```
In [27]:
```

```
import numpy as np
import matplotlib.pyplot as plt
import pynbody
from michaels functions import center and r vir, remove bulk velocity
from matplotlib.colors import LogNorm
In [28]:
path = "bulk1/data 2/hydro 59/output/"
data = pynbody.load(path + "output_00050")
aexp = data.properties['a']
data.physical units()
print path
print "a =", aexp
print z = 1./aexp -1
bulk1/data 2/hydro 59/output/
a = 0.600005205268
z = 0.666652207716
In [29]:
r_vir = center_and_r_vir(data, aexp, path)
('shifting on Stars:', SimArray([ 0.00308878, -0.03302971, -0.046767
32], 'kpc'))
('virial radius:', SimArray(152.40432611, 'kpc'))
In [30]:
re = 0.1 * r vir
print r_e
15.240432611151682
In [31]:
sph_5 = pynbody.filt.Sphere(radius = '%f kpc' %(r_e*1.4))
region = data[sph_5]
In [32]:
rho = region.gas["rho"].in_units("m_p cm^-3")
In [33]:
Z = region.gas["metal"]
```

```
In [34]:
```

```
f = open(data.filename + "/info "+data.filename[-5:]+".txt","r")
lines = f.readlines()
f.close()
for line in lines:
    if line[0:13]=="unit l
        print line[:-1]
        unit l = float(line[14:-1])
    if line[0:13]=="unit d
        print line[:-1]
        unit d = float(line[14:-1])
    if line[0:13]=="unit t
        print line[:-1]
        unit t = float(line[14:-1])
    if line[0:13]=="omega b
        print line[:-1]
        omega b = float(line[14:-1])
omega b
            = 0.450000017881393E-01
unit l
            = 0.682025380323961E+26
unit d
           = 0.123367583719985E-28
            = 0.163687521954501E+18
unit t
In [35]:
turb = np.sqrt( region.g["turb"] * 2./3. ) * unit 1 / unit t / 1e5
turb = pynbody.array.SimArray(turb, units = "cm s**-1")
c_s = np.sqrt(region.gas["p"] / region.gas["rho"])
c s = c s.in units('cm s**-1')
M = turb / c s
region.g["mach"] = M.in units("1")
In [36]:
turb
Out[36]:
SimArray([29.15456777, 44.73850117, 68.11498304, ..., 29.26368001,
          16.37539853, 25.15026196], 'cm s**-1')
In [37]:
c s
Out[37]:
SimArray([ 3276673.11939746, 12738195.66072513, 9202021.83758316,
          14469186.19848063, 13460450.29314729, 14119970.07822348],
'cm s**-1')
```

```
In [38]:
Μ
Out[38]:
SimArray([8.89761252e-06, 3.51215371e-06, 7.40217577e-06, ...,
          2.02248279e-06, 1.21655652e-06, 1.78118380e-06], '1.00e+0
0')
In [39]:
m p 1 = pynbody.array.SimArray(1.0, pynbody.units.m p)
n_H = rho / m_p_1
In [40]:
n H
Out[40]:
SimArray([0.00242818, 0.00016367, 0.00038948, ..., 0.00032273, 0.000
23647,
          0.00029291], 'cm**-3')
In [41]:
m p = pynbody.array.SimArray(1.672621777e-24, "g")
K b = pynbody.array.SimArray(1.38064852e-16, "cm**2 g s**-2 K**-1")
G = pynbody.array.SimArray(6.67259e-8, "cm**3 g**-1 s**-2")
T mean = pynbody.array.SimArray(10., "K")
G o = pynbody.array.SimArray(1.0, "1")
n_H_mean = pynbody.array.SimArray(1e2, "cm**-3")
In [42]:
lambda jeans = (c s) / np.sqrt(4* np.pi * G * n H * m p)
lambda jeans
Out[42]:
SimArray([5.61490010e+22, 8.40766919e+23, 3.93723266e+23, ...,
          6.80104626e+23, 7.39131101e+23, 6.96656552e+23], 'cm')
In [ ]:
'''vel = region.g["vel"] * unit_l / unit_t / 1e5
vel = pynbody.array.SimArray(vel, units = "cm s**-1")'''
In [ ]:
'''sigma s = pynbody.array.SimArray(vel, "1")
sigma s'''
In [ ]:
'''s bar = -0.5*(sigma s**2)
s_bar'''
```

```
In [ ]:
 '''smin = -7*sigma_s + s_bar
smax = 7*sigma_s + s_bar
 ds = (smax - smin)/1040042'''
In [ ]:
  '''smax[-1]'''
In [ ]:
  '''ds[-1]'''
In [ ]:
  '''smin[-1]'''
In [ ]:
  '''s = np.zeros(1040042)
for i in range(0, 1040042):
               s = smin + i*ds'''
In [ ]:
  '''n H 2 = n_H * np.exp(s)'''
In [ ]:
 '''pdf = (1/np.sqrt(2*np.pi*(sigma_s**2))) * (np.exp(-0.5*(((s - s_bar)/sigma_s))) * (np.exp(-0.5*(((s - s_bar)/sigma_s))) * (np.exp(-0.5*(((s - s_bar)/sigma_s)))) * (np.exp(-0.5*(((s - s_bar)/sigma_
 **2)))
pdf'''
In [ ]:
  '''integral1 = 0.0
 for i in range(0, 1000):
                integral1 += np.exp(s[i]) * pdf[i] * ds[i] #this should be = 1
               #plotting(n H, pdf, lambda jeans, X H2)
 integral1'''
In [ ]:
 '''plt.scatter(np.log10(n_H), pdf)
plt.xlabel('log(n_H)')
plt.ylabel('log(pdf)')
plt.grid(b=True, which='both', axis='both')
plt.title('log(n H) vs log(pdf)')
plt.show()'''
```

```
In [43]:
```

```
def calc_n_LW(n_H, G_o, lambda_jeans):
    kappa = 1000 * m_p
    rad_field_outside = G_o #in solar units
    exp_tau = np.exp(-kappa * n_H * lambda_jeans)
    n_LW = rad_field_outside * exp_tau
    return n_LW
```

