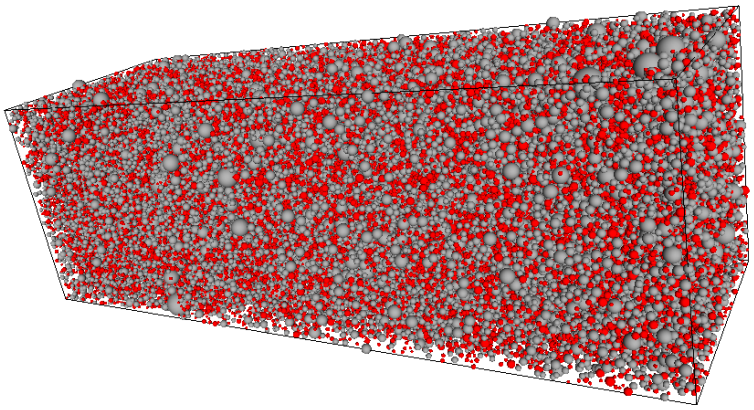
User Manual
for
RocPrepack

Authors: **Thomas L. Jackson & L. Chris Mink**
University of Florida
Date: **15 December 2016**



Point of contact: Dr. Thomas L. Jackson, tlj@ufl.edu

User Manual for *RocPrepack*

Preamble

This manual supersedes and replaces all previous manuals.

Overview

RocPrepack is a numerical tool that calculates the particle size distribution for three-dimensional, heterogeneous solid propellants. Different distribution types can be specified, such as log-normal or single size. The particles are assumed to be spherical, and the volumes that the code calculates can be for cubic, cylindrical or spherical. The output of ***RocPrepack*** is newpackformat_out. This output is the one used by the latest version of ***Rocpack***. The output of ***RocPrepack*** feeds into ***Rocpack,*** and the output of ***Rocpack*** feeds into ***Rocfire***.

Four examples using ***RocPrepack*** will be provided for four different blends of propellant.

Folders

Formulations_data: contains propellant blends in text files. Each file contains the details of each blend. These blend names are also contained in the file filenames.list. Each respective blend has its own mixture of propellants and each propellant has its own particle size distribution.

Ingredients_data: contains text files of different propellant ingredients. Each file contains the distribution of particle sizes in microns and percentages. For example, using miller_ap20.dat, there are two columns of numbers. The left column is the particle size in microns and the right column is the percentage of the particle distribution for which that particle size occupies. The right column must sum to 100.

Execution

- Compiling — type “gfortran –o a.exe *.f” into the command prompt ensuring beforehand that the correct directory is used: compiles all codes in the folder and generates the executable file “a.exe”
- Running code — type “a” or ./a.exe into command prompt after compiling to run code

Subroutines

- rocprepack_1.f
  - main code: contains an in-depth description of parameters and variables (internal and user defined)
- rocprepack_2a.f
  - subroutine cuts: computes the number of particles within each cut, takes into account the packing fraction, inputs: diam, dnj, Vfrackept, outputs: dN, V_total
  - subroutine consolidate: combines all cuts of particles into a distribution and calculates the total number of particles within the distribution, outputs: itotal, solidname(i), dN-final(i), D_final(i)
  - subroutine output: prints information to run packing code, computes dimensions of mesoscale volume, computes mass and density of that same volume of propellant

    - subroutine mix_and_rnd: combines like particles, do not call if there is aluminum in propellant
    - subroutine num_fraction: computes number fractions for each cut
    - subroutine ludcmp, lbksb: used for linear solver
- rocprepack_2b.f
    - input_pack_setup: pulls information from filenames.list to generate the packing fraction
- rocprepack_2c.f
    - subroutine w2v: converts weight fraction to volume fraction
    - subroutine lognormal: computes the log-normal distribution for an initial distribution of AP or aluminum
- rocprepack_3.h
    - global variables declaration file

USER SUPPLIED INPUT PARAMETERS:

