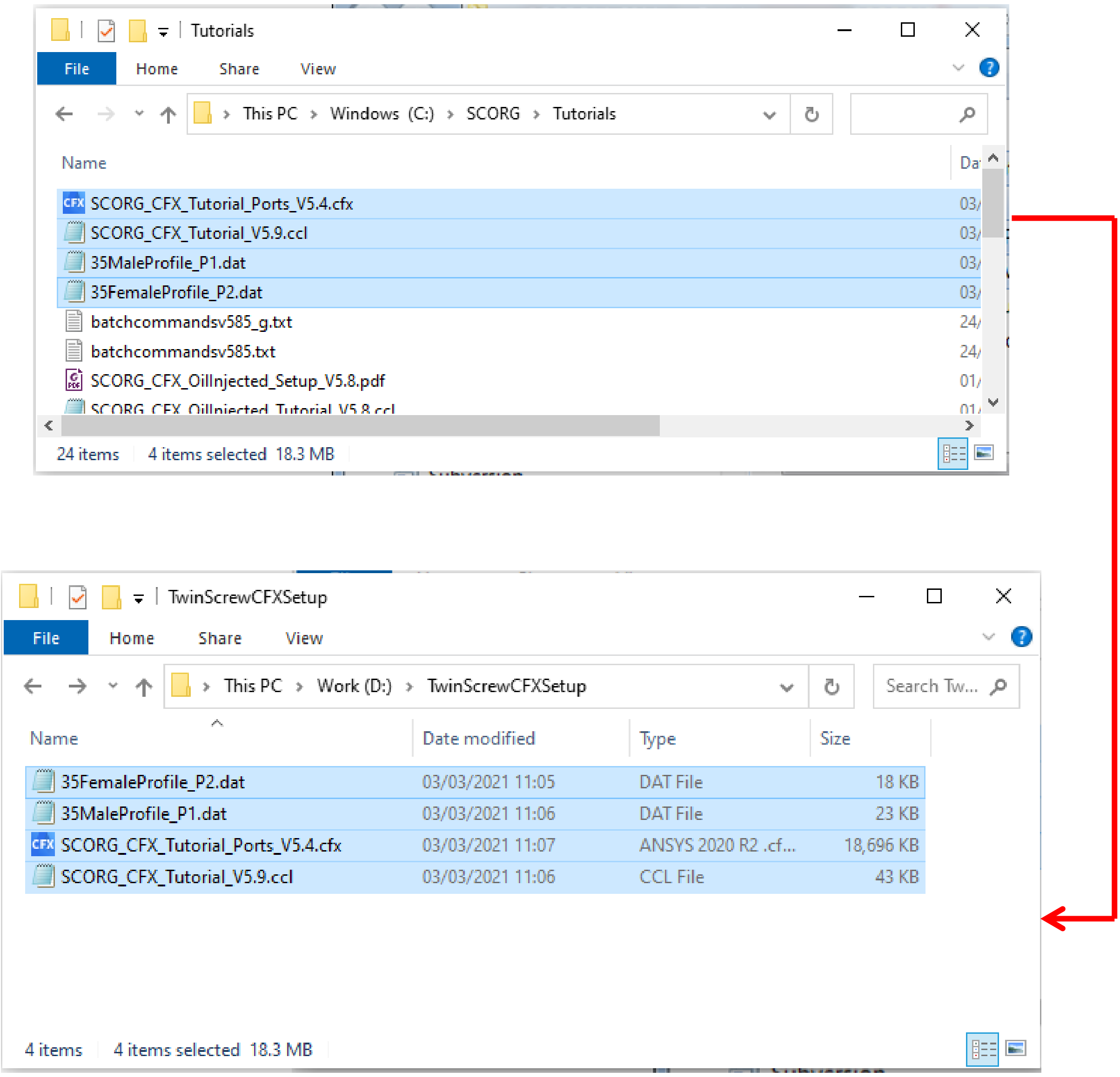
- The GUI of SCORG™ in the figure bellow shows the mains items of the front panel.



- In Units Tab, Select Length units as ‘m’. This selection has to be the same as the units in which input profile coordinates are available.



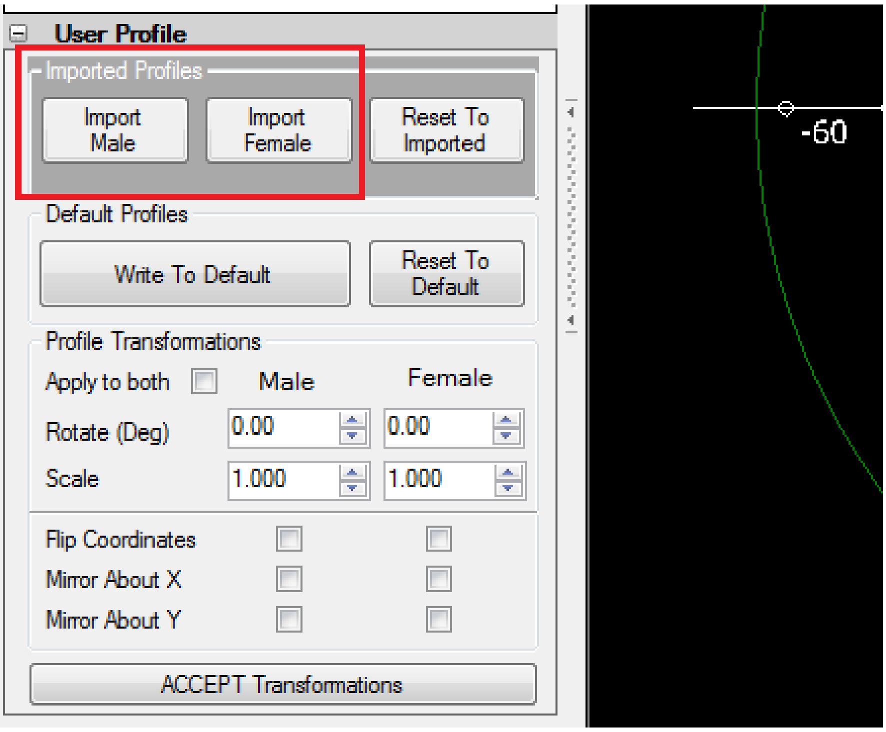
- Go to Help → Tutorials → Folder opens



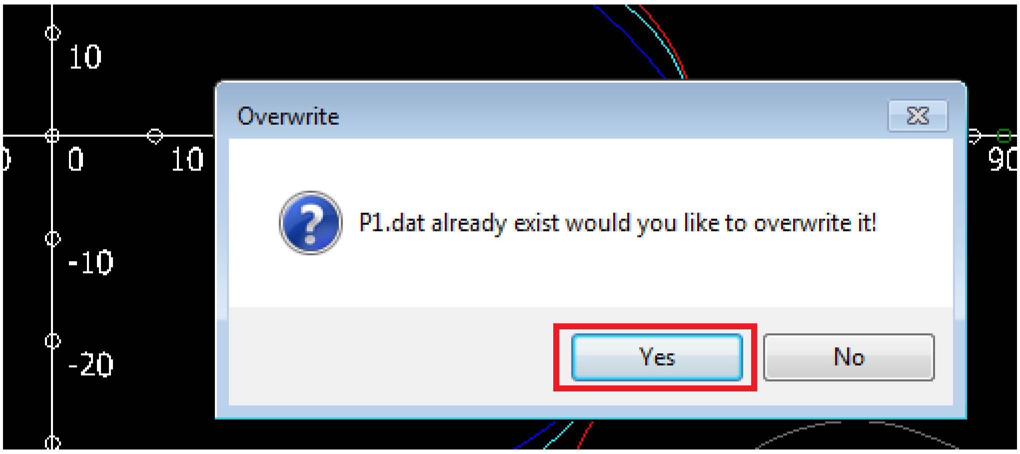
- Copy the compressor rotor profile files → [*35MaleProfile_P1.dat* and *35FemaleProfile_P2.dat*]
- Copy the compressor suction and discharge port grids → [*SCORG_CFX_Tutorial_Ports_V5.4.cfx*]

- Copy the CFX setup script → [*SCORG_CFX_Tutorial_V5.9.ccl*]
- Paste these files in the working directory → TwinScrewCFXSetup
-
- Go to User Profile → Browse and Select the Male Rotor Profile from working directory.

  35MaleProfile_P1.dat



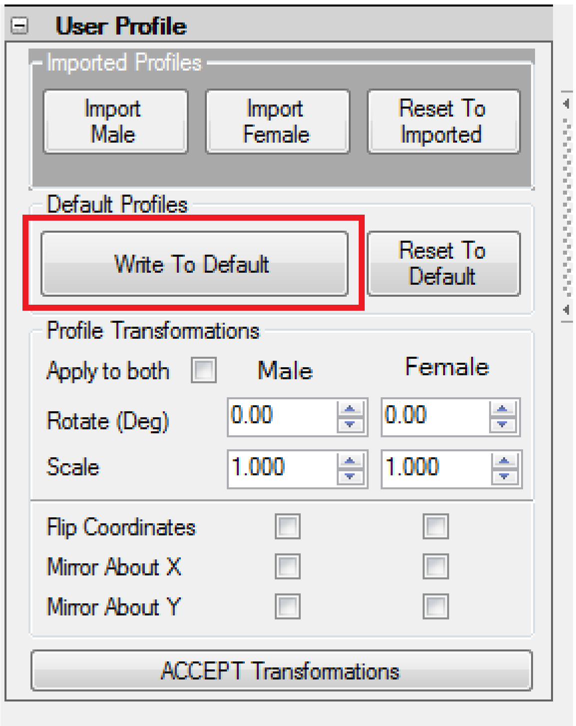
- Click 'Yes' to overwrite P1.dat.



- Similarly Select the Female Rotor Profile.

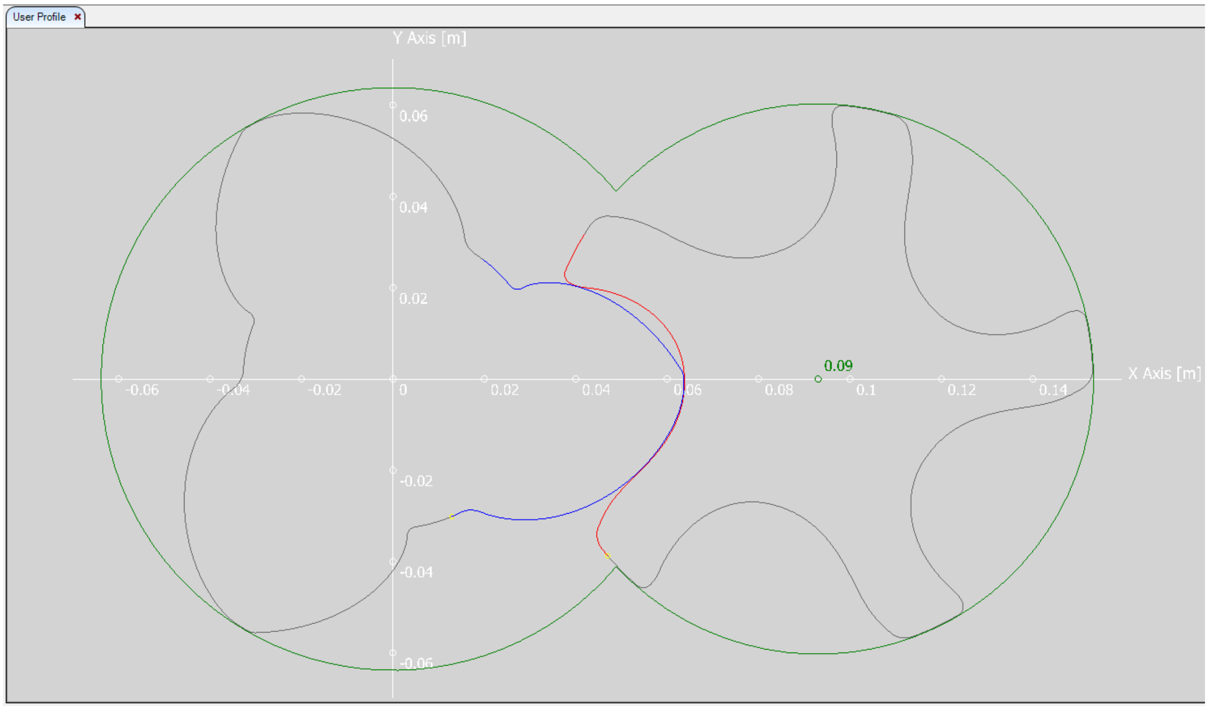
  35FemaleProfile_P2.dat

- Click Write To Default.

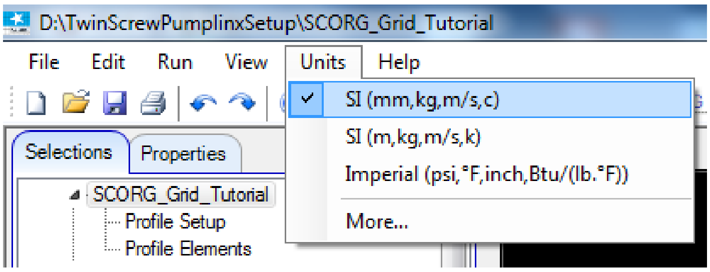


- Click Refresh to view new profiles.

- Inspect the Rotor Profile in the GUI for gaps in the tips, starting points of the profile indicated by the small yellow circles. Below is the required orientation.



