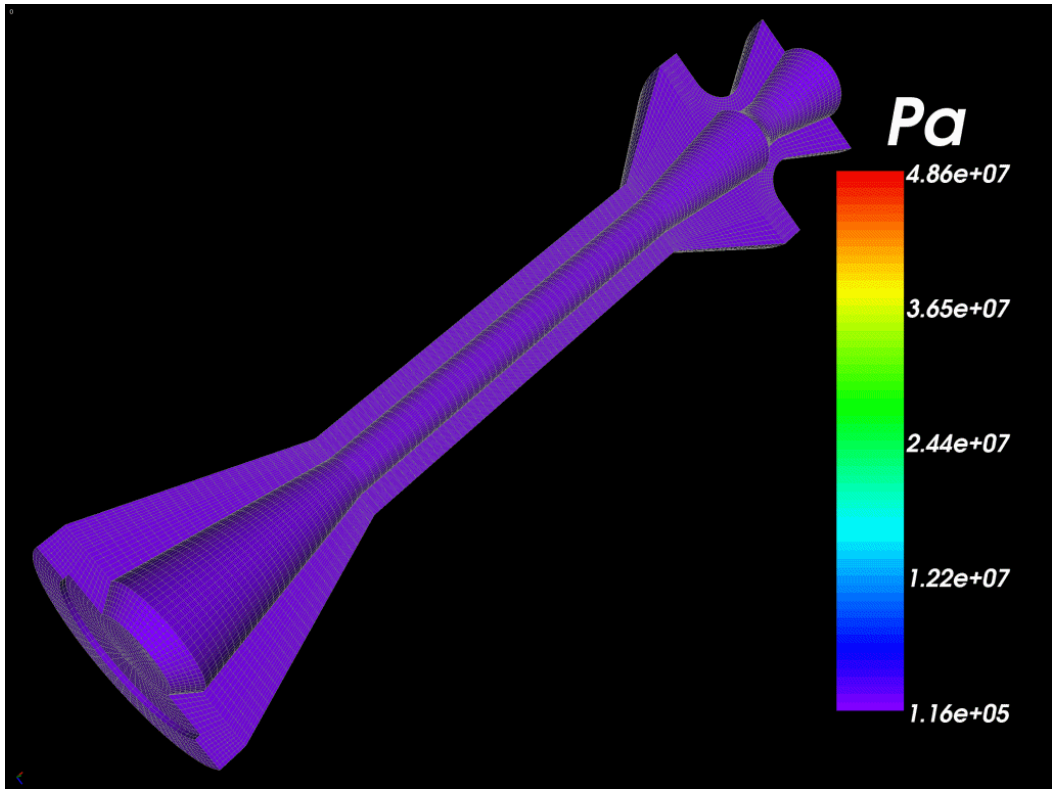
Section 13: Use Case 1

Attitude Control Motor

Problem Description

- Small (2 inch) Attitude Control Motor (ACM)
- Regressing burning surface
- Fluid-combustion coupling
- Rocflo model – block-structured hexahedral grid
- Goal: assemble and run moving-boundary fluid-combustion coupled run with Rocflo



File Checklist

- Rocstar
  - RocstarControl.txt
- Rocman
  - RocmanControl.txt
- RocburnAPN
  - RocburnAPNControl.txt
- Rocflo
  - RocfloControl.txt
  - ACM.inp
  - ACM.bc
  - ACM-COBALT.bcmp
  - ACM-COBALT.bc
  - ACM-COBALT.inp
- Gridgen
  - ACM.gg
  - ACM.dba

Rocstar does not use these files directly

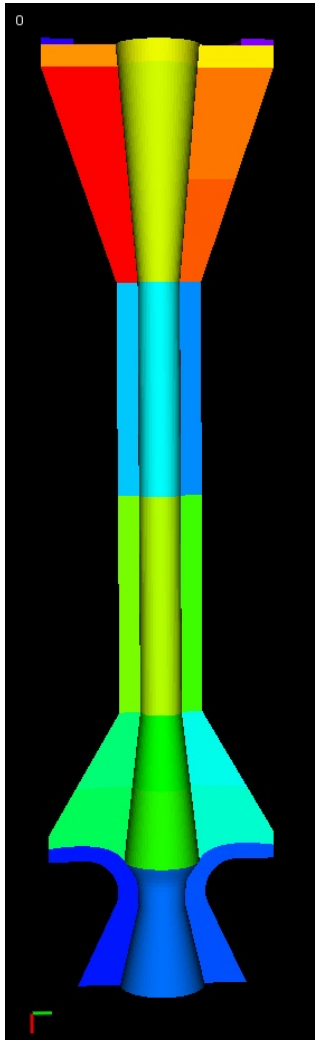
Preparing *Rocflo* Input

Outline

- Produce CAD model
  - Pro/Engineer exports IGES format
  - Can make simple geometries in Gridgen
- Generate meshes, set BC flags
  - Gridgen – block-structured Hex meshes for *Rocflo*

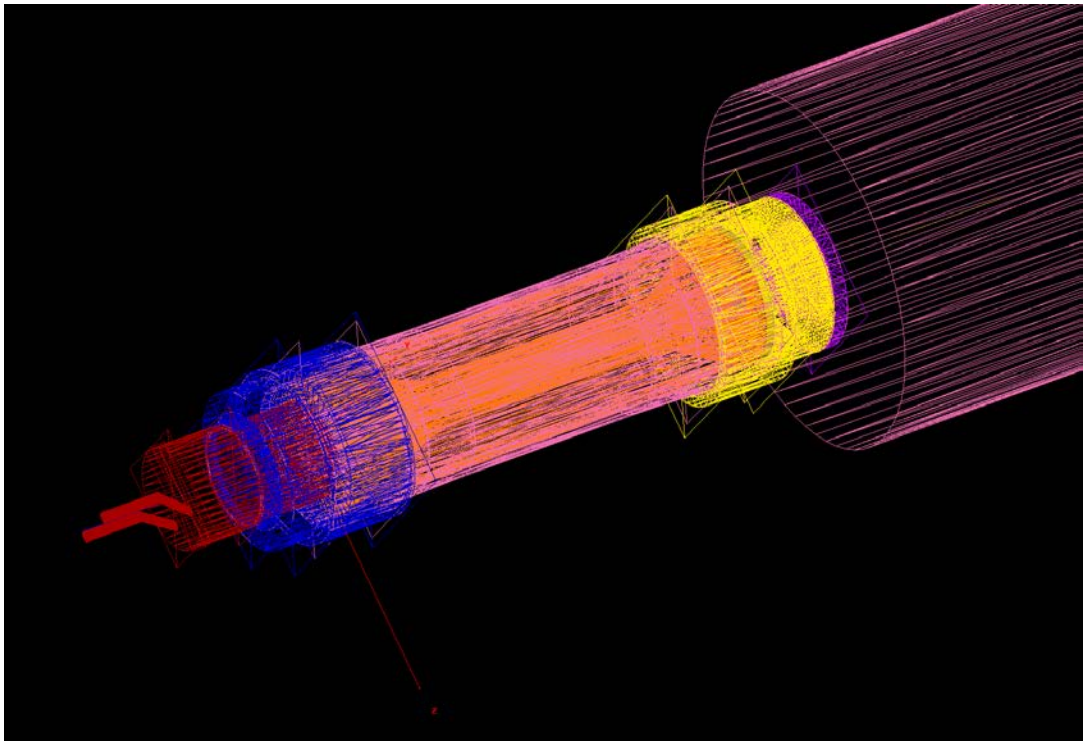
- Set up NDA with grids and input files
  - Choose a “casename”; ACM for this example
  - Grid, boundary condition map file
  - Basic input, boundary conditions, control
- Preprocess and partition
  - Use *Rocprep* on NDA
- Check input again!