- container
    - the shape of the mesoscale simulation, ‘cuboid’, ‘cylinder’, ‘annulus’
- idim
    - shape of particles, 2 (disks, disabled) or 3 (spheres)
- height
    - height of the 3D domain, if height > 0, then height is given in microns, if height < 0, then height is the nondimensional aspect ratio
    - for a cuboid the volume = L_x*L_y*L_z (length*width*height), if the height > 0, then height = L_y and L_x = L_z which implies that the volume = L_x^2*height, if the height < 0, then L_y = |height|*L_x and the volume = L_x^3*|height| and L_x = L_z = (volume/|heigh|)^(1/3)
    - for a cylinder the volume = π*R^2*height where R is the radius of the cylinder, if the height > 0, then L_y = height, L_x = the radius and the volume = π*L_x^2*height, if the height < 0, then L_x = the radius, L_y = 2*|height|*L_x, the volume = 2* π*L_x^3*|height| and L_x = (volume/(2* π*|height|))^(1/3) and L_y = 2*|height|*L_x (L_z is not used)
    - for an annulus the input file has two rows; row 1: L_y = height in microns, row 2: L_x = the inner radius in microns, let L_z = the outer radius in microns, the volume = π*(L_z^2-L_x^2)*L_y which implies that L_z = sqrt(L_x^2+volume/(π*L_y))
- iblend_max
    - number of cuts to be combined to form a propellant matrix; e.g. a blend with AP 20 micron, AP 50 micron and AP 200 micron means that iblend_max = 3
- ntot
    - total number of particles in a pack, this must be an integer
- density_binder
    - the density of the binder (units: g/cm^3)
- cut_name
    - name of propellant cut, predefined cuts located in directory Ingredients_data
    - e.g. Miller_AP_200 has a distribution of particle sizes with a mean of 200 micron
- cut_type(i)
    - type of solid

    - e.g. AP, Al, PETB, HMX, ADN
- density(i)
    - density for cut_type(i)
- w_frac(i)
    - weight fraction for cut_type(i), all values are in weight percent which is converted to volume percent in subroutine w2v which generates v_frac(i)
- dcutoff(i)
    - cutoff diameter for cut_type(i); smallest particle diameter to be considered for the pack
    - all particles below dcutoff will be homogenized into the binder to create a blend
- coating(i)
    - coating parameter for cut_type(i), coating is a radial displacement on the particles, contact radius of the particles is equal to half of the particle diameter + the coating thickness (coating is not currently used)

INTERNAL PARAMETERS AND VARIABLES:

- rho_v
    - theoretical packing fraction, assumed to be equal to the total solid volume packing fraction
- iflag
    - iflag = 0 uses volume to compute number fractions, iflag = 1 uses diameter to compute number fraction, code is hardwired for iflag = 0
- iblend
    - iblend the number of propellant cuts
- nmode(iblend)
    - the number of different particles for cut iblend
- diam(iblend,i)
    - the particle diameter
- vfrac(iblend,i)
    - the volume fraction, is equal to percent(iblend,i)/100
- dN(iblend)
    - the number of particles after consolidation for cut iblend
- Ni
    - the integer value after roundoff, equal to delNj_final(iblend,i)

Input Files

- filenames.list: this file contains preloaded blends. All blend names are commented out in the normal fashion in the Fortran language with "!" appearing at the beginning of every line. In order to pick a particular blend to run in ***RocPrepack***, ensure that the desired blend is the only uncommented line in the file. Once the blend has been uncommented, filenames.list must be saved. Then ***RocPrepack*** can be compiled and run again with the new blend. If the desired blend does not appear on the list, then the blend can be created if its characteristics are known. A new blend is created by placing the name of the blend into filenames.list as all other blend names appear and to put its characteristics into the Formulations_data folder in a new file under the same name that was put into filenames.list.

Output Files

- newpackformat_out: this is the output file that is read in by ***Rocpack.***

EXAMPLE PROBLEMS

Single_size_100

The information regarding the details of Single_size_100 is located in the directory RocPrepack -> Formulations_data -> Single_size_100. This blend only contains one propellant cut. This one propellant cut is AP at 100 micron. This propellant cut also does not have a distribution of particle sizes, hence the name Single_size_100. The input variables are shown in Table 1. When the blend details for Single_size_100 are opened, the screen will appear as seen in Fig. 1. The mesoscale volume is cuboid as seen in Fig. 1.

TABLE I
INPUT VARIABLES

VARIABLE	VALUE
idim	3
height	-1
iblend_max	1
ntot	1000
density_binder	0.92

Table of input variables for the Single_size_100.

```
'Single cut, Single size 100 micron AP'
'Cuboid'
3                       # idim
-1                    # height

1           # iblend_max
1000            # ntot, total number of particles
0.92                    # binder density

singlesize      # cut name
AP          # cut type
100.0           # diameter for single size
1.95                    # density
0.6         # weight fraction
5.0         # d_cutoff
0d0         # coating parameter; micron
```

Fig. 1. Screenshot of Single_size_100.