- Set Project Units to SI



- Set the following Profile Parameters to get desired clearance size:

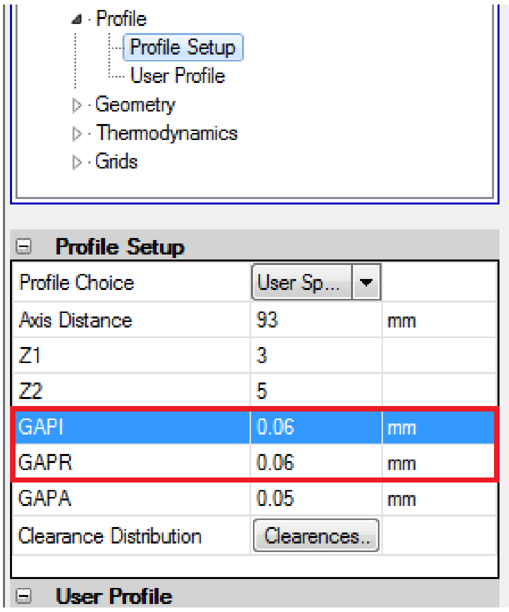
GAPI = 0.06mm

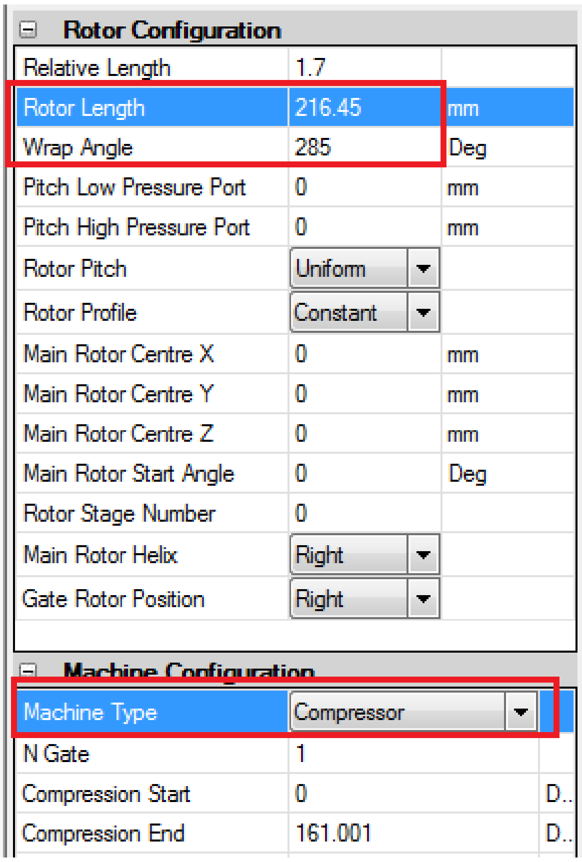
GAPR = 0.06mm

GAPA = 0.05mm

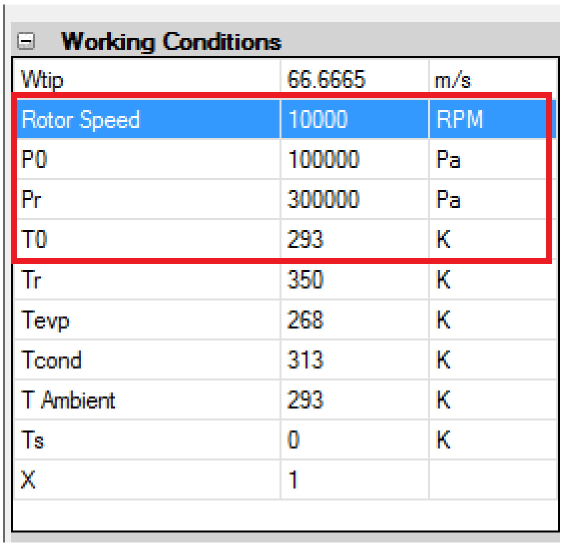
*Setting GAPI = 0.06 sets the minimum interlobe clearance as the GAPI.

- Go to Geometry → Set the following parameters:





- Go to Thermodynamics → Set the following parameters:



- Save the Project.

3 SCORG™ Mesh Generation

SCORG™ is stand-alone numerical CAD-CFD interface used to generate a numerical mesh of rotating parts of a screw machine and to transfer it to a general finite volume numerical solver. The program generates a block structured hexahedral numerical grid for rotor flow domains, solid rotor domains, inlet and outlet ports.

Inputs Required

In this step the rotor domain mesh is generated in SCORG™. The inputs required for this mesh generation are: (Kovacevic, et al., 2007).

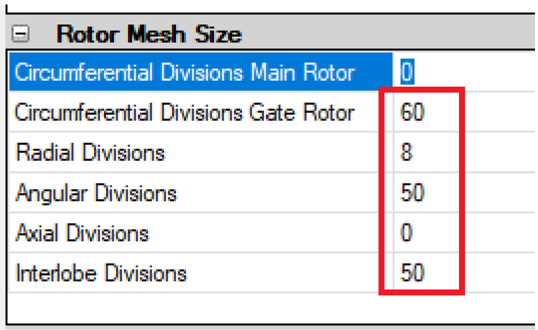
Control Parameters:

- Type of the machine.
- Number of mesh divisions along the lobe in circumferential direction.
- Number of mesh divisions in radial direction.
- Number of Angular divisions of the rotation.

Control Switches:

These Inputs are used to specify the method used for Rotor Profile Input and the required mesh calculation options.

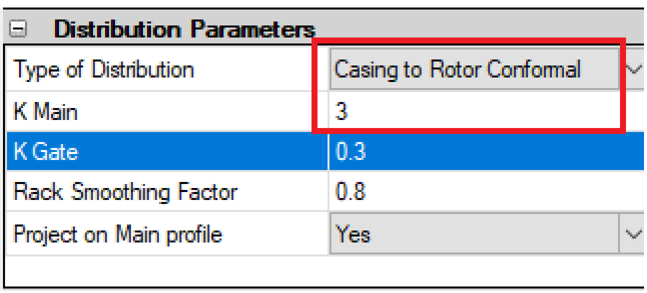
- Click Grid Module in the project tree
- In Mesh Type Size set:
  - Circumferential Main = 0
  - Circumferential Gate = 60
  - Radial = 8
  - Angular = 50
  - Interlobe Divisions = 50



- Distribution Parameters:

These inputs are used for adaptation and distribution of the grid points on the boundaries of the domain and for smoothing of rack (Rack is the curve representing a rotor with infinite radius which uniquely separates the flow domains of the male and female rotors).

  - Type of Distribution → Casing to Rotor Conformal



- Meshing Parameters:

Meshing parameters provide control over the distribution of the internal mesh points in each cross section of the rotors.

Meshing Parameters	
Mesh Orthogonality and Sm…	
Relaxation Factor (0 - 1)	1
Tolerance Factor (1 - 100)	100
Inflation Layer Control	
Radial Bias Factor (0 - 1)	0.5
Radial Bias Intensity (1 - 10)	1

  - both the distribution and meshing parameters can be changed later

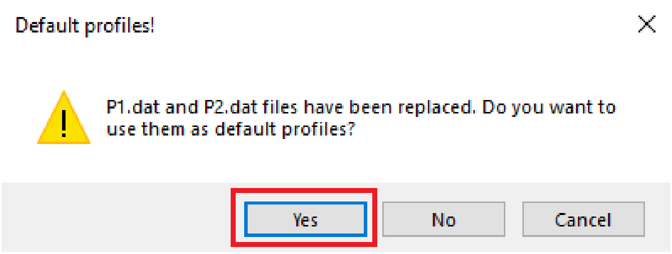
- Start Grid Generation through a three step process as below.

- Select Rack Refinement Points = 400

Control Switches	
Rack Generation	Off
Rack Refinement Points	400
Boundary Generation	Off
Fluid Rotor Grid	Off
Solid Rotor Grid	Off
Inlet Port Grid	Off
Outlet Port Grid	Off
Preprocessor Input File	Off
Vertex Files Start Number	1
Vertex Files End Number	50

- Click Numerical Rack Generation

This operation produces the rack curve between the two profiles. It is required to be executed only once in the grid generation process.



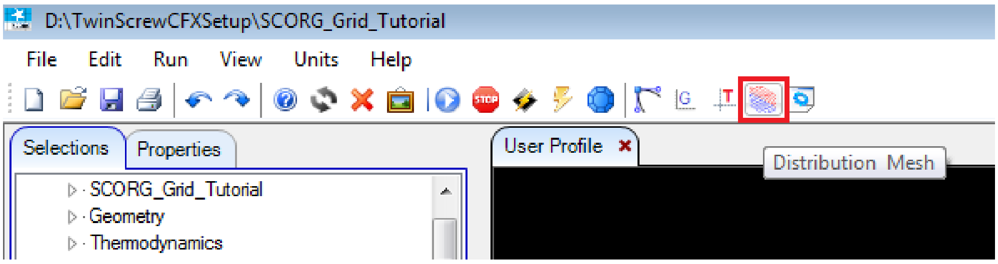
- Click Boundary Distribution Generation

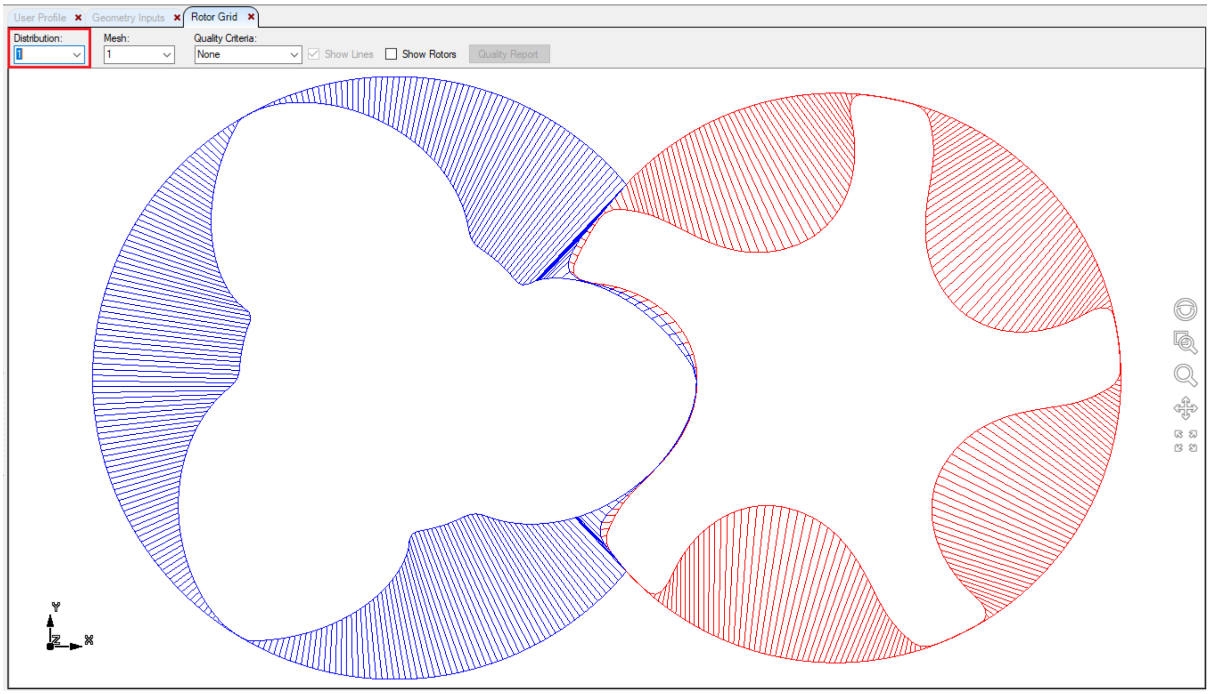
Information about the progress of the selected activities in the meshing procedure is displayed in the output window. Any warning or error and their locations are indicated. If errors occur, it is important to manually tune the input parameters which will produce a mesh without errors. Graphically the mesh distribution in each section can be visualized and checked for any deviation from requirements. The detailed description of methods used for distribution, adaptation and generation of numerical mesh is available through the Help in the drop down menu.

- Inspect report and check that there are no distribution warnings listed

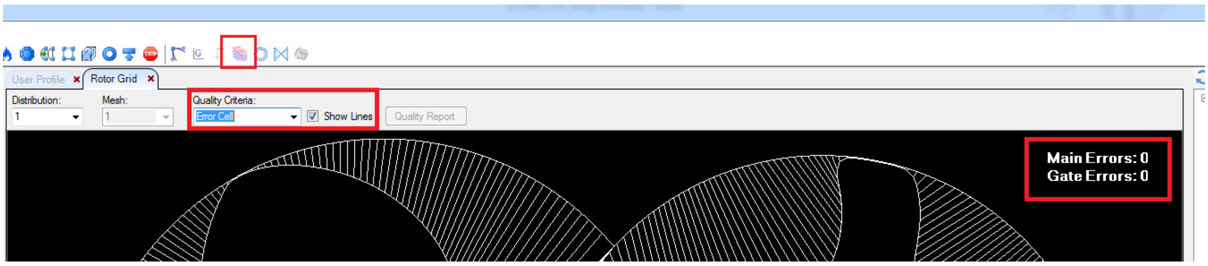
```
C:\SCORG\Grid>echo off

 .......................................................................
 InstallPath = C:\SCORG
 ProjectPath = D:\TwinScrewCFXSetup\SCORG_Grid_Tutorial
 ........................................................................

  SCORG - Screw Compressor Rotor Geometry grid  generator V.5.9
 ...................................................................... 3/ 3/2021...
 Screw compressor/p wrap =  283.2    RPM=12344.     Vel=  82.3    Ncel= 566400
  Z1/Z2= 3/5   d1=127.38 [mm]  d2=120.32 [mm]  a= 93.00 [mm]  len=216.45 [mm]
 ........................................................................
  Nfi    Nr    Nz Nadd  Rot Rack Boun Mesh RotM InpP OutP Prep RaSm Line  Oil
   60     8  118   50    3    1    1    0    0    0    0    0    1    1    0
 ........................................................................
 Calculation:  ROTOR       1:  0.00 Dist  0.00 Cos   2: 0.00 Ang.  0.00 Sin
 Calculation:  RACK        Smoothing factor:  0.80   Smooth: ON
 Calculation:  BOUNDARY    Male =  300               Female =  300
 Initial Smoothing Distribution:Casing to Rotor Conformal
  TFI_Mesh routine - Rotor          1
  TFI_Mesh routine - Rotor          2
 Initial Smoothing GRID  RelaxFac, TolFac, RadBFac, RadBInt, InterlobeBInt
                              1.0      100      0.5      1.0        2
  PDE Interlobe mesh routine
  Distribution Type: Casing to Rotor Conformal
 ........................................................................
 Distribution: Casing to Rotor Conformal
 ........................................................................
 Cell statistics        Overall number of cells        0
 .Rotor fluid          0          .Inlet  port         0
 .Rotor solid          0          .Outlet port         0
 ......................................................................
  Start: 11:23:18    End: 11:24: 2    Running time: 0h: 0m:43s =    42 sec
 ...................................................................... 3/ 3/2021...
  SCORG - Screw Compressor Rotor Geometry grid generator - Ver. 5.9
```