Cutaway of Block Model



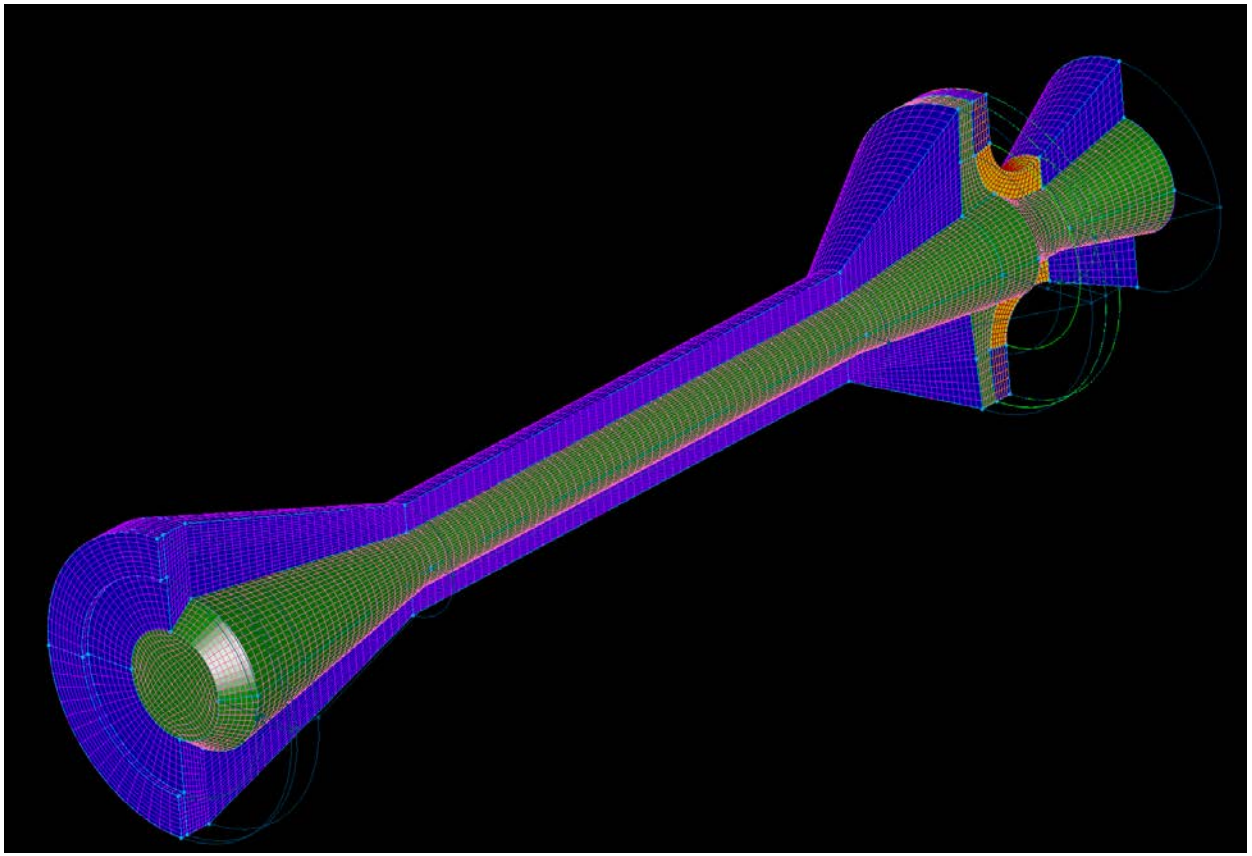
Database

- Made with Pro-Engineer; exported as iges
- Import into Gridgen
  - Almost always significant cleanup necessary; spurious surfaces, lines that don't connect
  - DB to the right has many extraneous elements



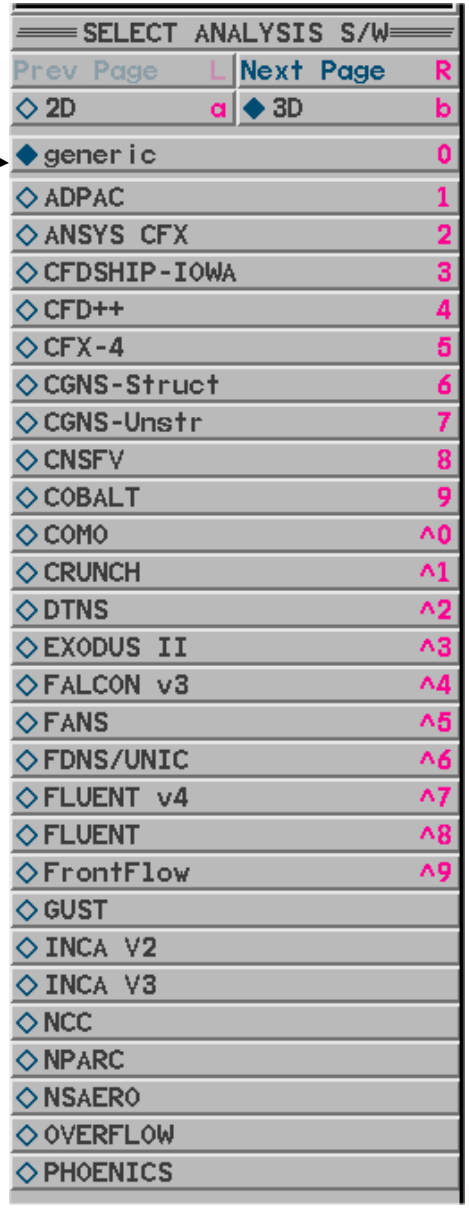
Assemble Block System

- Once DB is clean, assemble connectors, domains, and blocks
- Some blocking restrictions
  - Core block with four quarters
  - Can't combine quarter "wrap" blocks