### In [44]:

```
def calc_n_LW_ss(n_H, n_H2, G_o, lambda_jeans):
    kappa = 1000 * m_p
    rad_field_outside = G_o #in solar units
    exp_tau = np.exp(-kappa * n_H * lambda_jeans)
    N_H2 = n_H2*lambda_jeans
    term1 = (0.965/((1+(N_H2/5e14))**2))
    term2 = ( (0.035/np.sqrt(1+(N_H2/5e14))) * np.exp(-1*np.sqrt(1+(N_H2/5e14))/
1180) )
    S_H2 = term1 + term2
    n_LW_ss = rad_field_outside * exp_tau * S_H2
    return n_LW_ss, S_H2, N_H2
```

# In [45]:

#### In [46]:

```
def calc_X_CO(n_H, n_H2, n_LW):
    rate_CHX = 5.e-10 * n_LW
    rate_CO = 1.e-10 * n_LW
    x0 = 2.e-4
    k0 = 5.e-16 #cm3 s-1
    k1 = 5.e-10 #cm3 s-1
    factor_beta = rate_CHX/(n_H*k1*x0)
    beta = 1./(1.+factor_beta)
    factor_CO = rate_CO/(n_H2*k0*beta)
    X_CO = 1./(1.+factor_CO)
    return X_CO
```

#### In [47]:

```
def calc_n_CO(n_H, X_CO):
    abundance_Ctot = 1e-4 # n_C/n_H as defined by nucleosynthesis
    return n_H * abundance_Ctot * X_CO # CO/cc
```

#### In [48]:

```
n_LW = calc_n_LW(n_H, G_o, lambda_jeans)
X_H2_a = calc_X_H2(n_H, Z, n_LW)
n_H2_a = n_H * X_H2_a
```

```
In [49]:
```

```
n_LW_1, S_H2_1, N_H2_1 = calc_n_LW_ss(n_H, n_H2_a, G_o, lambda_jeans)
X_H2_1 = calc_X_H2(n_H, Z, n_LW_1)
n_H2_1 = n_H * X_H2_1
```

### In [50]:

```
n_LW_2, S_H2_2, N_H2_2 = calc_n_LW_ss(n_H, n_H2_1, G_o, lambda_jeans)
X_H2_2 = calc_X_H2(n_H, Z, n_LW_2)
n_H2_2 = n_H * X_H2_2
```