- Click Distribution Mesh to visually inspect the distribution in each cross section





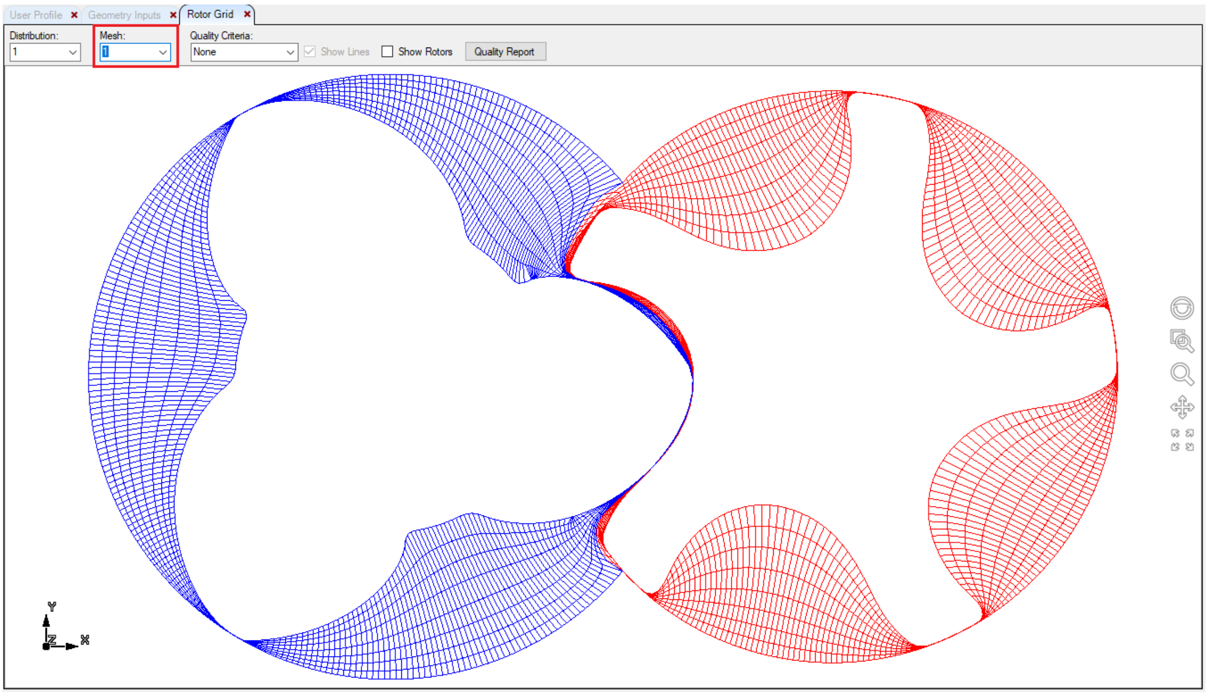
- In the Distribution Display → Select Quality Criteria = Error Cell



- Inspect all the distribution positions and ensure that 0 error are reported in each position.

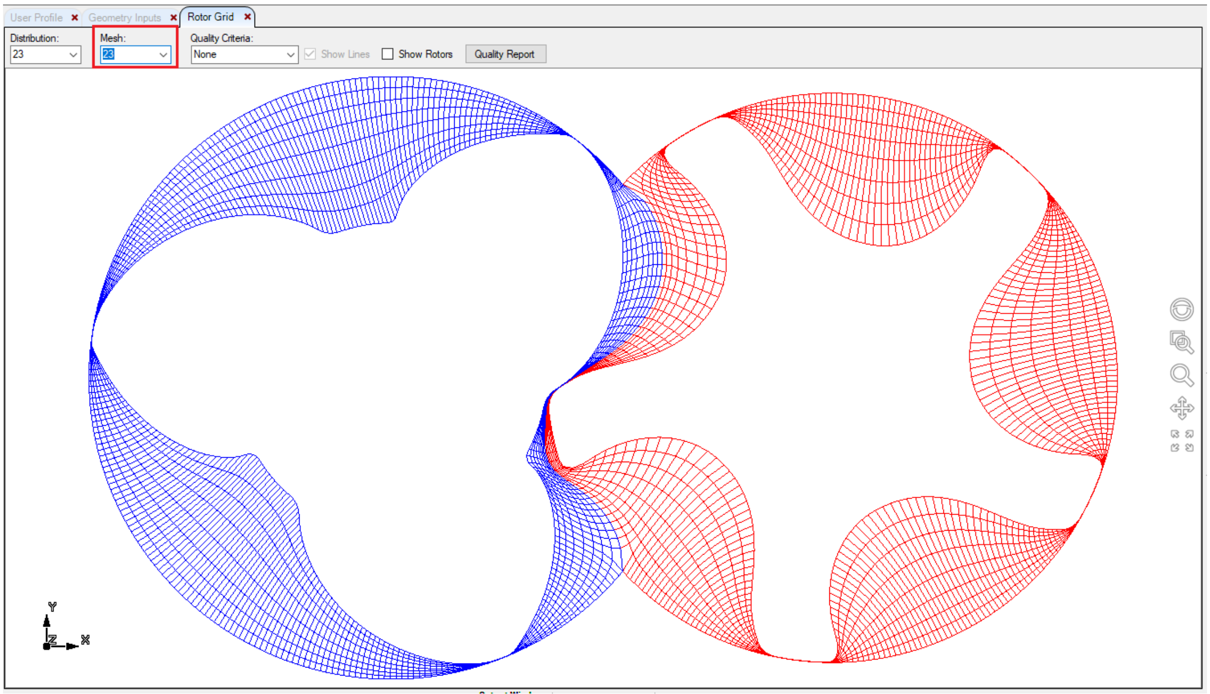
- Click Rotor Grid Generation

- Inspect report and check that there are no grid errors listed

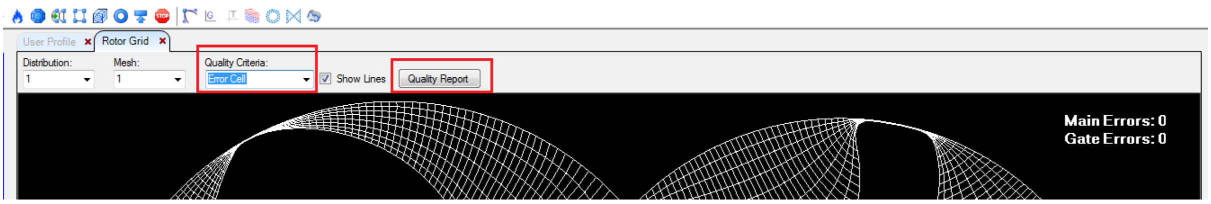


```
C:\SCORG\Grid>echo off

 .........................................................................
 InstallPath = C:\SCORG
 ProjectPath = D:\TwinScrewCFXSetup\SCORG_Grid_Tutorial
 ..........................................................................

  SCORG - Screw Compressor Rotor Geometry grid  generator V.5.9
 .............................................................. 3/ 3/2021...
 Screw compressor/p Wrap =  283.2   RPM=12344.    Vel=  82.3   Ncel= 566400
  Z1/Z2= 3/5  d1=127.38 [mm]  d2=120.32 [mm]  a= 93.00 [mm]  len=216.45 [mm]
 ..........................................................................
  Nfi    Nr   Nz Nadd  Rot Rack Boun Mesh RotM InpP OutP Prep RaSm Line  Oil
   60    8  118   50    0    0    0    1    0    0    0    0    1    1    0
 ..........................................................................
 Calculation:  FLUID GRID  RelaxFac, TolFac, RadBFac, RadBInt, InterlobeBInt
                               1.0     100     0.5     1.0        2
  TFI_Mesh routine - Rotor          1
  TFI_Mesh routine - Rotor          2
  PDE_mesh routine - Rotor          1
  PDE_mesh routine - Rotor          2
  PDE_Interlobe_mesh2 routine: Smooth Interlobe
 ..........................................................................
  Check_Grid - Rotor:           1
  Check_Grid - Rotor:           2
  Write 2D Grid Data

  Grid Data Count:
   Male rotor domain, Vertices:  321300, Cells  283200
 Female rotor domain, Vertices:  321300, Cells  283200
 Written Control.dat
 ..........................................................................
 Cell statistics        Overall number of cells          0
 .Rotor fluid          0            .Inlet  port         0
 .Rotor solid          0            .Outlet port         0
 .........................................................................
  Start: 11:29:31    End: 11:29:42    Running time: 0h: 0m:10s =     2 sec
 .............................................................. 3/ 3/2021...
  SCORG - Screw Compressor Rotor Geometry grid generator - Ver. 5.9
```

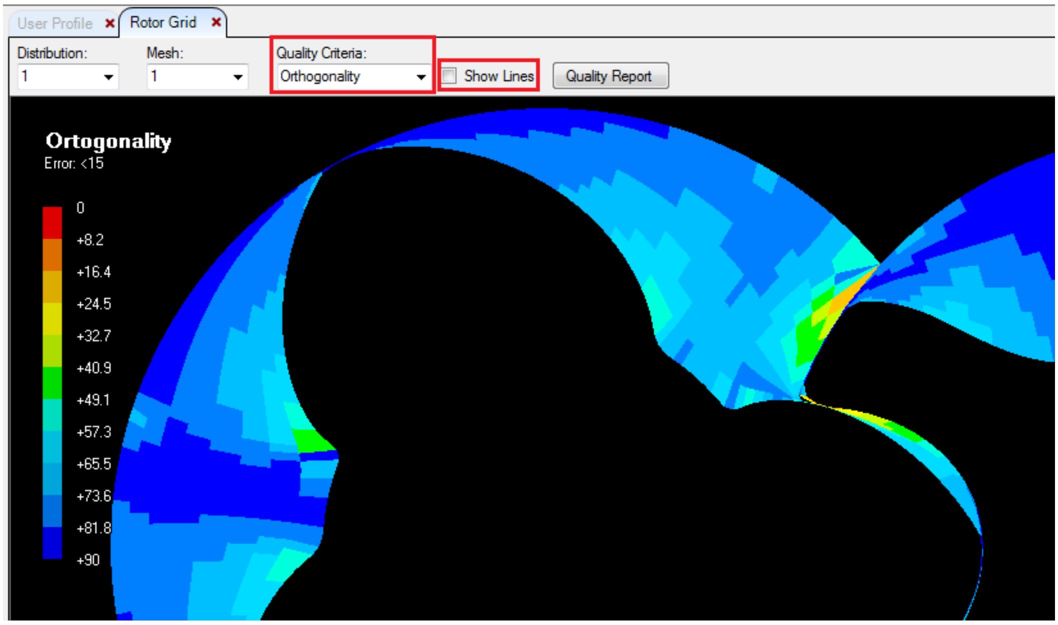
- Click Rotor Grid 2D Mesh to visually inspect the grid in each cross section



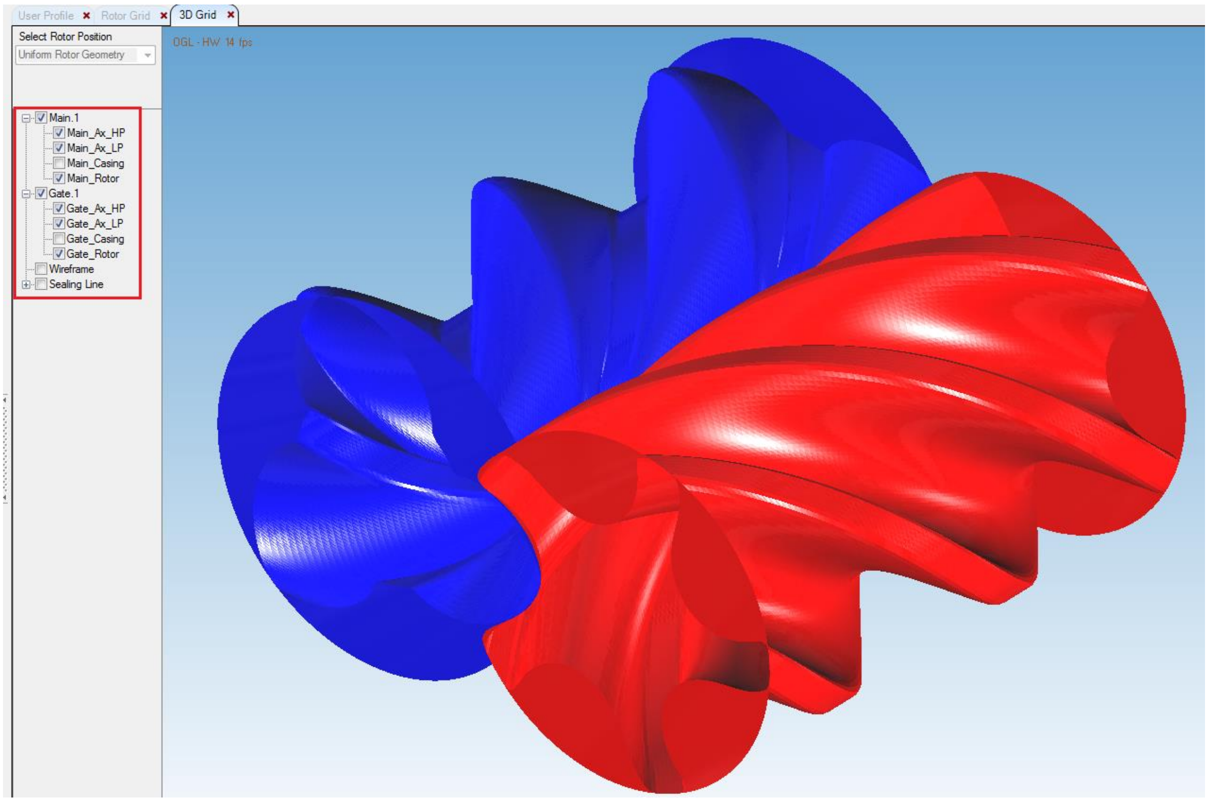
- Click Quality Critera → Error Cell and Inspect.