Rocflo Boundary Conditions

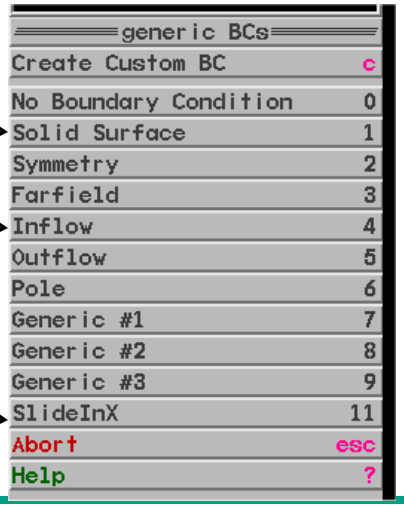
- Make sure Analysis Software is set to generic (Plot3D)
  - Can't fix after setting BCs!
- Make sure all external surfaces have a BC
- Make sure no internal inter-block surfaces do (all Type -1)
- Make note of BC numbers, as they will be needed for the .bcmp file
  - Custom BC numbers are accurate
  - Pre-set BC numbers are off by one (low)



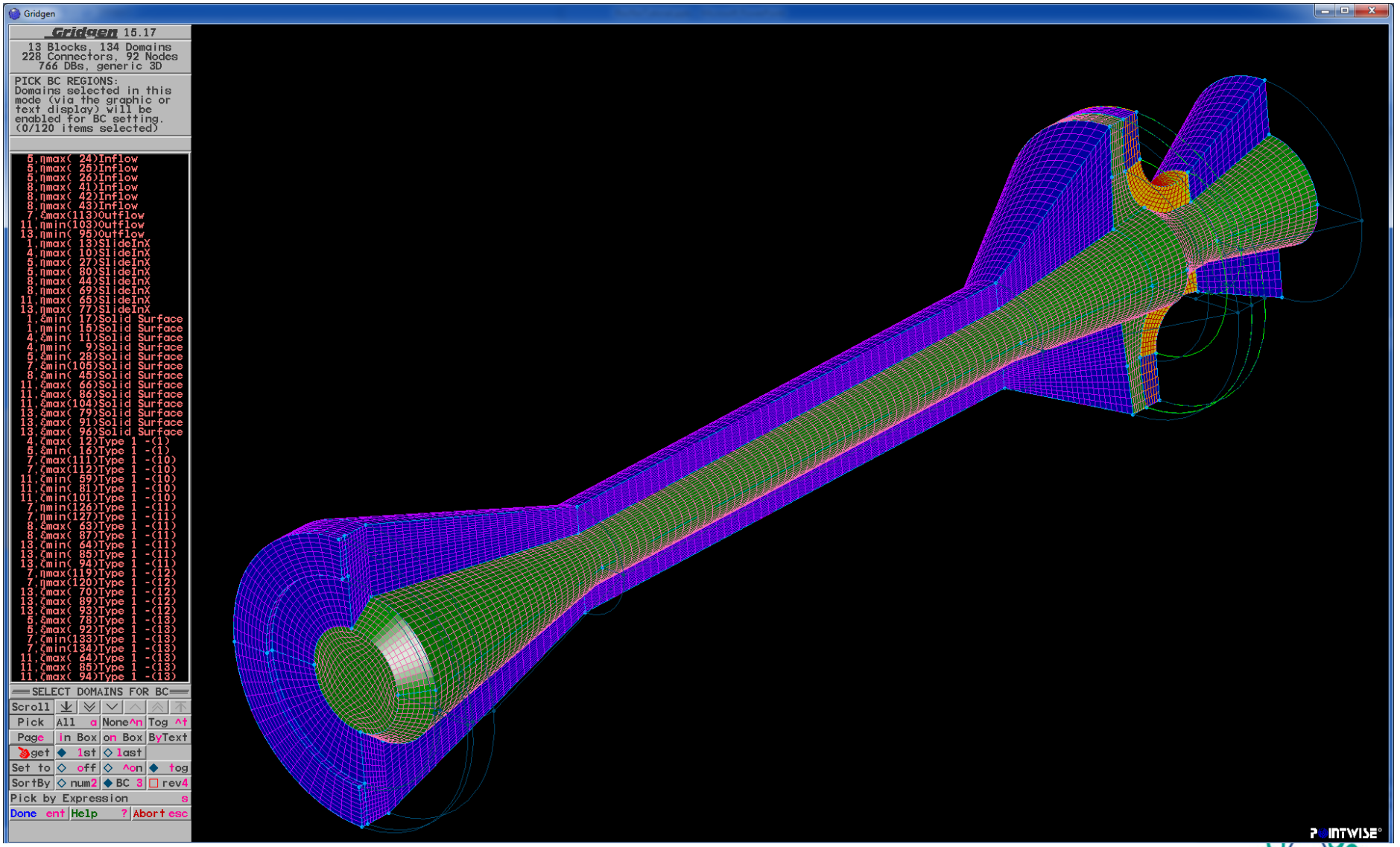
Will be 2 when output

Will be 5 when output

Will be 11 when output

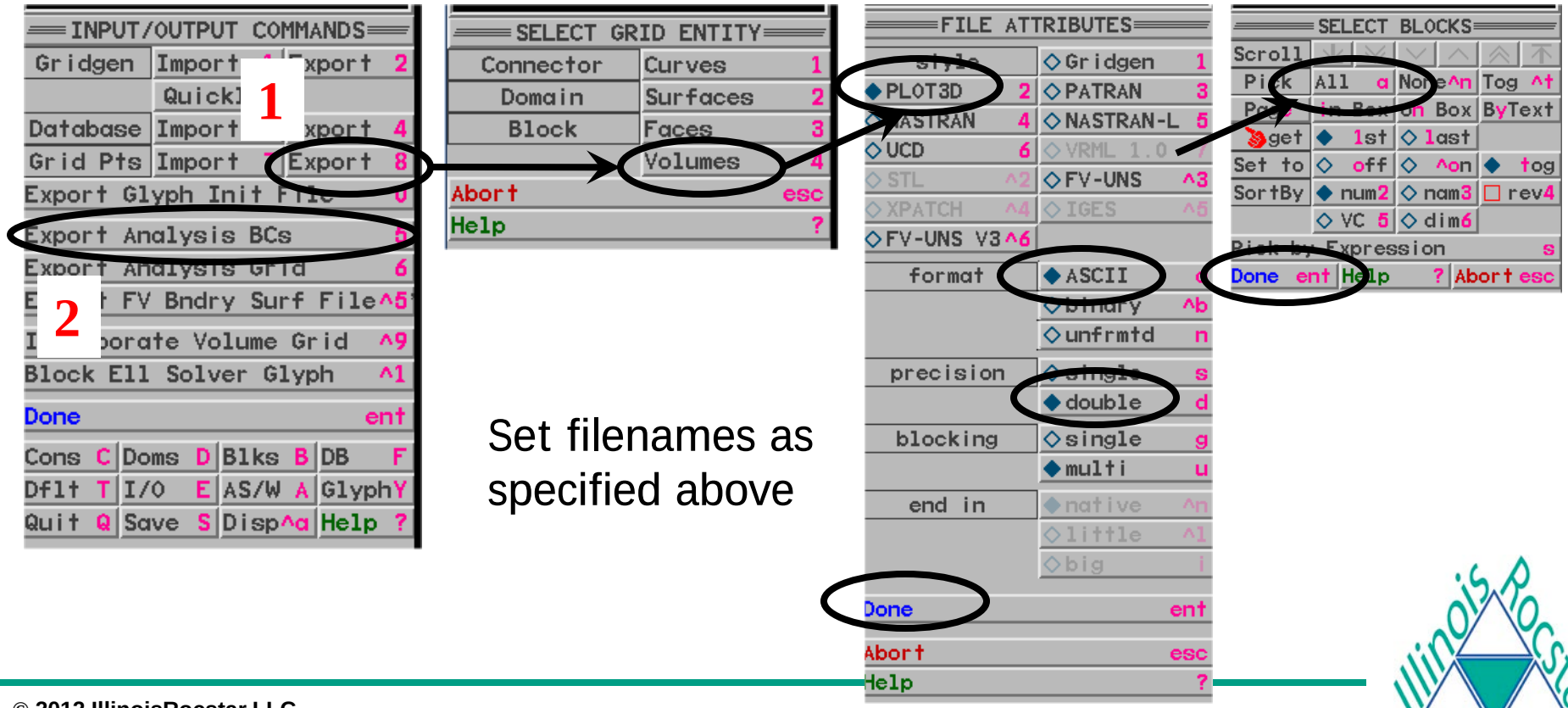


Boundary Conditions Complete



Export *Rocflo* Grid

- Export files:
  - Block volumes: <casename>-PLOT3D.grd – example: ACM-PLOT3D.grd
  - BC file <casename>-PLOT3D.inp – example: ACM-PLOT3D.inp
- If working on Windows, run dos2unix on them once on Linux
  - Fortran doesn't like cross-platform line endings



Boundary Condition Map

- Must map Gridgen BC numbers to Rocflo BC numbers
  - Form text file <casename>-PLOT3D.bcmp

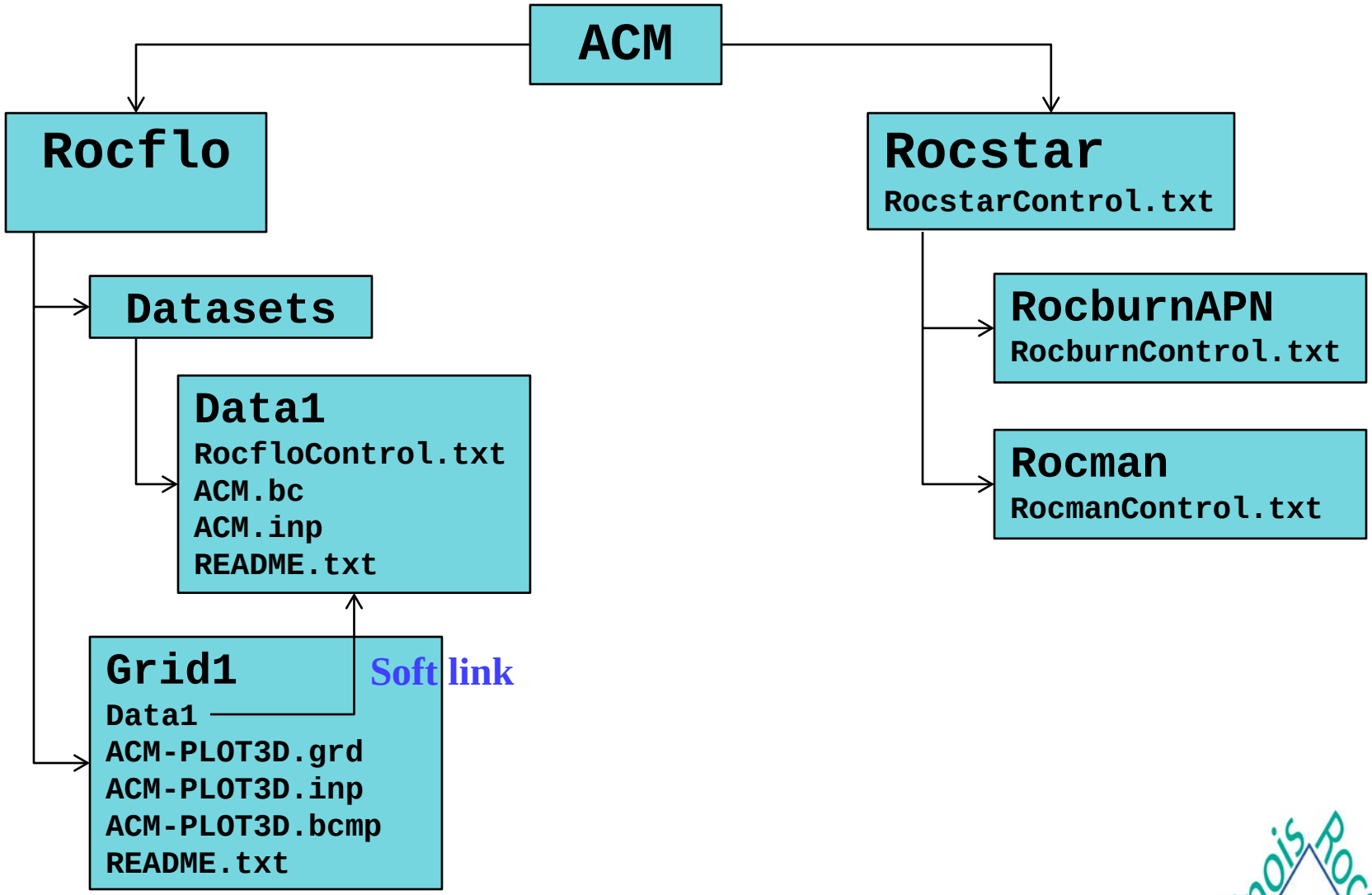
```
# This file is line-oriented.
# A '#' begins a comment line.
# Other lines define a boundary condition, with the format:
#  <gridgen bc number> <rocfloMP bc number> <coupled flag>
#
#####################################################
#Gridgen type 2-- "solid surface-slip wall, fixed“; last zero means non-interacting