#### In [51]:

```
n_LW_3, S_H2_3, N_H2_3 = calc_n_LW_ss(n_H, n_H2_2, G_o, lambda_jeans)
X_H2_3 = calc_X_H2(n_H, Z, n_LW_3)
n_H2_3 = n_H * X_H2_3
```

### In [52]:

```
n_LW_4, S_H2_4, N_H2_4 = calc_n_LW_ss(n_H, n_H2_3, G_o, lambda_jeans)
X_H2_4 = calc_X_H2(n_H, Z, n_LW_4)
n_H2_4 = n_H * X_H2_4
```

#### In [53]:

```
n_LW_5, S_H2_5, N_H2_5 = calc_n_LW_ss(n_H, n_H2_4, G_o, lambda_jeans)
X_H2_5 = calc_X_H2(n_H, Z, n_LW_5)
n_H2_5 = n_H * X_H2_5
```

## In [54]:

```
n_LW_6, S_H2_6, N_H2_6 = calc_n_LW_ss(n_H, n_H2_5, G_o, lambda_jeans)
X_H2_6 = calc_X_H2(n_H, Z, n_LW_6)
n_H2_6 = n_H * X_H2_6
```

### In [55]:

```
n_LW_7, S_H2_7, N_H2_7 = calc_n_LW_ss(n_H, n_H2_6, G_o, lambda_jeans)
X_H2_7 = calc_X_H2(n_H, Z, n_LW_7)
n_H2_7 = n_H * X_H2_7
```

## In [56]:

```
n_LW_8, S_H2_8, N_H2_8 = calc_n_LW_ss(n_H, n_H2_7, G_o, lambda_jeans)
X_H2_8 = calc_X_H2(n_H, Z, n_LW_8)
n_H2_8 = n_H * X_H2_8
```

### In [57]:

```
n_LW_9, S_H2_9, N_H2_9 = calc_n_LW_ss(n_H, n_H2_8, G_o, lambda_jeans)
X_H2_9 = calc_X_H2(n_H, Z, n_LW_9)
n_H2_9 = n_H * X_H2_9
```

```
In [58]:
```

```
n_LW_10, S_H2_10, N_H2_10 = calc_n_LW_ss(n_H, n_H2_9, G_o, lambda_jeans)
X_H2_10 = calc_X_H2(n_H, Z, n_LW_10)
n_H2_10 = n_H * X_H2_10
```

```
In [59]:
```

```
n_LW_ss, S_H2, N_H2 = calc_n_LW_ss(n_H, n_H2_10, G_o, lambda_jeans)
X_H2 = calc_X_H2(n_H, Z, n_LW_ss)
n_H2 = n_H * X_H2
```

## In [60]:

```
X_{CO} = calc_X_{CO}(n_H, n_H2_a, n_LW)
```

### In [61]:

```
n_CO = calc_n_CO(n_H, X_CO)
```

### In [62]:

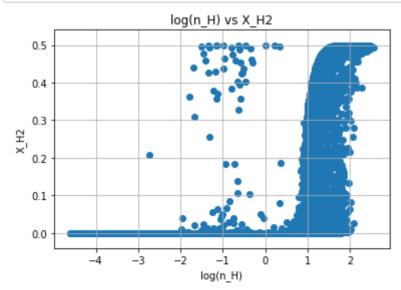
X H2

#### Out[62]:

SimArray([2.42520898e-12, 1.85451271e-13, 4.17934370e-13, ..., 3.49206881e-13, 2.15039016e-13, 2.99809526e-13])

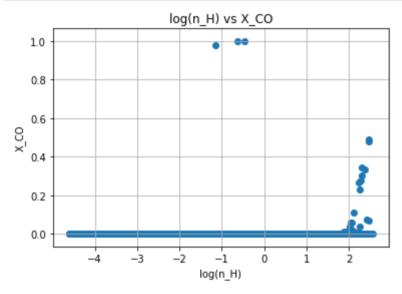
## In [63]:

```
plt.scatter(np.log10(n_H), X_H2)
plt.xlabel('log(n_H)')
plt.ylabel('X_H2')
plt.grid(b=True, which='both', axis='both')
plt.title('log(n_H) vs X_H2')
#plt.savefig('log(n_H)vsX_H2.png'.format())
plt.show()
```