- Click Quality Critera → Orthogonality and Inspect.



- Inspect the 3D mesh



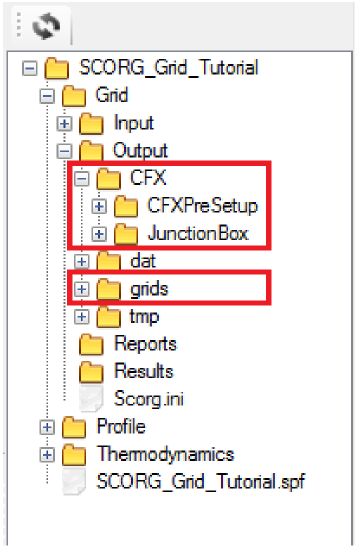
- In Control Switches → Preprocessor Input File select → ANSYS CFX
- Set Vertex Files Start = 1
- Set Vertex Files End = 50 [= Number of Angular Divisions]

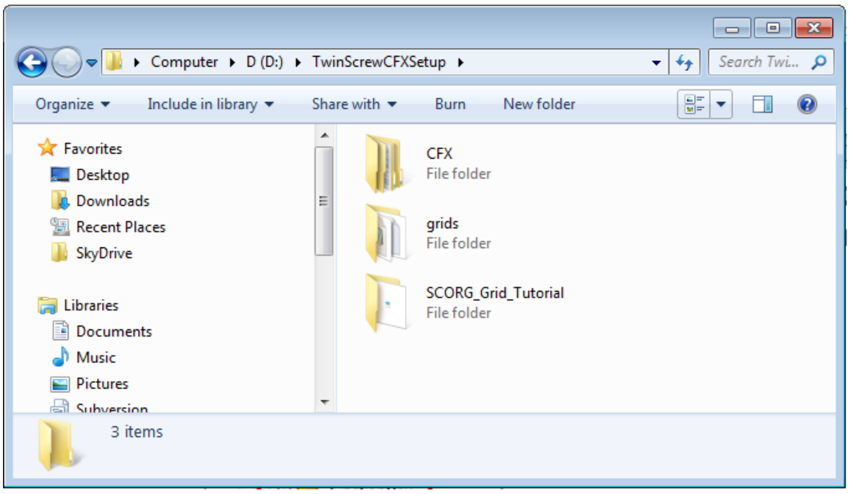
Control Switches	
Rack Generation	Off
Rack Refinement Points	400
Boundary Generation	Off
Fluid Rotor Grid	On
Solid Rotor Grid	Off
Inlet Port Grid	Off
Outlet Port Grid	Off
Preprocessor Input File	ANSYS CFX
Vertex Files Start Number	1
Vertex Files End Number	50

- Calculate Preprocessor Files Generation

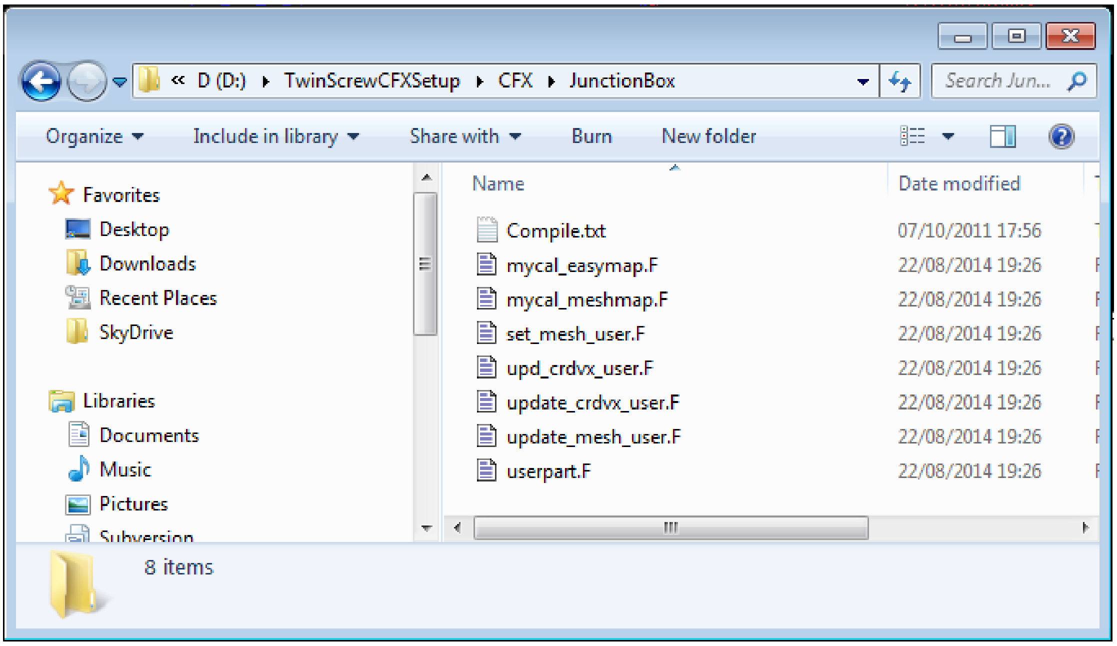

```
C:\SCORG\Grid>echo off

 .......................................................................
 InstallPath = C:\SCORG
 ProjectPath = D:\TwinScrewCFXSetup\SCORG_Grid_Tutorial
 ........................................................................
  All control parameters for grid generation are disabled

 ........................................................................

 Conformal
 ----Generation of Port Pre Processor files
 Low Pressure Port not calculated
 Pre-Processing Skipped
 High Pressure Port not calculated
 Pre-Processing Skipped

 ----Generation of Rotor Pre Processor files
 Checking volumes in Male
 Min/Max Volume=  1.0739071E-11  1.4677777E-08
 Checking volumes in Female
 Min/Max Volume=  8.2917484E-12  1.8342320E-08

 CFX SETUP Grids written

 Generation of time step grid files
   Start time step:          1
   End   time step:         50

Rotor     1,  Grid position     1
Rotor     1,  Grid position     2
Rotor     1,  Grid position     3
```

- With this the SCORG™ Project is complete and the CFX setup can be started.
- In the directory structure of SCORG™ Project → Grid → Output with consist of CFX and grids folder.
- Copy these two folders in the project working directory → TwinScrewCFXSetup
- The CFX folder consists of two sub folders
  - CFXPreSetup
  - JunctionBox





- JunctionBox folder consists of the Fortran codes that need to be compiled to generate an external library that will be linked to the CFX solver during executions in order to be able to read the set of grids generated by SCORG™



4 Compiler Environment setup [*One time procedure*]

Intel Fortran Compiler is required in the initial stages of the case setup. It is not required to repeat this step for every CFX case setup.

For Windows OS,

- Install Microsoft Visual Studio 2008 or any later version.

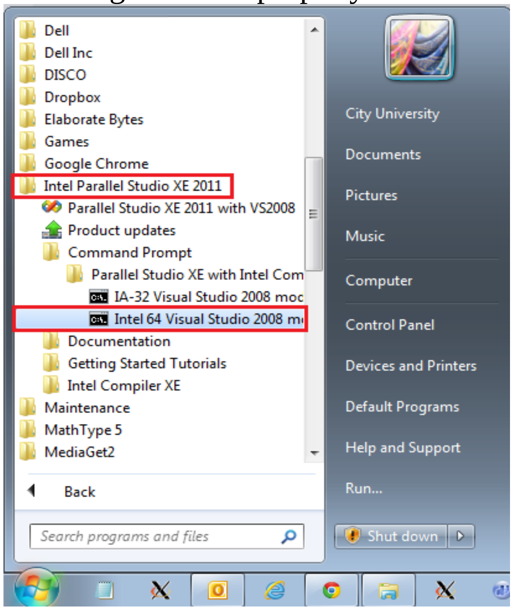
- Install Intel Parallel Studio XE 2011 for the Fortran compiler.

Below are some links that provide these installers (Evaluation Editions), but if you have other Fortran compiler then it can be used.

http://www.microsoft.com/en-gb/download/details.aspx?id=40787

https://software.intel.com/en-us/intel-parallel-studio-xe/

You can then access the Intel Fortran compiler command prompt as shown below. Try to run **ifort** command to check if it is recognized and properly works.



For Linux, check if either of F77, F90, G77, G90 or a Portland compiler is installed.

4.1 Compilation of Junction box Subroutines

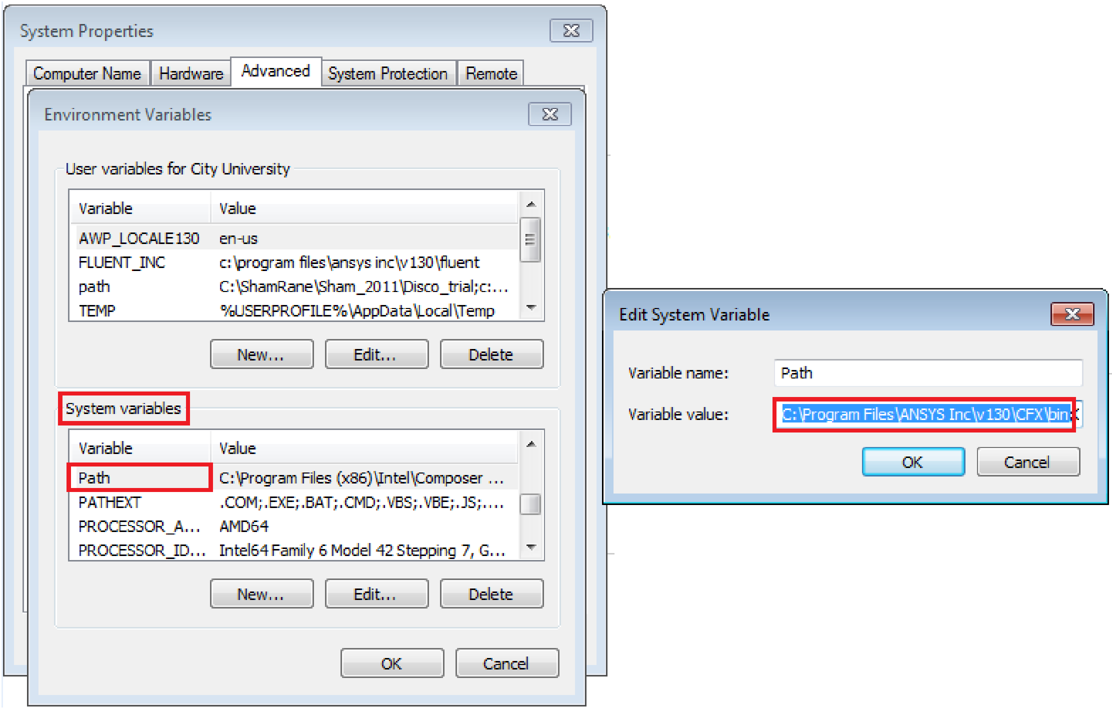
Junction box subroutines are used by CFX solver to read the new mesh coordinates of the rotor domain every time step. The source code and compilation command used for this purpose is available in the [**TwinScrewCFXSetup\CFX\JunctionBox**] folder.

For Windows,

In order to create the library and link the object files compiled by Fortran compiler we will use the cfx command **'cfx5mkext'**. For this you need to first set the environment variable 'Path' and point to the CFX installation directory.

System Properties → Advanced → Environment Variables → System Variables → Path.

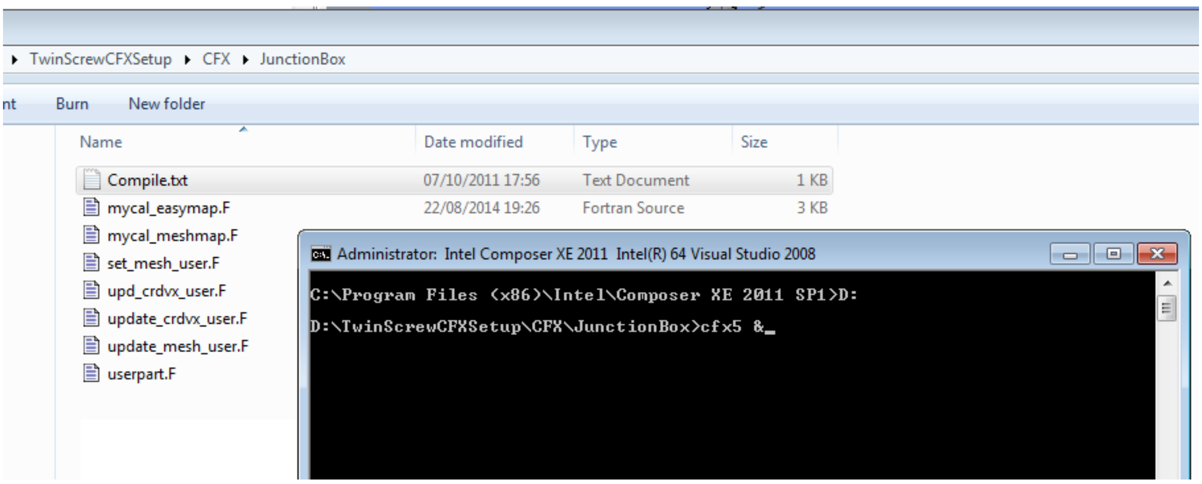
Add the path of [..*AnsysInc\v130\CFX\bin*] to the variable separated by a semicolon from others.