2  62  0
#####################################################
# Gridgen type 5-- "inflow"
# This is an ignition boundary-- a burning surface; last 1 means interacting
5  90  1
#####################################################
# Gridgen type 6-- "outflow"
# This is a supersonic/subsonic exit
6  20  0
#####################################################
# Gridgen type 11-- "SlideInX"
# Internal Communication BC
11  63  0
#####################################################
# Unspecified condition (default)
0  999  0
```

Rocflo Boundary Condition Numbers

http://www.csar.illinois.edu/CSARdocs/DocumentsPub/uguides/rocflo_ug.pdf

- 10 – inflow
- 20 – outflow
- 30 – block boundary (continuous grid)
- 60 – slip wall, grid freely moved on fixed surface by Rocflo
- 61 – slip wall, grid freely moved on fixed surface by Rocprop
- 62 – slip wall, grid and surface fixed
- 63 – slip wall, surface may slide or stretch in x-direction by Rocprop
- 64 – slip wall, surface may slide or stretch in y-direction by Rocprop
- 65 – slip wall, surface may slide or stretch in z-direction by Rocprop
- 66 – slip wall, surface may slide in plane by Rocprop
- 70 – noslip wall
- 80 – far field
- 90 – injection
- 100 – symmetry
- 110 – translational periodicity
- 120 – rotational periodicity