Since the blend is only a single size of 100 micron, the distribution of sizes does not need to be computed. The input variables for this blend can be found in Table 2.

TABLE II
VARIABLES FOR AP

VARIABLE	VALUE
density(AP)	1.95
d_cutoff	5.0
coating(AP)	0d0
coating(AP)	0d0

Table of variables for the lognormal distribution of aluminum in Single_size_100.

Once the blend name has been uncommented in filenames.list in the same manner as described below with Miller_blend_24_Thiokol, the program can be run. Fig. 2 is an example of what newpackformat_out should look like after ***RocPrepack*** has been run with Single_size_100. The output of other blends look similar, but they can vary greatly in size depending on blend complexity.

```
# pack -vD -f  0.41441458504307827

# create a pack
import "shapes/adn"
import "shapes/cube"
import "shapes/hmx"
import "shapes/petn"


set packing_fraction =   0.41441458504307827      ;
set seed = 13;
set growth_rate = 1.0;
boundary {box   1.0000000000000000        1.0000000000000000        1.0000000000000000       periodic}

create         1000  sphere  size    100.00001372447760      tag           1 color 0.6 0.6 0.6 ;



***   Single_size_100
***   Single cut, Single size 100 micron AP
***   Yr: 2016  Mo: 10  Day: 25  Time:  9:44:51

***   Propellant Density  1.34685E+00  gm/cm^3
***   Propellant Mass     1.70170E-03  gm

        AP             -0.00000017  !(V_{AP,total} - V_{AP,spheres}) / (Length Width Height)
    Binder              0.58558559  ! V_{Binder} / (Length Width Height)
       1081.07215196712559        ! Length
       1081.07215196712559        ! Width
       1081.07215196712559        ! Height
          0.41441441441441        ! Theoretical packing density
          0.41441458504308        ! Packing density
                      1000        ! Total number of particles
                         1        ! Total number of different diameters
         1        1000            AP          100.000013724478
```

Fig. 2. Screenshot of newpackformat_out after running Single_size_100.

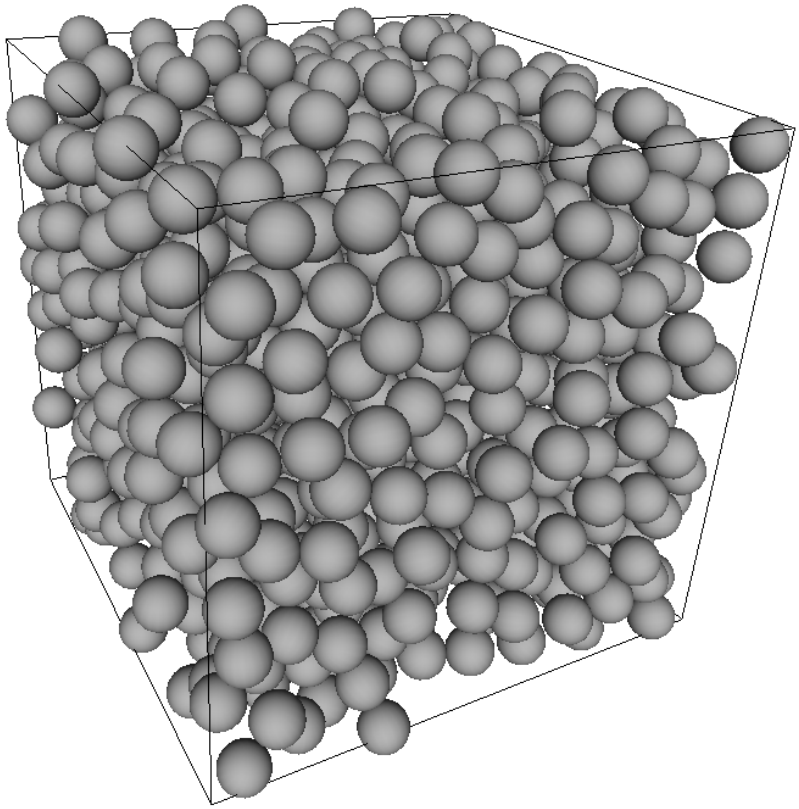


Fig. 3. Single_size_100 output image from ***Rocpack***. ***Rocpack*** run time is 1 second.