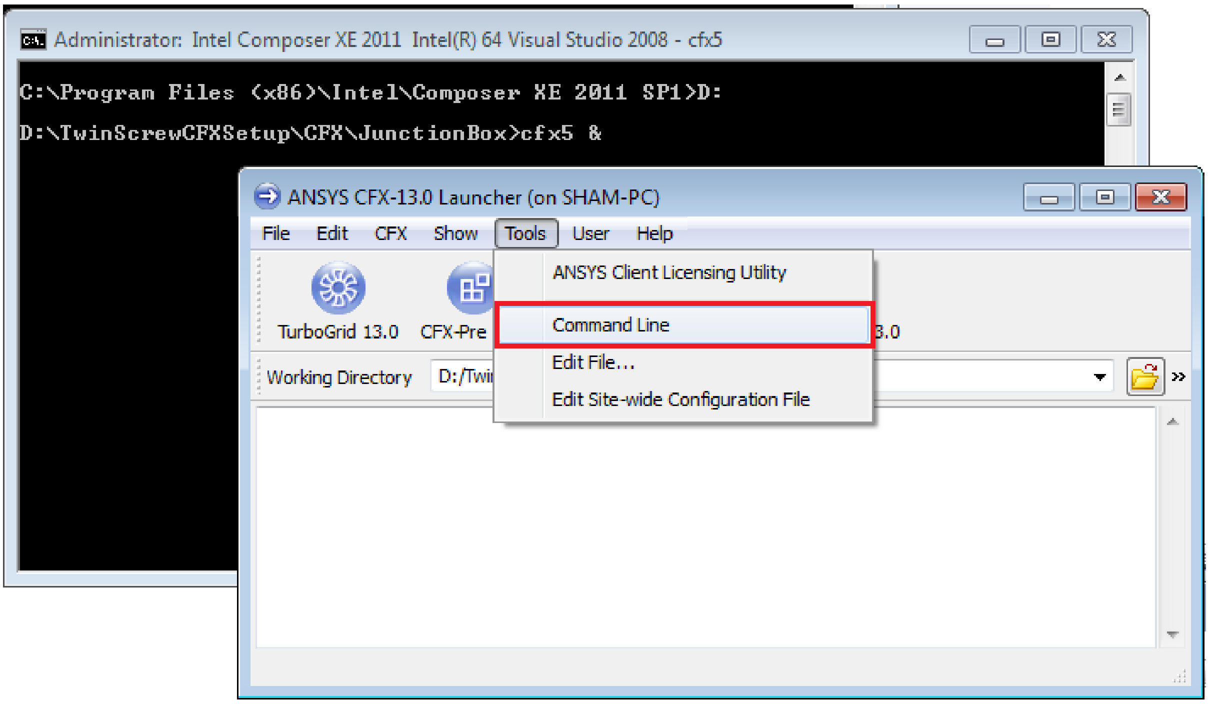


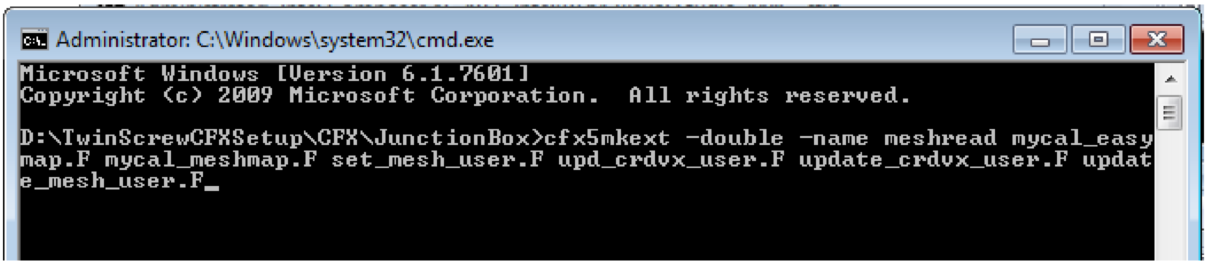
Once the path is set, launch Intel Fortran Compiler command prompt. Change the working directory. Issue the command mentioned in **Compile.txt** file.

-double is a flag for double precision CFX simulation. You need to remove it for Single precision simulations.

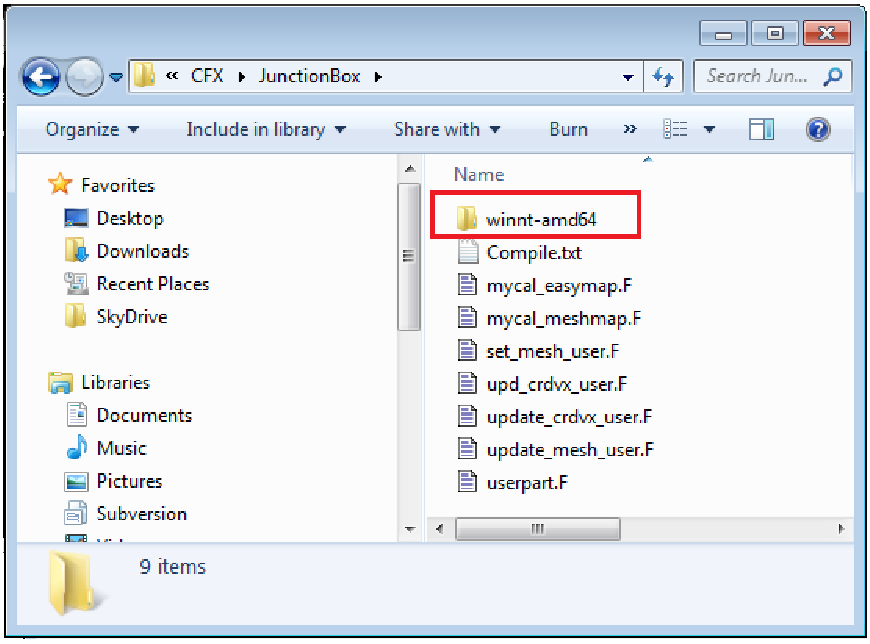
-name is a flag for the routine object and is called by the solver.







- Copy the created library “winnt-amd64” in the C:\windows folder for easy access and subsequent reuse

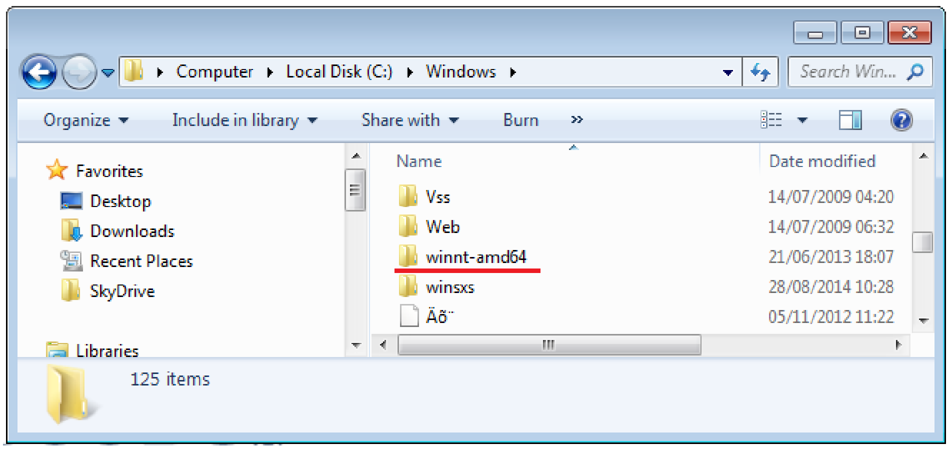


For Linux,

Go to the working directory using Linux command prompt and issue the following commands.

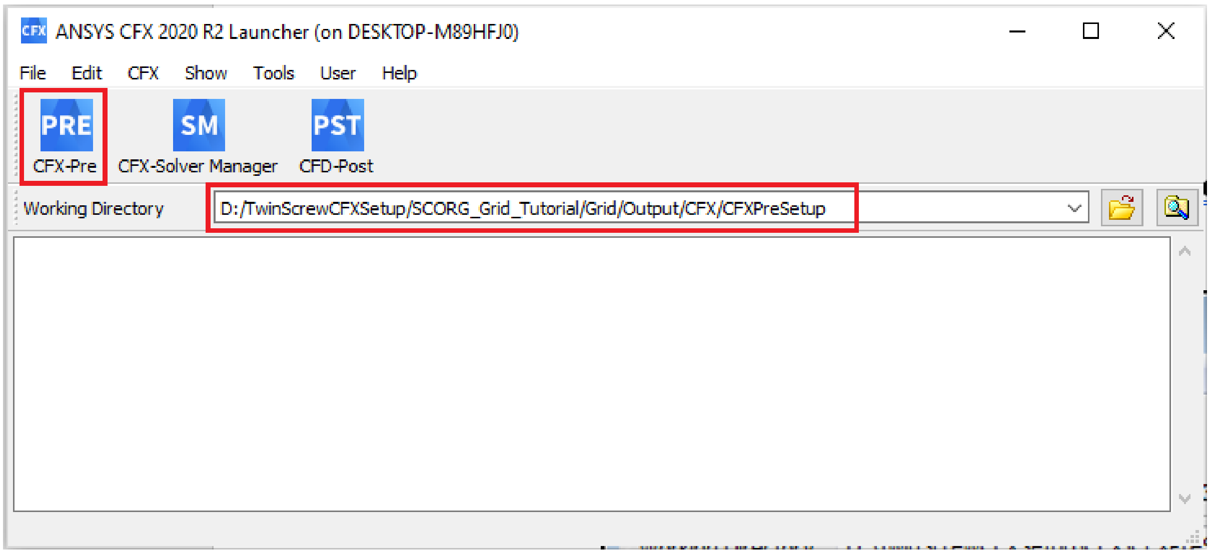
- Use Intel Fortran Compiler 2015
- The procedure for compilation is same as for windows.
- A folder **linux-amd64** will be created when this step is successful.

It is not required to repeat this step for every CFX case setup and the folder **winnt-amd64/linux-amd64** can be just copied and used again in another case. But this library is specific to a given operating system and a given architecture. So in case you are running on a 32 bit OS or any other OS (Win 8) etc. you need to execute this step and provide the library so created to the CFX solver definition file. The library is common for Serial and Parallel Simulations.

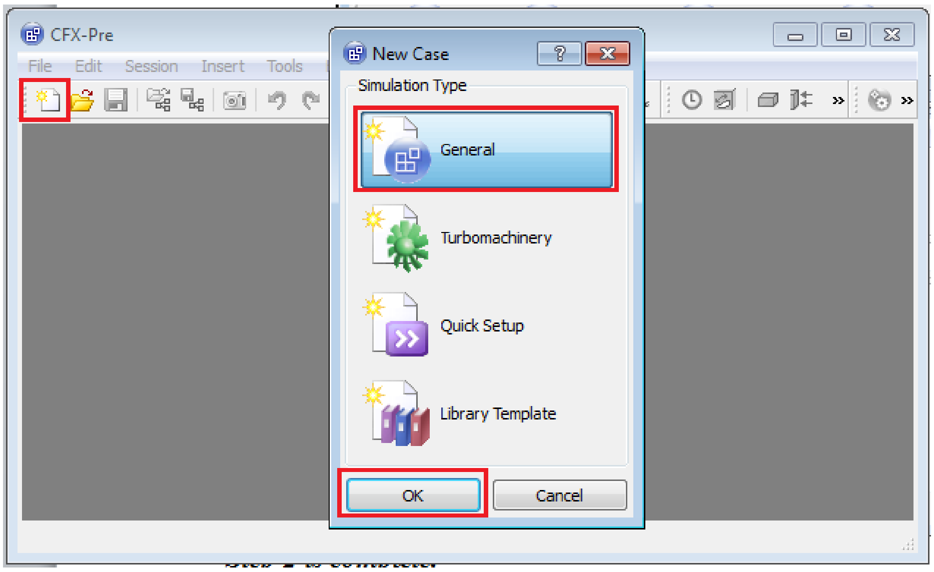


5 CFX Pre case setup

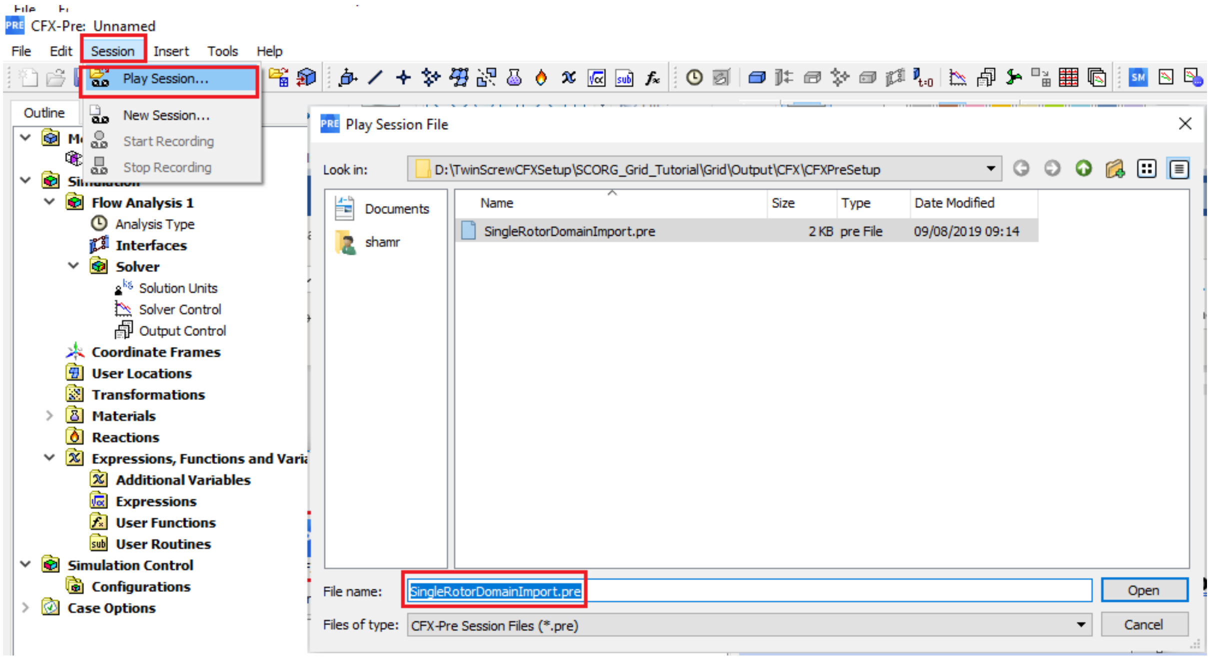
- Launch CFX from [**TwinScrewCFXSetup\CFX\CFXPreSetup**] folder