Set up NDA



Steps in Setting Up NDA

- Produce the following directory hierarchy:
  - `mkdir ACM; cd ACM`
  - `mkdir Rocstar; mkdir Rocflo`
  - `cd Rocstar`
  - `mkdir RocburnAPN; mkdir Rocman; cd ../Rocflo`
  - `mkdir Grid1; mkdir Datasets; cd Datasets; mkdir Data1`
  - `cd ../../Grid1; ln –s ../Datasets/Data1 Data1`
- Go to directory where tutorial files for ACM have been placed
- Place files in NDA:
  - Place `RocstarControl.txt` in the `Rocstar` directory
  - Place `RocburnControl.txt` in the `Rocstar/RocburnAPN` directory
  - Place `RocmanControl.txt` in the `Rocstar/Rocman` directory
  - Place `RocfloControl.txt`, `ACM.inp` and `ACM.bc` in the `Rocflo/Datasets/Data1` directory
  - Place `ACM-PLOT3D.bcmp`, `ACM-PLOT3D.bc` and `ACM-PLOT3D.inp` in the `Rocflo/Grid1` directory

Run *Rocprep* on NDA

```
rocprep –A –o 1 1 -b –d /IR/NDAs/ACM –t ./ACM34 –n 34 [–p ~/build/bin/]
```