Miller_blend_24_Thiokol:

The information regarding the details of Miller_blend_24_Thiokol is located in the directory RocPrepack -> Formulations_data -> Miller_blend_24_Thiokol. This blend is a blend of three different propellant cuts: thiokol_ap200.dat, thiokol_ap50.dat, and thiokol_ap20.dat. The input variables are shown in Table 3. When the blend details for Miller_blend_24_Thiokol are opened, the screen will appear as seen in Fig. 4. The mesoscale volume is cuboid as seen in Fig. 4.

TABLE III
INPUT VARIABLES

VARIABLE	VALUE
idim	3
height	-1
iblend_max	3
ntot	10000
density_binder	0.92

Table of input variables for the blend Miller_blend_24_Thiokol.

```
'Propellant: Miller Blend 24; Thiokol AP'
'Cuboid'
3                       # idim
-1                    # height

3                       # iblend_max
10000                   # ntot, total number of particles
0.92                    # binder density

thiokol_ap200.dat   # cut name
AP                      # cut type
1.95                    # density
0.3158           # weight fraction
5.0                 # d_cutoff
0d0          # coating parameter; micron

thiokol_ap50.dat    # cut name
AP                      # cut type
1.95                    # density
0.4211           # weight fraction
5.0                 # d_cutoff
0d0          # coating parameter; micron

thiokol_ap20.dat    # cut name
AP                      # cut type
1.95                    # density
0.1368           # weight fraction
5.0                 # d_cutoff
0d0          # coating parameter; micron

```

Fig. 4. Screenshot of Miller_blend_24_Thiokol.

As an example, the details of thiokol_ap20.dat cut can be found in the directory RocPrepack -> Ingredients_data -> thiokol_ap20.dat. The details of all cuts can be found in the Ingredients_data folder. The input variables for thiokol_ap200.dat can be found in Table 4.

TABLE IV
VARIABLES FOR THIOKOL_AP200.DAT

VARIABLE	VALUE
density(AP)	1.95
w_frac(AP)	0.3158
d_cutoff	5.0
coating(AP)	0d0

Table of variables for the cut thiokol_ap200.dat.

To run the program for Miller_blend_24_Thiokol, this blend must be uncommented in filenames.list and all other blends must be commented out. This is accomplished by deleting the exclamation point in front of Miller_blend_24_Thiokol and the exclamation point needs to be replaced in front of all other blends. This can be seen in Fig. 5.

```
13  !Single_size_100
14  !Single_Thiokol_20
15  !Single_Thiokol_50
16  !Single_Thiokol_200
17  !Single_Miller_20
18  !Single_Miller_50
19  !Single_Miller_90
20  !Single_Miller_200
21  !
22  !
23  !     These Miller blends use the Thiokol AP cuts
24  !       Run times < 3 mins
25  !
26  Miller_blend_24_Thiokol
27  !Miller_blend_23_Thiokol
28  !Miller_blend_19_Thiokol
```

Fig 5. Screenshot of filenames.list showing Miller_blend_24_Thiokol being uncommented.