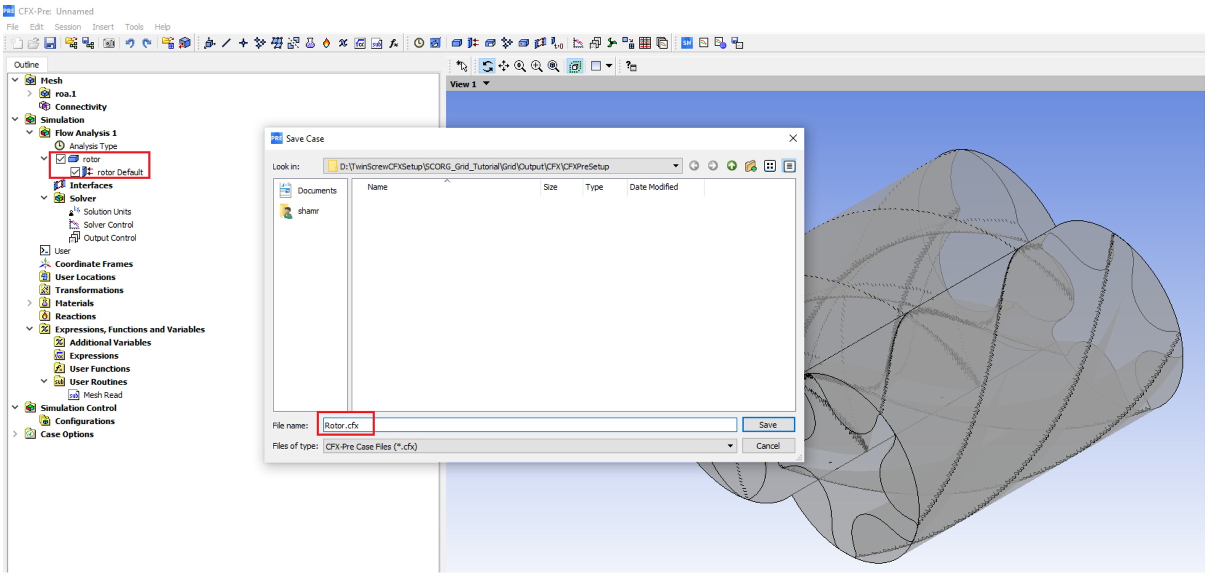
- Select New → General



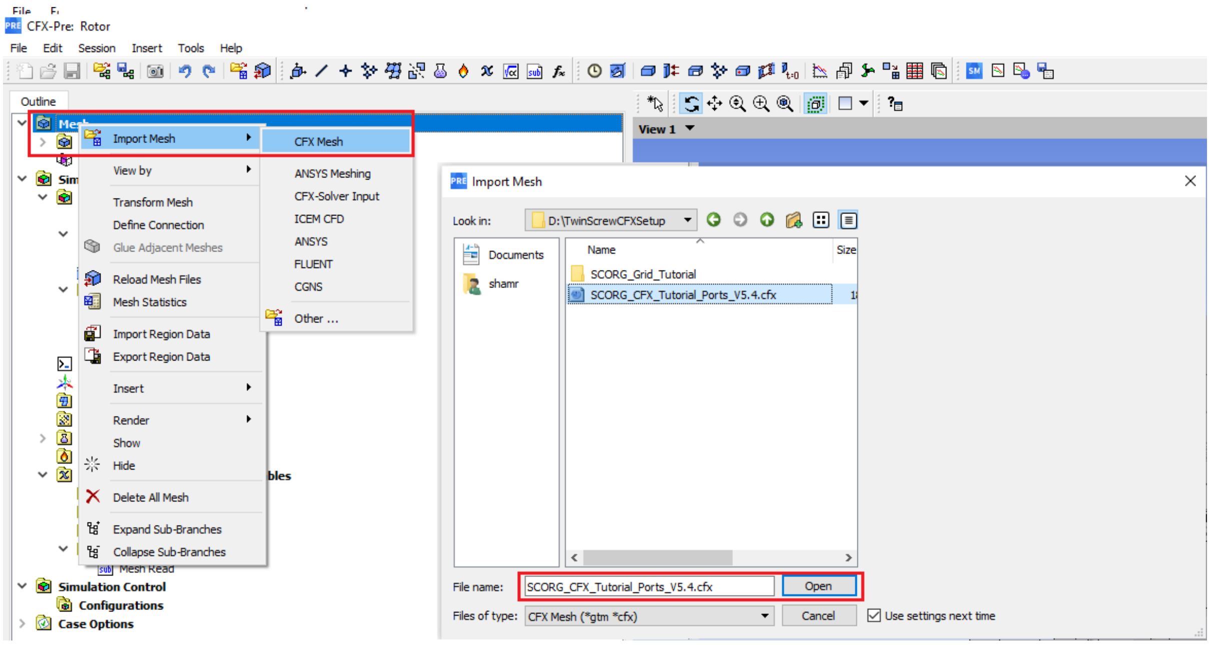
- Go to → Session → Play Session → Select SingleRotorDomainImport.pre



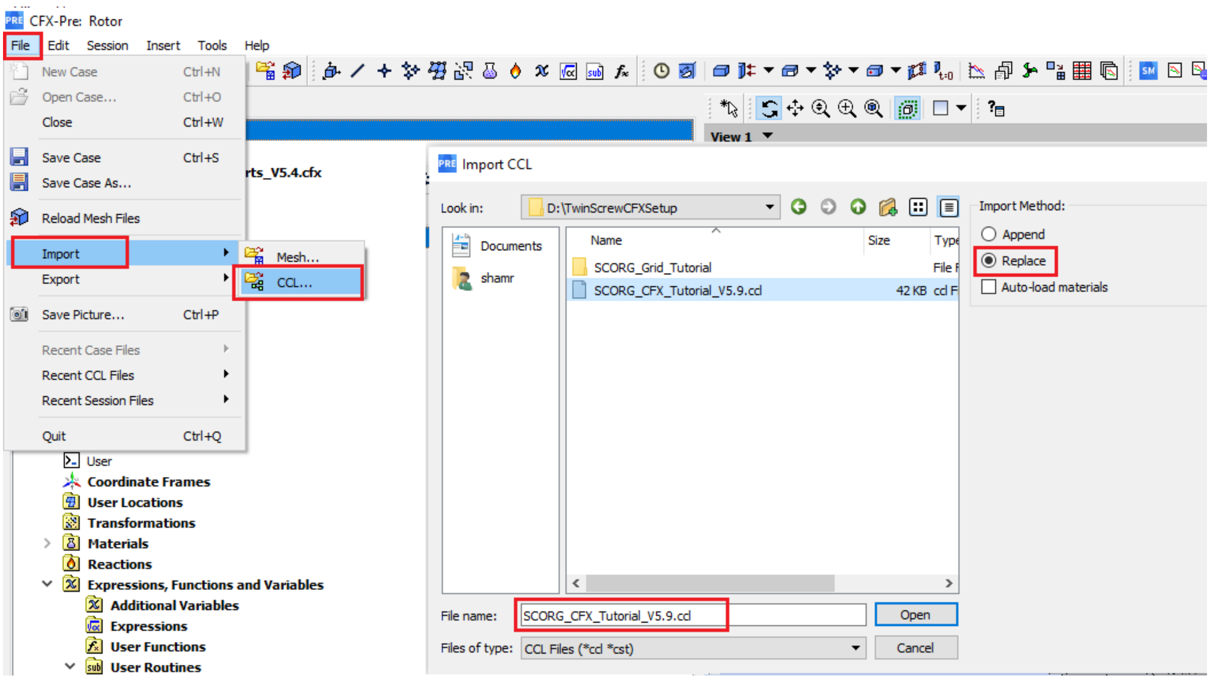
- This imports the rotor grid in starting position and single domain rotor is created in the setup.
- Save case as Rotor.cfx



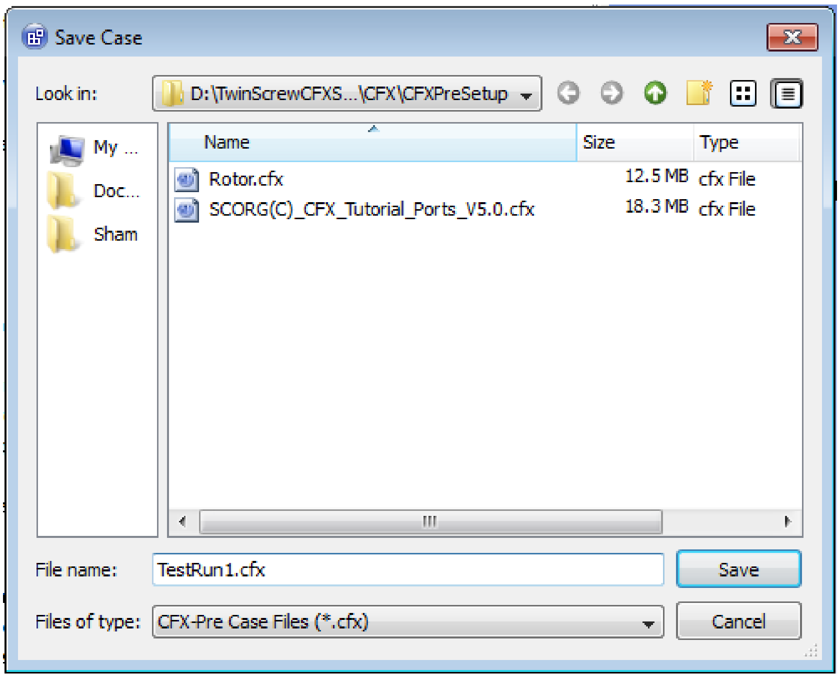
- Right click Mesh → Import Mesh → CFX Mesh → Select SCORG_CFX_Tutorial_Ports_V5.4.cfx