Extract from NDA and preprocess to make full Rocstar dataset

Process Data1 and Grid1 for Rocflo

Extract Rocburn

Root directory for NDA problem to be processed

Target dir for dataset

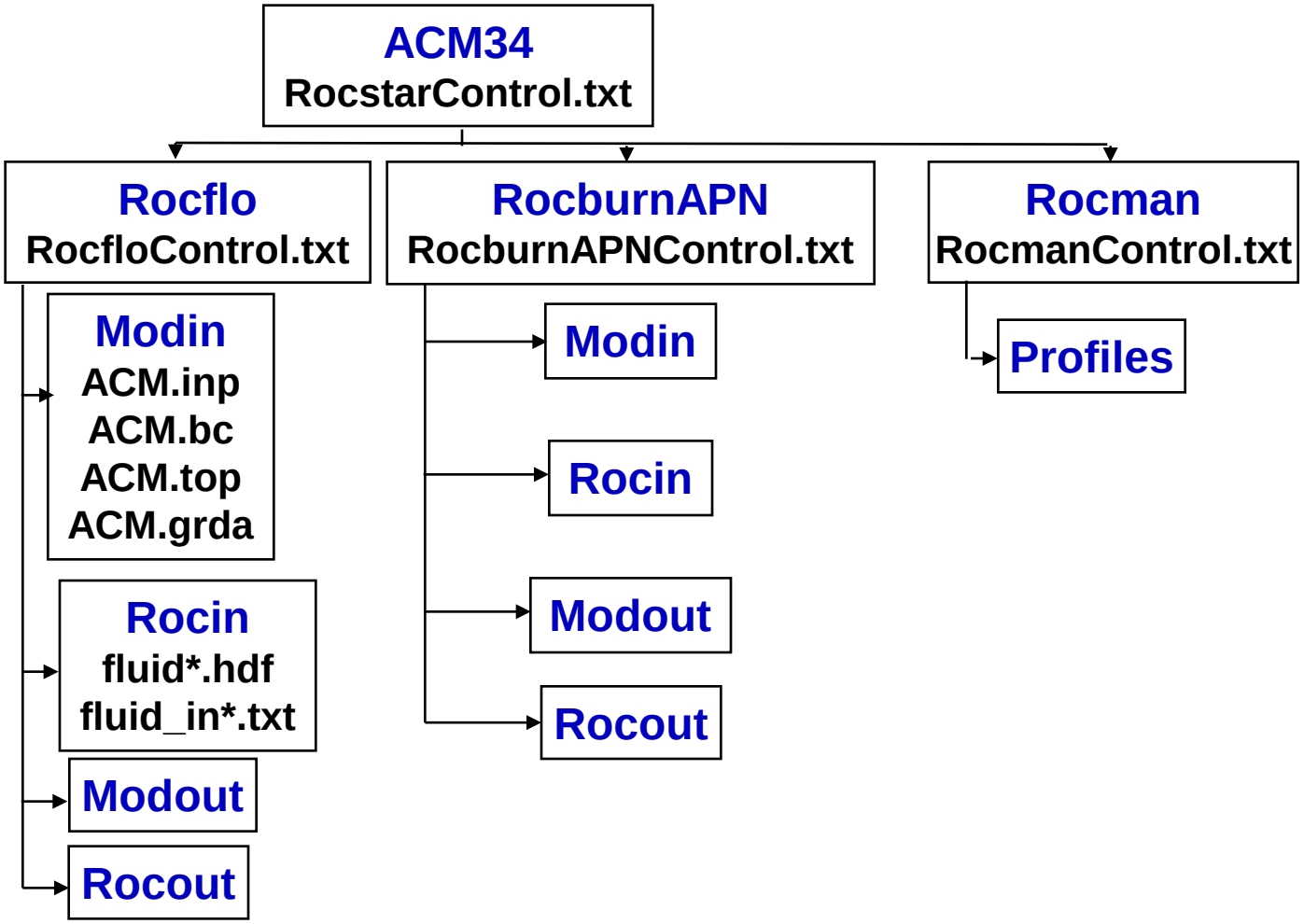
Number of partitions to make

Optional path to pre-processing tools

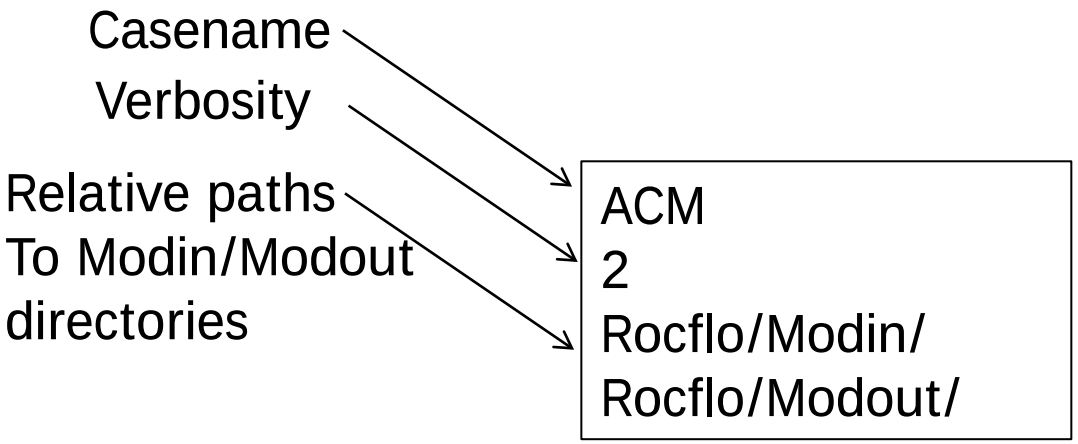
Execute *Rocprep* with no arguments for help screen:

```
[mdbrandy@taubh1 Modin]$ ~/Rocprep/Rocprep.pm
First switch must be mode switch -A|C|E|P|U, not:

********************************************************************************
Usage: /home/mdbrandy/Rocprep/Rocprep.pm -A|C|E|P [OPTION]...

Major modes of operation:
  -A, --all         extract and preprocess
  -C, --check       check an existing dataset at -d <path>
  -E, --extract     copy NDA files to target at -t <path>
  -P, --preprocess  run module preptools on data at -d <path>

Physics module selection:
  -o [m] [n]     Rocflo preprocessing, optional NDA Data<m> & Grid<n> dirs
  -u [m] [n]     Rocflu preprocessing, optional NDA Data<m> & Grid<n> dirs
  -f [m] [n]     Rocfrac preprocessing, optional NDA Data<m> & Grid<n> dirs
  -s [m] [n]     Rocsolid preprocessing, optional NDA Data<m> & Grid<n> dirs
  -b             Rocburn preprocessing

Module-specific flags:
  -r <m>         specify <m> regions (rocflu only), default is -n value
  -splitaxis <n> force split along n=0,1, or 2 axis (rocflo only)
  -un <units>    convert model units to meters (rocfrac only)

General options:
  -i <o|u|f|s>   surfdive interface meshes, default infers from physics options
  -d <path>      path to source data, default is current working directory
  -h, --help     print this help message and terminate
  -n <m>         specify <m> processors/partitions
  -t <path>      target path for new rocstar dataset
  -p <path>      path to preptool binaries, default will use shell path
  -x, --ignore   ignore RocprepControl.txt control file

Example: /home/mdbrandy/Rocprep/Rocprep.pm -A -o 1 1 -f 2 4 -d archiveDir/ -t newDataset/ -n 8
********************************************************************************
```

Resulting Rocstar Dataset



Examine RocfloControl.txt



- Note: Casename is critical. It is used for *Rocprep* and *Rocflo* to know what other files are called. Make sure it is used consistently.
- Normally the other three lines will always be the same

Examine ACM.bc

- Boundary condition definitions that will be used by *Rocflo*

Don't forget space…

Start #

End #

```
# BC_INJECT       ! This is BC 90 in *.bcmp file
BLOCK     0  0    ! applies to block ... (0 0 = to all)
PATCH     0  0    ! applies to patch ... (0 0 = to all patches of BLOCK)
EXTRAPOL  0       ! order of extrapolation to dummy cells (0 or 1)
DISTRIB   0       ! single value (=0) or distribution (=1)
MFRATE    5.7429  ! mass flow rate [kg/(m^2*s)] (if distrib=0)
MAXCHANGE 0.2
TEMP      2855.0  ! injection temperature [K] (if distrib=0)
#
```

Ignored when Rocburn used; But must be here

Almost always 0 0, but can have Multiple BCs with Different blocks

```
# BC_OUTFLOW      ! This is BC 20 in *.bcmp file
BLOCK     0  0    ! applies to block (0 0 = to all)
PATCH     0  0    ! applies to patch (0 0 = to all patches from range of blocks)
TYPE      0       ! 0=supersonic only, 1=subsonic only, 2=mixed
DISTRIB   0       ! single value (=0) or distribution (=1)
MODEL     1       ! 0=standard model, 1=partly non-reflecting
PRESS     1.0E+5  ! static pressure [Pa] (if type=1 or 2)
NRCOEF    1.0     ! non-reflecting coefficient (default=1.)
#

# BC_SLIPW        ! This is BC 62 and 63 in *.bcmp file
BLOCK     0  0    ! applies to block ... (0 0 = to all)
PATCH     0  0    ! applies to patch ... (0 0 = to all patches of BLOCK)
EXTRAPOL  0       ! order of extrapolation to dummy cells (0 or 1)
MAXCHANGE 0.2
#
```

Examine ACM.inp (1)

- Problem definition file: physical and numeric parameters
- Can get complex for multiphysics simulations
- Delimited (#...#) blocks can be in any order

Always the same for *Rocstar*

```
# BLOCKMAP
NBLOCKS 0
#
```

Always the same for *Rocstar*

```
# FORMATS
GRID      0     ! 0 - PLOT3D ASCII,
SOLUTION  2     ! 0 - ROCFLO ASCII, 1 - ROCFL0 binary, 2 -  HDF
#
```

These change depending on whether you want a viscous flow or not, and whether the grid should move or not

```
# FLOWMODEL
BLOCK    0 0
MODEL    0      ! 0 - Euler, 1 - Navier-Stokes
MOVEGRID 1      ! 0 - static grid, 1 - moving grid
#
```

ACM.inp (2)

Number of ghost cell layers: can't be changed after pre-processing!

```
# INITFLOW
BLOCK    0 0
NDUMMY   2
VELX     0.0
VELY     0.0
VELZ     0.0
PRESS    1.0E+5
DENS     1.16
#
```

Initial velocities in simulation. Care should be taken not to set values that will not change too abruptly

Initial simulation pressure And density. Care should be taken to ensure that these are consistent with the desired simulation temperature since Rocflo will calculate the temperature. Inconsistent values will cause instabilities.

ACM.inp (3)

- Probe and thrust files have text data that can be processed in spreadsheets, Tecplot, etc.

```
# REFERENCE
GAMMA    1.2259          ! Ratio of specific heats
CP       1905.849        ! Specific heat at constant pressure
#

# PROBE
NUMBER 2
0 0.015 0.0 0.0   !0 x y z. Alternative: Block# i j k
0 0.0495735 0.0 0.0
#
WRITIME 0.000005
OPENCLOSE 1
#

! thrust -----------------------------------------------------------------

# THRUST
TYPE       2     ! 0=none, 1=momentum thrust only, 2=momentum and pressure thrust
PLANE      1      ! 1: x=const, 2: y=const, 3: z=const. plane
COORD      0.0495735   ! coordinate of the plane
PAMB       1.E+5  ! ambient pressure (only if TYPE=2)
WRITIME    1.E-5  ! time offset [s] to store thrust history
WRIITER    10     ! offset between iterations to store thrust history
OPENCLOSE  1      ! open & close file with thrust every time (0=no, 1=yes)
#
```

Initial zero indicates using x, y, z location

This line generates ACM.prb_0001 in Modout

This line generates ACM.prb_0002 in Modout

How often to write probe file (seconds)

Whether to open and close every write (1=yes, 0=no)

Generates ACM.thr in Rocflo/Modout

ACM.inp (4)