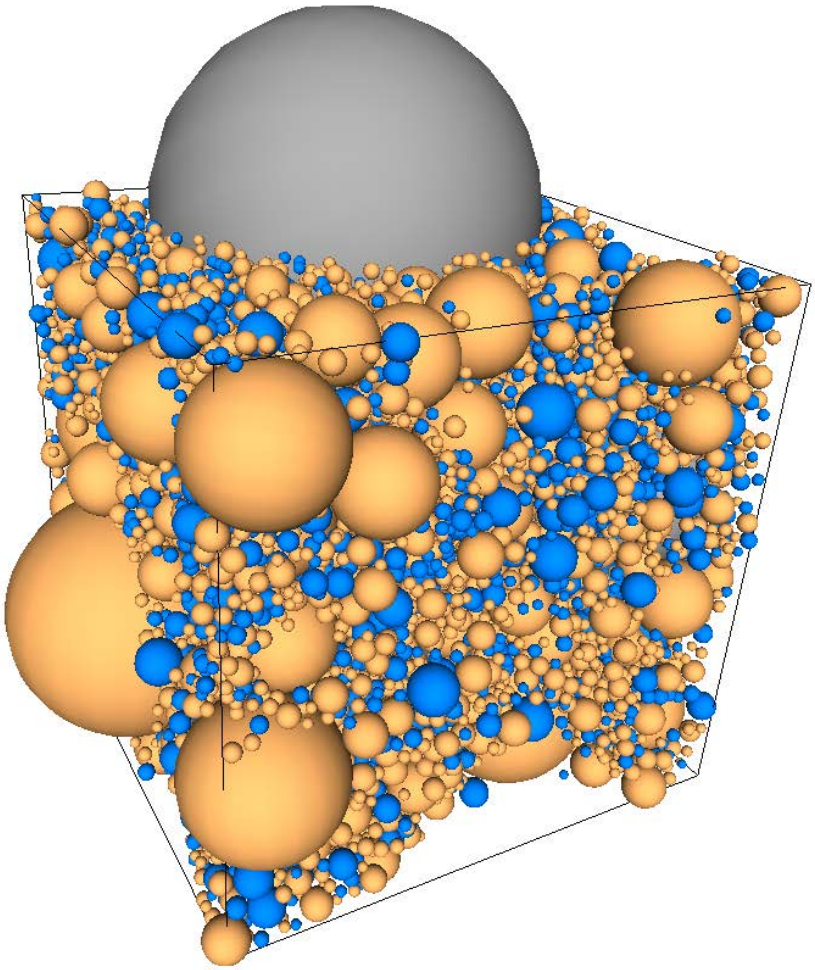


Fig. 6. Miller_blend_24_Thiokol output image from ***Rocpack***. ***Rocpack*** run time is 110 seconds.

Borne01

The information regarding the details of Borne01 is located in the directory RocPrepack -> Formulations_data -> Borne01. This blend is a blend of only one propellant cut: HMX with a lognormal distribution. This cut does not have its own .dat file as seen in the blends for Miller_blend_24_Thiokol. However, the distribution for this cut is calculated in rocprepack_2c.f in the subroutine lognormal. The input variables are shown in Table 5. When the blend details for Borne01 are opened, the screen will appear as seen in Fig. 7. The mesoscale volume is cuboid as seen in Fig. 7.

TABLE V
INPUT VARIABLES

VARIABLE	VALUE
idim	3
height	-4
iblend_max	1
ntot	900
density_binder	0.90

Table of input variables for the blend Borne01.

```
'Propellant: Example for Borne; 70% wgt HMX and 30% wgt wax'
'Cube'
3                       # idim
-4                    # height

1                       # iblend_max
900                     # ntot, total number of particles
0.90                    # binder density

lognormal             # cut name
hmx                        # cut type
1.902                      # density
0.70              # weight fraction
5.0                   # d_cutoff
0d0           # coating parameter; micron
0.8                        # bcoeff
250.0                       # diam_Peak
200.0                        # diam_Min
300.0                 # diam_Max

```

Fig. 7. Screenshot of Borne01.

The calculations for the lognormal cut of HMX can be found in the directory RocPrepack -> rocprepack_2c.f in the subroutine lognormal. The input variables for this distribution of HMX can be found in Table 6.

TABLE VI
VARIABLES FOR LOGNORMAL HMX

VARIABLE	VALUE
density(hmx)	1.902
w_frac(hmx)	0.70
d_cutoff	5.0
coating(hmx)	0d0
bcoeff	0.8
diam_Peak	250.0
diam_Min	200.0
diam_Max	300.0

Table of variables for the lognormal distribution of HMX in Borne01.

Once the blend name has been uncommented in filenames.list in the same manner as described with Miller_blend_24_Thiokol, the program can be run.

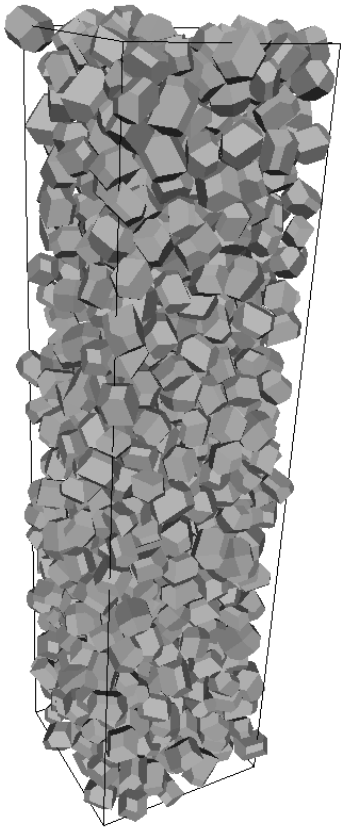


Fig. 8. Borne01 output image from ***Rocpack***. ***Rocpack*** run time is 35 seconds.