▶ Go to File → Import → CCL → Select SCORG_CFX_Tutorial_V5.9.ccl

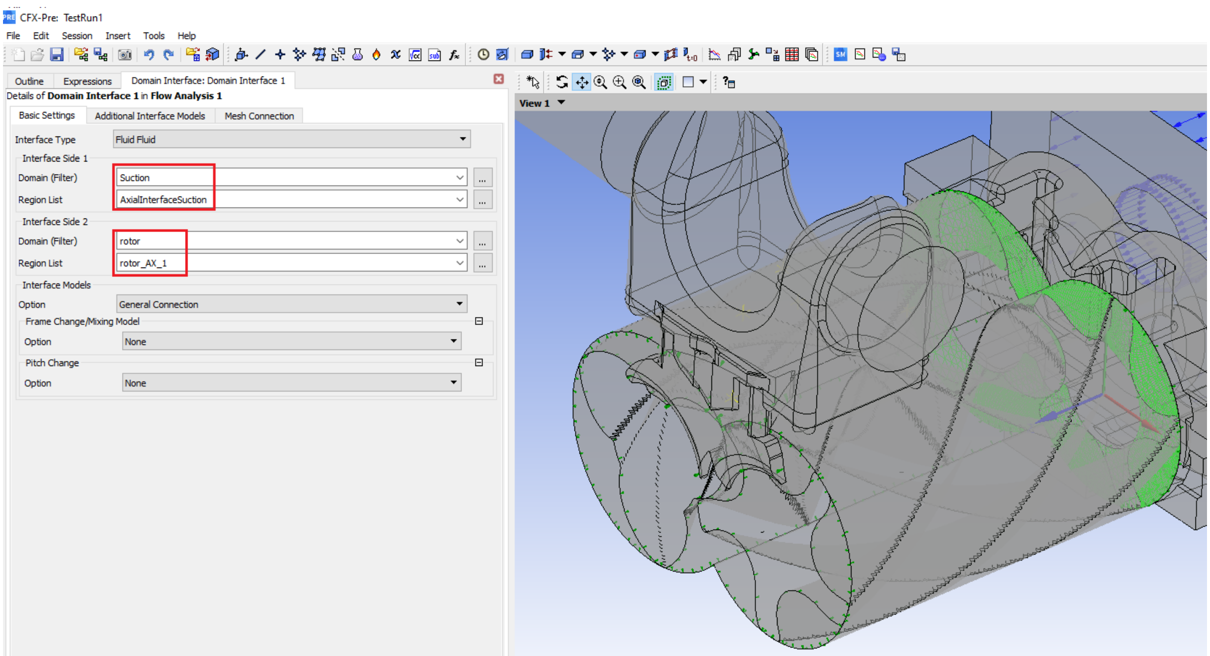


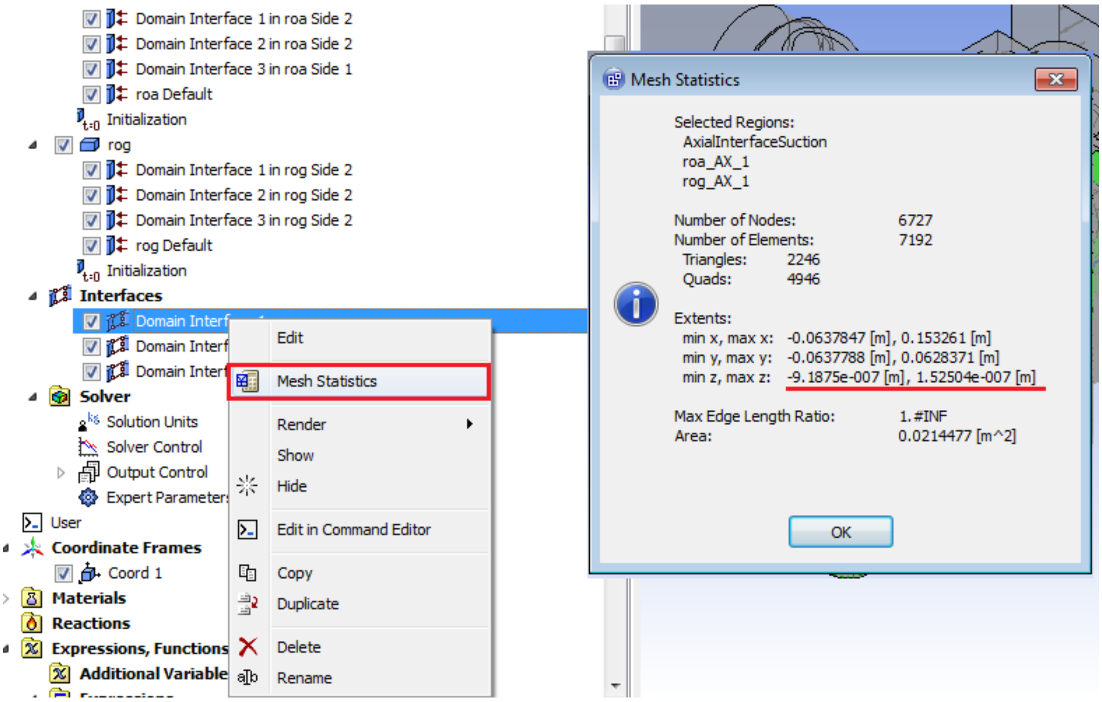
▶ Save case as Testrun1.cfx



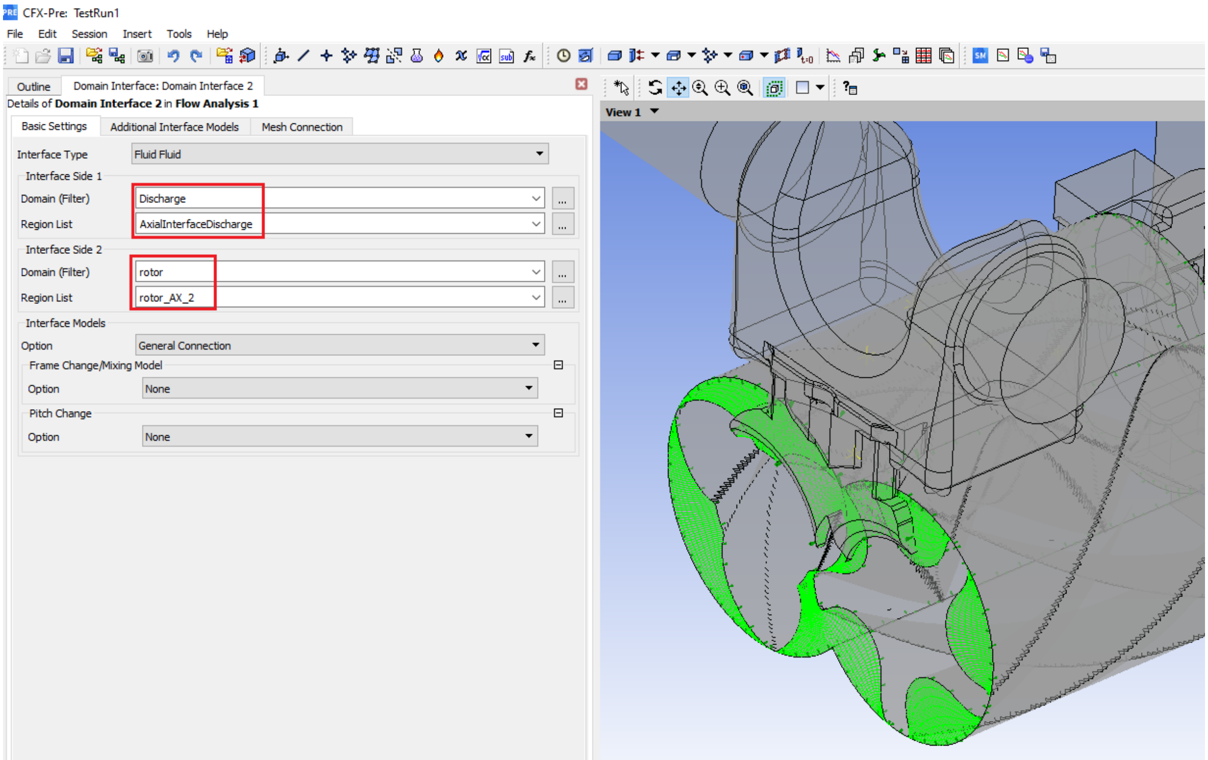
- In the setup there are three non-conformal grid interfaces
  - Domain Interface 1
  - Domain Interface 2
  - Domain Interface 3

- **Interface 1** is between the Suction Port and the two rotors.
  - Inspect the interface settings.
  - Right click Domain Interface 1 → Mesh Statistics → min / max z should match so that there is no gap between the faces.

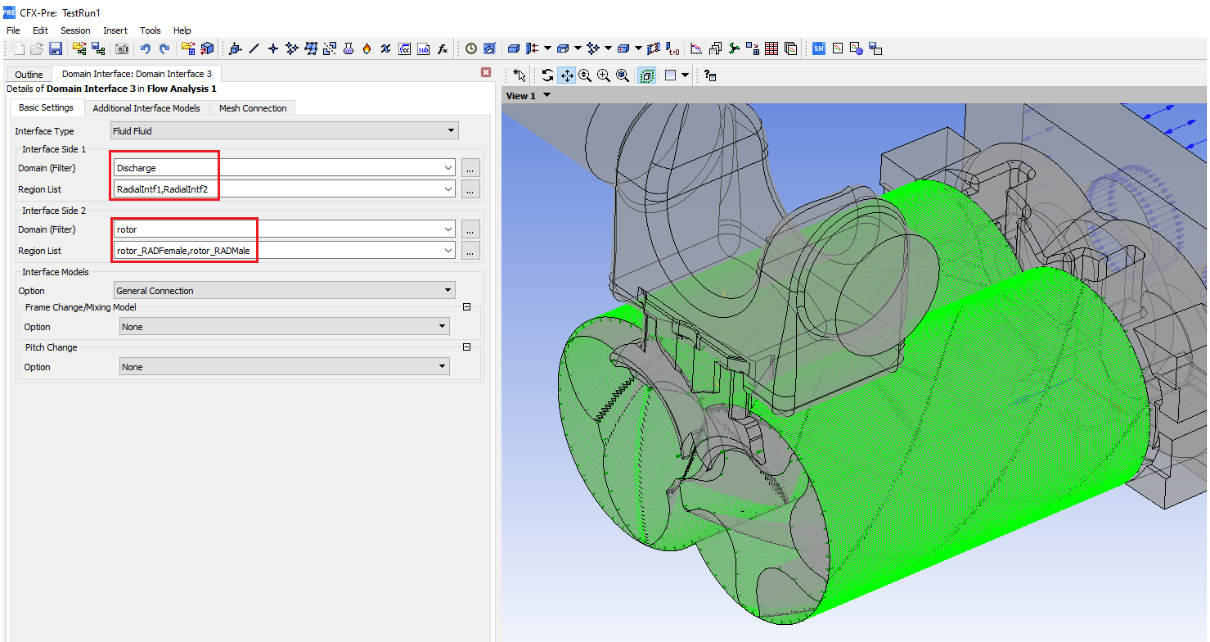




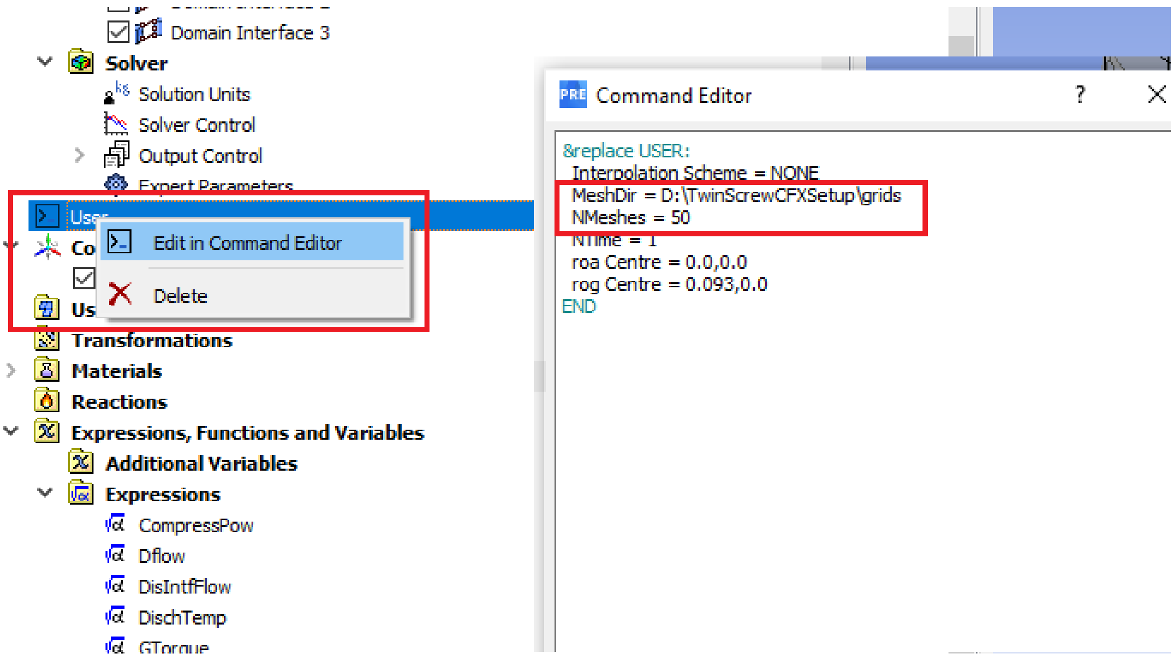
- **Interface 2** is between the Discharge Port and the two rotors.
  - Inspect the interface settings.
  - Right click Domain Interface 2 → Mesh Statistics → Min / Max Z should match so that there is no gap between the faces.



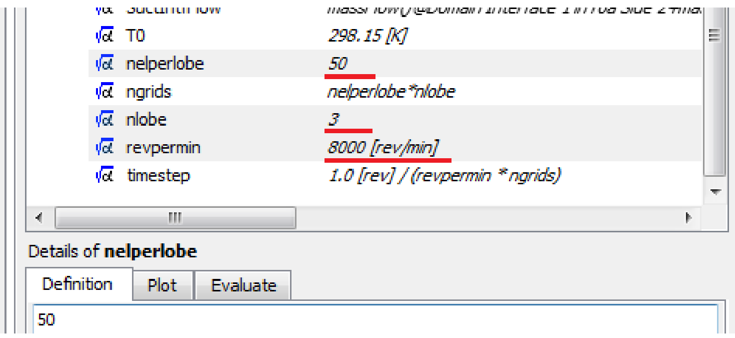
- **Interface 3** is between the two rotors and also with the Discharge Port and a special zone selection is required in such type of domain connection.
    - Inspect the interface settings.
    - Notice that the face zones form a cross exchange of boundaries as highlighted.



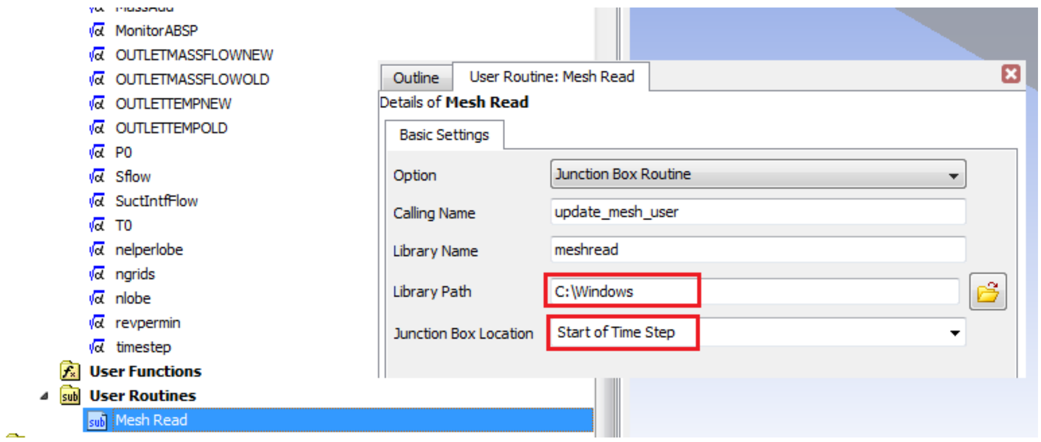
- Go to User → Edit in Command Editor → Set the correct MeshDir, NMeshes and rog Centre.