- Use global-WgLaplacian for motion where blocks need to move relative to each other

```
# GRIDMOTION
TYPE    2          ! 0=block-TFI, 1=block-WgLaplacian 2=global-WgLaplacian
                   ! 3=global-NuLaplacian 4=block-Elliptic 5=global-Elliptic
NITER   0          ! number Laplacian iterations (TYPE>0)
VITER   5          ! number volume elliptic PDE iterations (TYPE=4,5)
SITER  20          ! number surface elliptic PDE iterations (TYPE=4,5)
POWER   2.         ! power of inverse node distance in frame gm (TYPE=1,2,4,5)
AMPLIFX 1.20       ! 1.5 amplification factor for frame motion (TYPE=2,3,5)
AMPLIFY 1.0        ! 1.2 amplification factor for frame motion (TYPE=2,3,5)
AMPLIFZ 1.0        ! 1.2 amplification factor for frame motion (TYPE=2,3,5)
NEIGHBOR 48        ! 12 number of closest block-corner neigbours <=26 (TYPE=2,3,5)
NSURFMATCH 3       ! number iteration for block interface matching >=2 (TYPE=2,3)
ORTHODIR   0       ! orthogonality direction: 0=all, 1=I, 2=J, 3=K (TYPE=2,3,5)
ORTHOWGHTX 0.0     ! x-wghting factor for block lvl orthogonality (TYPE=2,3,5)
ORTHOWGHTY 0.0     ! y-wghting factor for block lvl orthogonality (TYPE=2,3,5)
ORTHOWGHTZ 0.0     ! z-wghting factor for block lvl orthogonality (TYPE=2,3,5)
WEIGHT     0.5     ! weighting factor for cell center averaging (TYPE=3)
ORTHOCELL  0.5     ! weighting factor for cell level orthogonality (TYPE=3)
#
```

ACM.inp (5)

- Numerics parameters critical to stability
  - CFL normally 1. Can be less. Can be higher but stability lessened
  - Order normally 2 in *Rocflo*. Will run with order 1; rarely needed
  - DISCR changes the discretization method. Central generally suffices.
  - K2 & 1/K4 numeric dissipation parameters. Ramp for turbulence simulations. K2=0 and 1/K4 = large (>20000) are desirable if stable
  - Other parameters normally not changed

```
# NUMERICS
BLOCK    0 0
SMOOCF   -0.7    ! coefficient of implicit residual smoothing (<0 - no smooth.)
CFL      1.0     ! CFL number
DISCR    0       ! Type of space discretization (0 – central, 1 - Roe, 2 - MAPS)
ORDER    2       ! Order of accuracy (1 - first, 2 - second)
K2       0.1
1/K4     128
PSWTYPE   1      ! 0=standard pressure switch, 1=TVD type (if discr=0)
PSWOMEGA  0.1    ! blending coefficient for PSWTYPE=1 (if discr=0)
LIMFAC   5.0     ! limiter coefficient (if discr=1)
ENTROPY  0.05    ! Entropy correction coefficient (if DISCR=1)
#
```

Examine *Rocstar* Control Files for ACM

RocstarControl.txt

```
CouplingScheme    =  FluidBurnAlone
FluidModule       =  "Rocflo"
BurnModule        =  "RocburnAPN"
OutputModule      =  "Rocout"

MaximumTime       =  0.016

CurrentTimeStep =     1.0E-06
OutputIntervalTime = 1.0E-04
ZoomFactor = 1.0

MaxWallTime = 43000

ProfileDir = "Rocman/Profiles"
```

Must be 1.0 to allow boundary regression

RocmanControl.txt

```
Verbose = 0

InterpolationOrder = 1

TractionMode = 1
P_ambient =  1.0E+05

Rhoc = 1703.0
Pressure =  6.8d6
BurnRate =  0.01

RFC_verb = 1
RFC_order = 2
RFC_iteration = 100
RFC_tolerance = 1.e-6

Face-offsetting = T

AsyncInput = F
AsyncOutput = F
```

Important

RocburnAPN for ACM

Careful with units when setting

```
0.77        a in rb=a*P^n,   rb in cm/sec and P in atm, a_p (cm/sec)
0.62        n in rb=a*P^n,   rb in cm/sec and P in atm, n_p
1           Maximum_number_of_spatial_nodes,_nxmax
2916.0      adiabatic flame temperature, Tf_adiabatic (K)
298.00      initial temperature        , To_read      (K)
Rocburn_2D_Output/Rocburn_APN
```

- Burn rate is one of the only places in *Rocstar* that is not strictly SI units (meters)

Run ACM problem

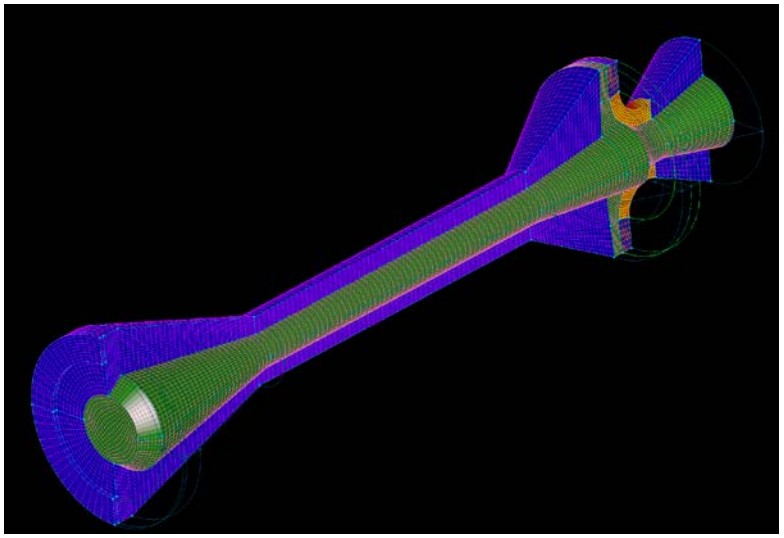
```
#!/bin/csh -f

#SBATCH --nodes=5                    # Number of nodes
#SBATCH --time=10:00:00               # Wall clock time
#SBATCH --account=FY127542              # WC ID
#SBATCH --job-name=ACMTest              # Name of job
set nodes=$SLURM_JOB_NUM_NODES
set cores=7
cd /gscratch2/aluketa/ACMTest
srun -n 34 /projects/Rocstar/Rocstar/bin/rocstar
```