AtlasV

The information regarding the details of AtlasV is located in the directory RocPrepack -> Formulations_data -> AtlasV. This blend is a blend of three different propellant cuts, and these cuts do not have their own .dat files as seen in the blends for Miller_blend_24_Thiokol. Two of the propellant cuts are AP and the third cut is aluminum. The input variables are shown in Table 7. When the blend details for AtlasV are opened, the screen will appear as seen in Fig. 9. The mesoscale volume is cuboid as seen in Fig. 9.

TABLE VII
INPUT VARIABLES

VARIABLE	VALUE
idim	3
height	2000
iblend_max	3
ntot	50000
density_binder	0.92

Table of input variables for the blend AtlasV.

```
'Propellant: ATLAS V Propellant'
'Cuboid'
3                       # idim
2000                    # height

3                       # iblend_max
50000                   # ntot, total number of particles
0.92                    # binder density

lognormal           # cut name
AP                      # cut type
1.95                    # density
0.35            # weight fraction
20.0                # d_cutoff
0d0         # coating parameter; micron
0.9                     # bcoeff
300.                    # diam_Peak
190.0                     # diam_Min
380.                # diam_Max

lognormal           # cut name
AP                      # cut type
1.95                    # density
0.35            # weight fraction
20.0                # d_cutoff
0d0         # coating parameter; micron
0.9                     # bcoeff
20.                   # diam_Peak
10.0                    # diam_Min
90.                 # diam_Max

lognormal           # cut name
Al                      # cut type
2.70                    # density
0.20            # weight fraction
10.0                # d_cutoff
0d0         # coating parameter; micron
0.8                     # bcoeff
20.                   # diam_Peak
5.0                     # diam_Min
90.                 # diam_Max
```

Fig. 9. Screenshot of AtlasV.

The calculations for the lognormal cut of AP and aluminum can be found in the directory RocPrepack -> rocprepack_2c.f in the subroutine lognormal. The input variables for this distribution of HMX can be found in Table 8.

TABLE VIII
VARIABLES FOR LOGNORMAL ALUMINUM

VARIABLE	VALUE
density(Al)	2.70
w_frac(Al)	0.20
d_cutoff	10.0
coating(Al)	0d0
bcoeff	0.8
diam_Peak	20.
diam_Min	5.0
diam_Max	90.0

Table of variables for the lognormal distribution of aluminum in AtlasV.

Once the blend name has been uncommented in filenames.list in the same manner as described on page 9 with Miller_blend_24_Thiokol, the program can be run.

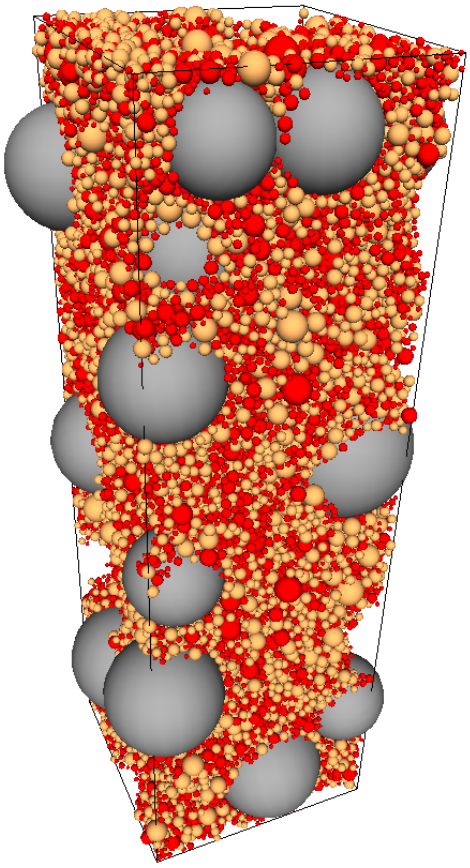


Fig. 10. AtlasV output image from ***Rocpack***. ***Rocpack*** run time is 1500 seconds.

References

[1] G.M. Knott, T.L. Jackson & J. Buckmaster (2001). "Random packing of heterogeneous propellants". AIAA Journal, Vol. 39(4), pp. 678-686.

[2] S. Kochevets, J. Buckmaster, T.L. Jackson & A. Hegab (2001). "Random propellant packs and the flames they support." AIAA J. of Propulsion and Power, Vol. 17, pp. 883-891.

[3] F. Maggi, S. Stafford, T.L. Jackson & J. Buckmaster (2008). "Nature of packs used in propellant modelling." Physical Review E, Vol. 77(4), 046107.