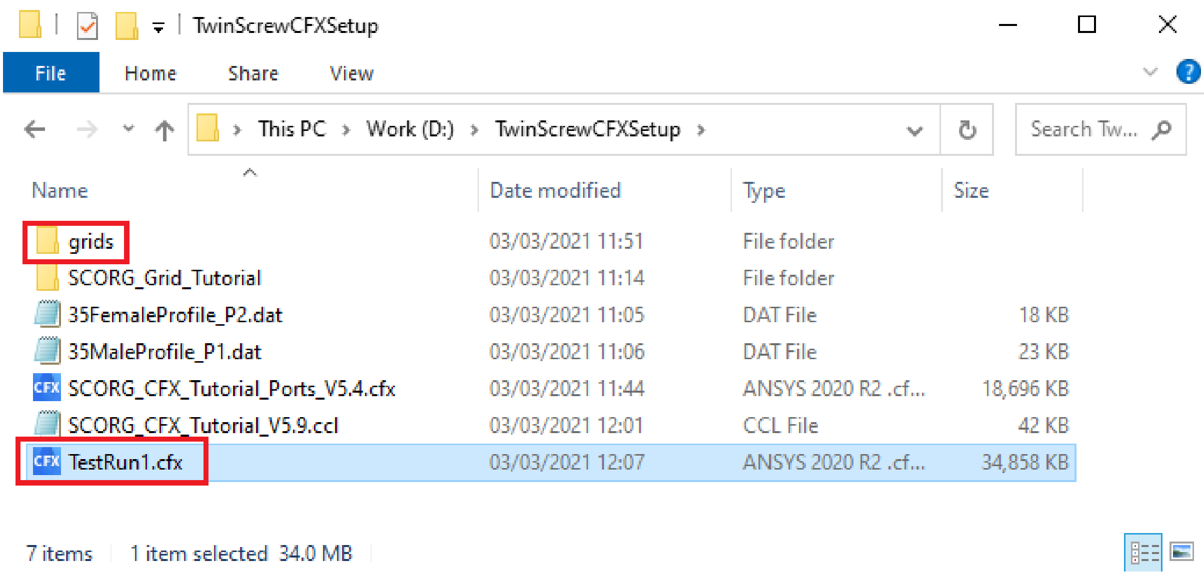
- Go to Expressions → Set the correct parameters
  - nelperlobe = Number of divisions in Angular = 50
  - nlobe = Number of Lobes on Male Rotor = 3
  - revpermin = rpm of Male rotor = 8000



- Go to Mesh Read → Set correct Library Path → Start of time Step
  - Library Path is the folder where winnt-amd64 has been placed

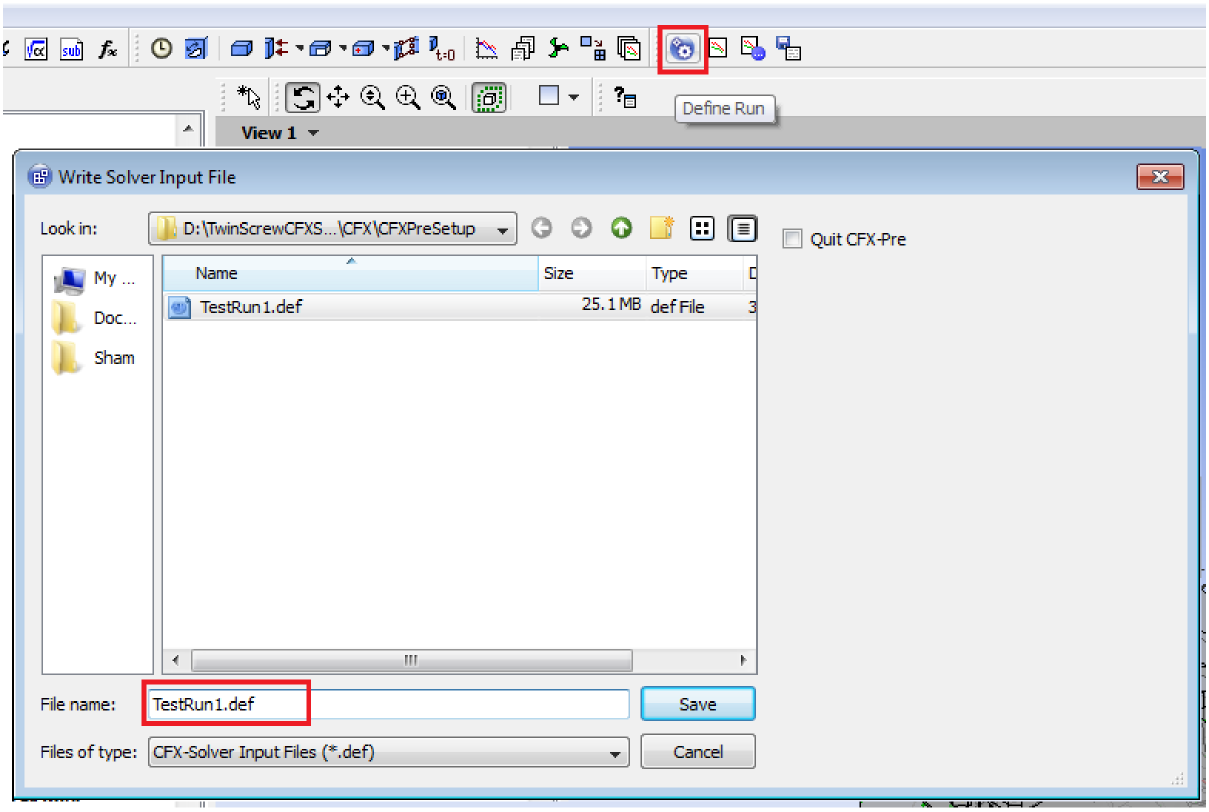


- Move TestRun1.cfx and grids folder → TwinScrewCFXSetup → Open TestRun1.cfx
  - Only rotor.1, rotor.2 etc file from grids folder will be used, other files can be deleted.

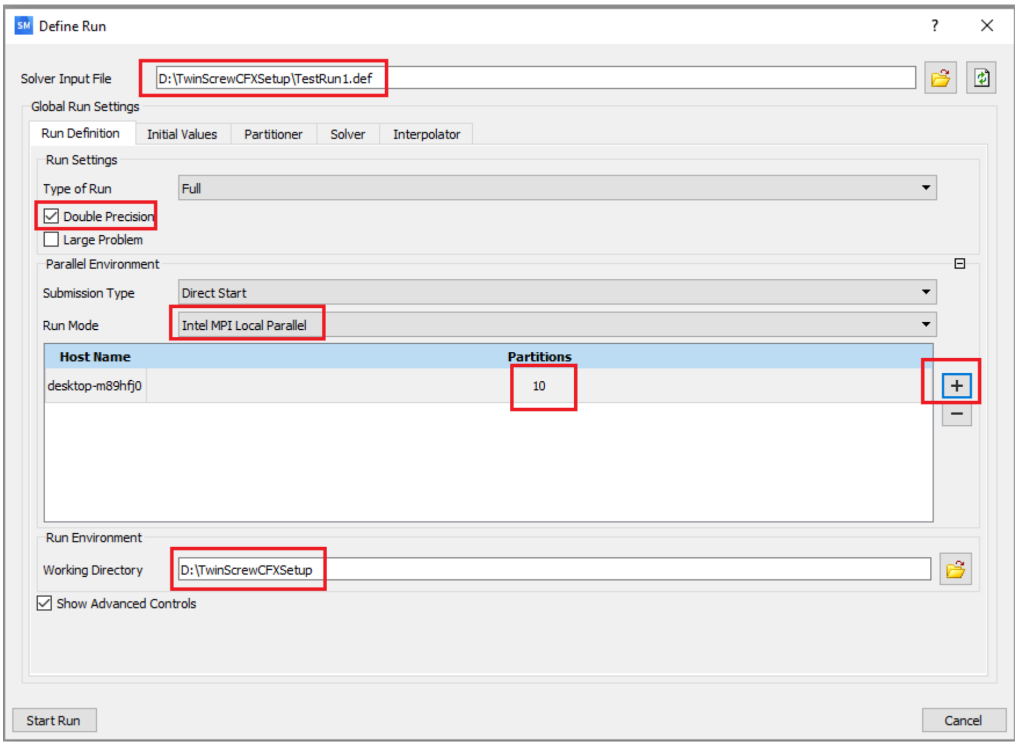


6 CFX Solver Calculation

- Click Define Run → Save Definition file as TestRun1.def



- Select → Double Precision → HP MPI Local Parallel → Start Run



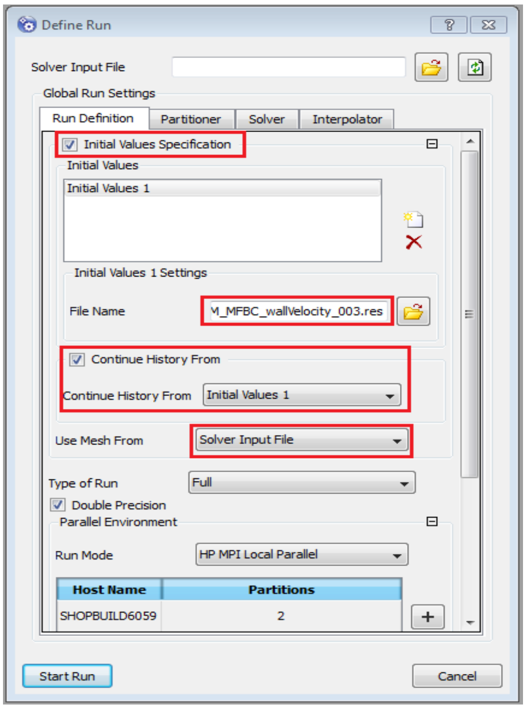
- In the Time stepping Information, mesh map generation and replacement with consecutive meshes should be reported

```
======================================================================
|                      Timestepping Information                      |
----------------------------------------------------------------------
|   Timestep    |    Courant Number     | Acoustic Courant Number |
+---------------+-----------------------+-------------------------+
|               |    RMS        MAX     |     RMS        MAX      |
+---------------+-----------------------+-------------------------+
|   5.0000E-05  |    0.10       2.75    |    724.04     999.99    |
----------------------------------------------------------------------
DOMAIN: rotor
Reading mesh for map generation
File read: D:\TwinScrewCFXSetup\grids\rotor.1
Number of vertices  =          636650
DOMAIN: rotor
File read: D:\TwinScrewCFXSetup\grids\rotor.2
Number of vertices  =          636650
+--------------------------------------------------------------------+
|                          Mesh Statistics                           |
+--------------------------------------------------------------------+
| Domain Name             | Orthog. Angle | Exp. Factor | Aspect Ratio |
+-------------------------+---------------+-------------+--------------+
|                         | Minimum [deg] |   Maximum   |   Maximum    |
+-------------------------+---------------+-------------+--------------+
| rotor                   |      14.0  !  |     990  !  |    1064  OK  |
| Global                  |       1.1  !  |   13142  !  |   11204  ok  |
+-------------------------+---------------+-------------+--------------+
|                         |  %!  %ok  %OK | %!  %ok  %OK | %!  %ok  %OK |
+-------------------------+---------------+-------------+--------------+
| rotor                   |  <1   10   90 | <1    1   99 |  0    0  100 |
| Global                  |  <1    9   91 |  4    2   94 |  0   <1  100 |
+-------------------------+---------------+-------------+--------------+
Domain interface: Domain Interface 1
    Non-overlap area fraction on side 1                  =    4.48E-01
    Non-overlap area fraction on side 2                  =    2.69E-01
Domain interface: Domain Interface 2
    Non-overlap area fraction on side 1                  =    4.13E-01
    Non-overlap area fraction on side 2                  =    8.11E-01
Domain interface: Domain Interface 3
    Non-overlap area fraction on side 1                  =    4.90E-04
    Non-overlap area fraction on side 2                  =    9.84E-01

======================================================================
TIME STEP =     1 SIMULATION TIME = 5.0000E-05 CPU SECONDS = 2.306E+02
----------------------------------------------------------------------
```

6.1 Restarting a Simulation from an intermediate Stop

You can stop the simulation at an intermediate step by hitting the stop button in CFXSolver GUI or through command line. This will complete the current coefficient loop iteration and close the solver. Results file is written for the current completed time step.

To restart from the same flow time specify this result file as the initialization file and check on the continue history from initial file. This will continue the residual monitors from the same time steps and also the junction box routine will call the corresponding mesh file from the grids directory.



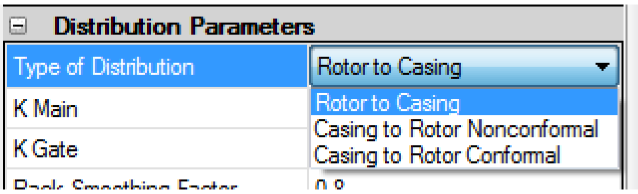
7 Distribution Options

There are three options available in the Type of Distribution (Rane, 2015)

a. Rotor to Casing
Generates a smooth rotor surface and node distribution on the rotor can be controlled using Distribution Adaptation factors. This gives good quality rotor profile in 3D.

b. Casing to Rotor Nonconformal
Generates an orthogonal cell structure with possibility to independently refine the interlobe leakage region. This gives better leakage predictions.

c. Casing to Rotor Conformal
Generates an orthogonal cell structure with a single domain containing both the rotors.



The selection of the type of distribution is dependent on the type of screw machine being solved and the CFD solver in consideration. For ANSYS CFX all the three options are available.

The preferred option is Casing to Rotor Conformal as this will generate a single block structured grid that has both the rotors and eliminates the interface between them

Refer to SCORG Help Manual for more details.

8 Summary

This document describes the steps to setup an ANSYS CFX model for Screw compressor CFD analysis starting from output data generated by SCORG™ Meshing tool. More detailed information on using SCORG and Screw compressor mesh generation can be found in user guide (SCORG, 2021). As mentioned earlier the compilation of junction box routines is a onetime process but has to be done whenever the operating system or its architecture changes. The set of mesh files generated for a complete cycle are reused cyclically when the simulation is run for more than one cycle. Thus it is possible to continuously run the simulation until repeatable results in the monitors and good convergence is obtained. It is also possible to stop and restart the simulation in between, change certain Boundary conditions, Solver control parameters or save the intermediate results. More details information on using ANSYS CFX, Transient simulations and Post-Processing can be found in user guide (ANSYS CFX, 2021).

9 Bibliography

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