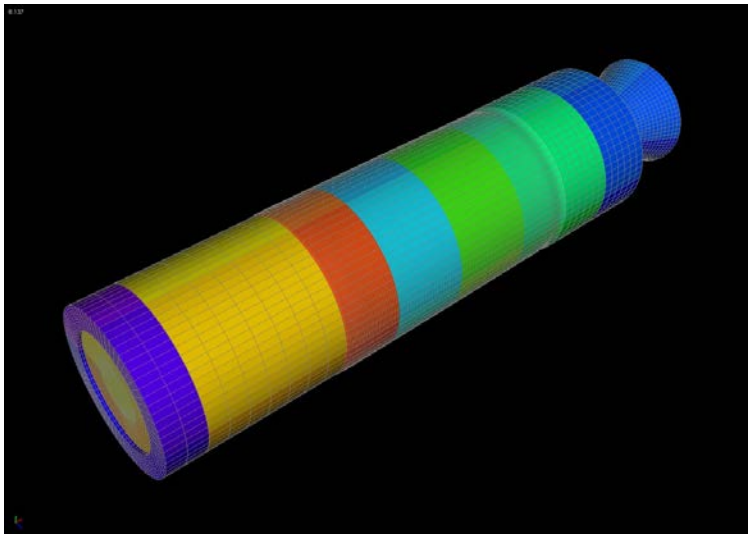
- Need to set up a batch-system specific job script for your system.
- Example for our system below for ACM

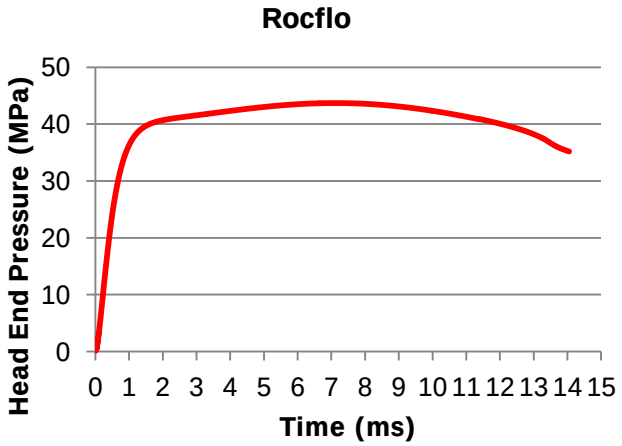
```
#!/bin/tcsh
#
# Requst 5 nodes, 7 procs each (i.e. 35 procs)
#PBS -l nodes=5:ppn=7
# For this long:
#PBS -l walltime=10:00:00
#
#PBS -N ACM
# Join the stdout and stderr into the output file
#PBS -j oe

# cd to the directory from which the job was submitted
cd ${PBS_O_WORKDIR}
mpirun -np 34 ./rocstar
```

ACM Expected Results

- This motor burns out in about 14 ms, and the *Rocflo* grid motion can handle most of the burnback







Monitor Standard out/err

- Large amounts of information is written to standard out/err

Monitor Probe File(s)

- Depending upon your setup, you can "watch" the probe files to monitor progress
- `cd Rocflo/Modout; tail –f ACM.prb_0001`

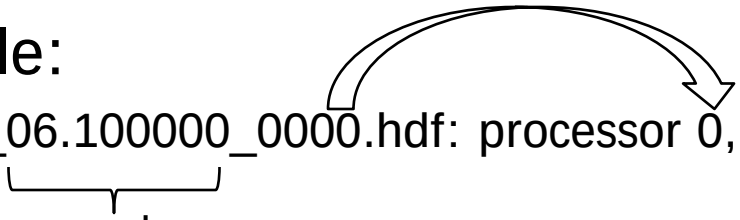
```
# probe data (iteration/time, density, u, v, w, p, T)
# region    14, icell     3, jcell     9, kcell     9
# x=  0.14856E-01, y=  0.21521E-07, z= -0.14945E-07
 2.7035969E-07  1.16000E+00 -1.06085E-14 -4.21347E-14  2.29825E-14  1.00000E+05  2.45467E+02
 5.0000000E-06  1.18107E+00 -4.35562E-02 -1.10686E-03 -1.55134E-03  1.02232E+05  2.46470E+02
 1.0000000E-05  2.60138E+00 -2.43497E+01 -2.06613E-03 -6.09490E-03  2.73136E+05  2.98969E+02
 1.5000000E-05  2.21299E+00 -2.76699E+01 -9.98801E-03  3.66079E-02  2.24079E+05  2.88318E+02
 2.0000000E-05  3.72242E+00 -7.31183E+01  8.72279E-03 -2.65008E-02  4.25827E+05  3.25730E+02
 2.5000000E-05  4.24793E+00 -1.10089E+02  1.99342E-02  9.96979E-03  5.02469E+05  3.36808E+02
 3.0000000E-05  4.82351E+00 -1.38443E+02 -3.53893E-02 -7.66165E-02  5.87183E+05  3.46625E+02
 3.5000000E-05  3.51547E+00 -1.72720E+02  1.88846E-02  4.85104E-02  3.98075E+05  3.22427E+02
 4.0000000E-05  4.88654E+00 -1.98719E+02 -9.84630E-03 -2.71287E-02  5.96106E+05  3.47354E+02
 4.5000000E-05  5.91230E+00 -1.71383E+02 -1.23496E-02 -4.90376E-02  7.56641E+05  3.64404E+02
 5.0000000E-05  4.86712E+00 -1.91427E+02  2.05179E-03  5.82279E-02  5.95716E+05  3.48512E+02
 5.5000000E-05  6.42790E+00 -1.81320E+02  9.75009E-03 -2.17876E-02  8.41403E+05  3.72722E+02
 6.0000000E-05  1.19800E+01 -1.42908E+02 -4.73421E-02 -2.96886E-02  1.83861E+06  4.37002E+02
 6.5000000E-05  1.30104E+01 -1.60689E+02 -2.81673E-02  9.27011E-03  2.05774E+06  4.50351E+02
 7.0000000E-05  9.95572E+00 -1.67150E+02  4.40584E-03  1.54315E-02  1.52269E+06  4.35500E+02
 7.5000000E-05  1.05171E+01 -1.55261E+02 -5.44063E-02 -1.11832E-04  1.71412E+06  4.64082E+02
 8.0000000E-05  1.45618E+01 -1.37359E+02 -1.81264E-02 -2.33013E-02  2.67457E+06  5.22986E+02
```

- The location of this probe is defined in ACM.inp

```
# PROBE
NUMBER 2
0 0.015 0.0 0.0
0 0.0495735 0.0 0.0
#
```

Visualize HDF Output

- Can use Rocketeer to visualize output
- Can also translate to Tecplot format
- Need to learn to read output file naming
- `cd Rocflo/Rocout; ls`
- Once a checkpoint has occurred, there will be one HDF file per processor per checkpoint
- Example:
  - fluid_06.100000_0000.hdf: processor 0, 0.10ms time



Means 0.10E06 nanoseconds,
Or 0.10 ms, or 0.0001 seconds

- `fluid_XX.XXXXX_XXX.hdf` are 3-D volume grid files
- `ifluid_Y_XX.XXXXX_XXXX.hdf` are surface grid files
  - Y: ni=non-interacting, b=burning

Pre-run Visualization Files

- For Rocflo ACM, pre-run visualization files are available for 0ms, 5 ms, 10 ms, 14 ms
- Load these into Rocketeer from the VizData directory (see tutorial in next lesson)

Transfer to Rocketeer Tutorial