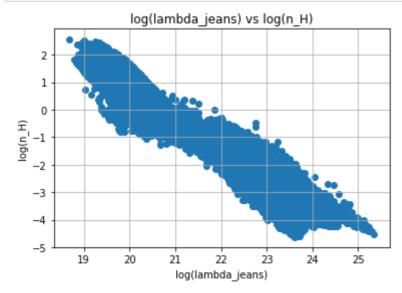
#### In [64]:

```
plt.scatter(np.log10(n_H), X_CO)
plt.xlabel('log(n_H)')
plt.ylabel('X_CO')
plt.grid(b=True, which='both', axis='both')
plt.title('log(n_H) vs X_CO')
#plt.savefig('log(n_H)vsX_CO.png'.format())
plt.show()
```



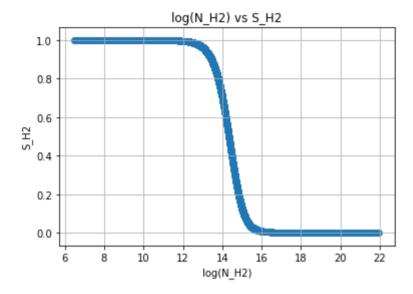
## In [65]:

```
plt.scatter(np.log10(lambda_jeans), np.log10(n_H))
plt.xlabel('log(lambda_jeans)')
plt.ylabel('log(n_H)')
plt.grid(b=True, which='both', axis='both')
plt.title('log(lambda_jeans) vs log(n_H)')
#plt.savefig('log(lambda_jeans)vslog(n_H).png'.format())
plt.show()
```



# In [66]:

```
plt.scatter(np.log10(N_H2), S_H2)
plt.xlabel('log(N_H2)')
plt.ylabel('S_H2')
plt.grid(b=True, which='both', axis='both')
plt.title("log(N_H2) vs S_H2")
#plt.savefig('log(N_H2)vsS_H2.png'.format())
plt.show()
```



## In [67]:

```
region.gas["lambda_jeans"] = lambda_jeans
```

## In [68]:

```
region.gas["n_H"] = n_H
```

## In [69]:

```
region.gas["X_H2"] = X_H2
```

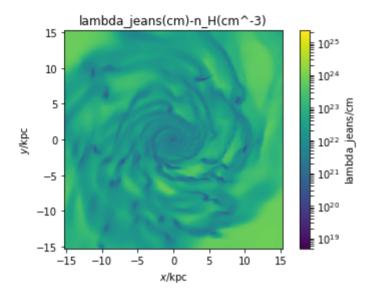
## In [70]:

```
region.gas["X_CO"] = X_CO
```

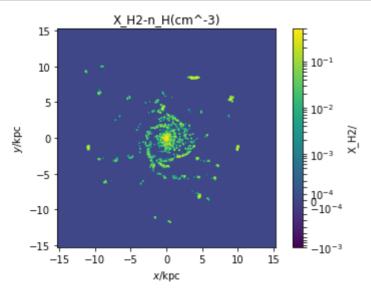
#### In [71]:

/home/cluster/mkrets/anaconda2/lib/python2.7/site-packages/pynbody-0.47-py2.7-linux-x86\_64.egg/pynbody/snapshot/\_\_init\_\_.py:1443: Runti meWarning: Conjoining derived and non-derived arrays. Assuming result is non-derived, so no further updates will be made.

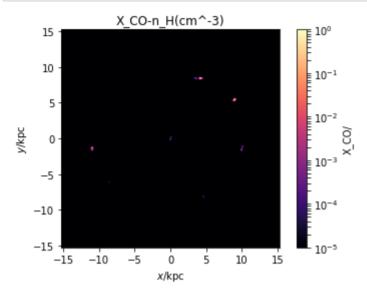
"Conjoining derived and non-derived arrays. Assuming result is non-derived, so no further updates will be made.", RuntimeWarning)



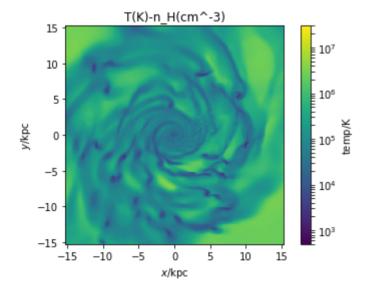
## In [72]:



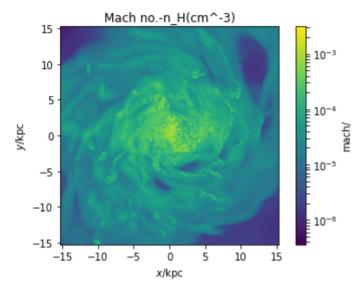
#### In [73]:



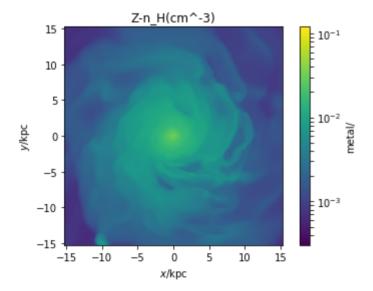
### In [74]:



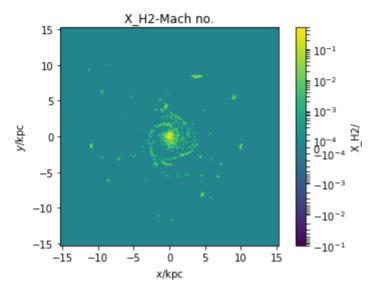
#### In [75]:



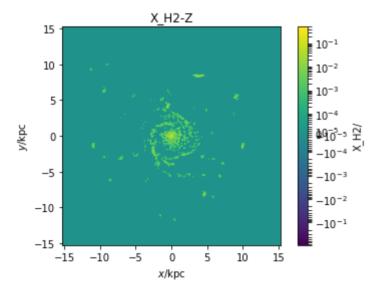
### In [76]:



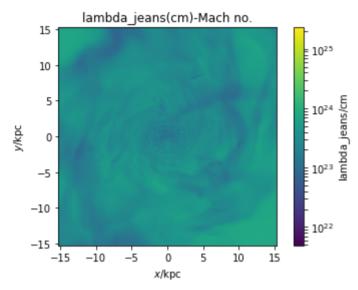
#### In [77]:



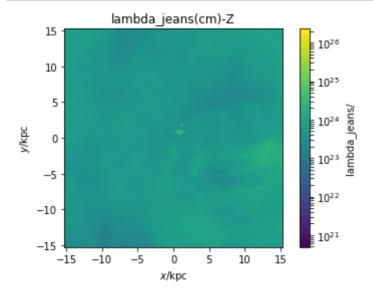
### In [78]:



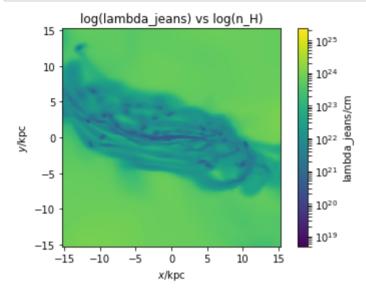
#### In [79]:



### In [80]:



#### In [81]:



#### In [82]:

#### In [83]:

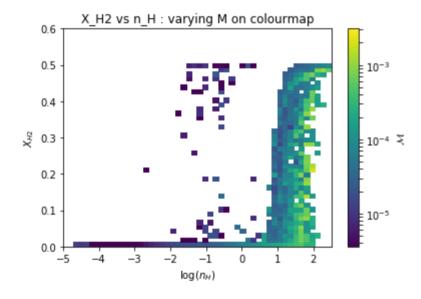
```
#Mach number - mass weighted - X_H2 vs n_H
plt.pcolormesh(xedges, yedges, histX_H2_M_mass/histX_H2_mass, norm=LogNorm(), vm
in=3.6e-6, vmax=3.1e-3)

plt.xlabel(r"$\log(n_H)$")
plt.ylabel(r"$X_{H2}$")
plt.colorbar(label=r"$\mathcal{M}$")
plt.title("X_H2 vs n_H : varying M on colourmap")
#plt.savefig('001_log(n_H)vsX_H2--M.png')
plt.show()
```

/net/cephfs/home/mkrets/anaconda2/lib/python2.7/site-packages/ipyker
nel\_launcher.py:2: RuntimeWarning: invalid value encountered in divi
de

/home/cluster/mkrets/anaconda2/lib/python2.7/site-packages/matplotli b/colors.py:1031: RuntimeWarning: invalid value encountered in less\_equal

mask |= resdat <= 0



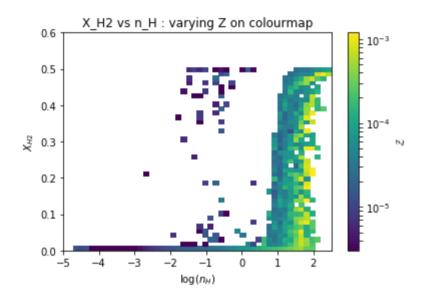
# In [84]:

#### In [85]:

```
#Z - mass weighted - X_H2 vs n_H
plt.pcolormesh(xedges, yedges, histX_H2_M_mass/histX_H2_mass, norm=LogNorm(), vm
in=3.03e-6, vmax=1.2e-3)

plt.xlabel(r"$\log(n_H)$")
plt.ylabel(r"$X_{H2}$")
plt.colorbar(label=r"$\mathcal{Z}$")
plt.title("X_H2 vs n_H : varying Z on colourmap")
#plt.savefig('002_log(n_H)vsX_H2--Z.png')
plt.show()
```

/net/cephfs/home/mkrets/anaconda2/lib/python2.7/site-packages/ipyker
nel\_launcher.py:2: RuntimeWarning: invalid value encountered in divi
de



## In [86]:

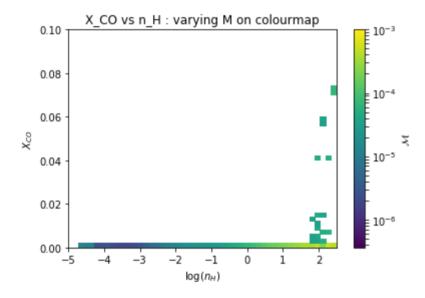
#### In [87]:

```
#M - mass weighted - X_CO vs n_H
plt.pcolormesh(xedges, yedges, histX_CO_M_mass/histX_CO_mass, norm=LogNorm(), vm
in=3.6e-7, vmax=1e-3)

plt.xlabel(r"$\log(n_H)$")
plt.ylabel(r"$X_{CO}$")
plt.colorbar(label=r"$\mathcal{M}$$")
plt.title("X_CO vs n_H : varying M on colourmap")
#plt.savefig('003_log(n_H)vsX_CO--M.png')

plt.show()
```

/net/cephfs/home/mkrets/anaconda2/lib/python2.7/site-packages/ipyker
nel\_launcher.py:2: RuntimeWarning: invalid value encountered in divi
de



# In [88]:

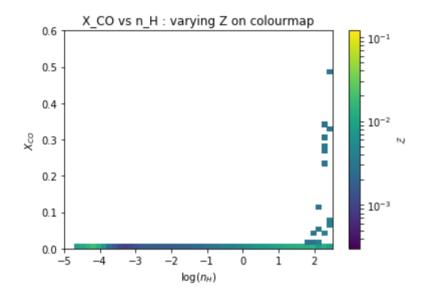
#### In [89]:

```
#Z - mass weighted - X_CO vs n_H
plt.pcolormesh(xedges, yedges, histX_CO_mass_Z/histX_CO_mass, norm=LogNorm(), vm
in=3.03e-4, vmax=1.2e-1)

plt.xlabel(r"$\log(n_H)$")
plt.ylabel(r"$X_{CO}$")
plt.colorbar(label=r"$\mathcal{Z}$")
plt.title("X_CO vs n_H : varying Z on colourmap")
#plt.savefig('004_log(n_H)vsX_CO--Z.png')

plt.show()
```

/net/cephfs/home/mkrets/anaconda2/lib/python2.7/site-packages/ipyker
nel\_launcher.py:2: RuntimeWarning: invalid value encountered in divi
de



```
In [90]:
```

np.min(Z)

Out[90]:

SimArray(0.000267)

In [91]:

np.max(Z)

Out[91]:

SimArray(0.11394659)

## In [92]:

# region.properties

```
Out[92]:
{'a': 0.600005205267563,
  'boxsize': Unit("2.21e+04 kpc"),
  'h': 0.6773999786376951,
  'omegaL0': 0.691100001335144,
  'omegaM0': 0.308899998664856,
  'time': Unit("7.68e+00 kpc s km**-1")}
```

In [93]:

region.gas.all\_keys()

Out[93]: ['tform', 'mass', 'temp', 'r\_mag', 'i\_mag', 'K lum den', 'vtheta', 'U lum den', 'vcxy', 'j2', 'I lum den', 'u mag', 'vr', 'vt', 'H\_lum\_den', 'V lum den', 'alt', 'i lum den', 'zeldovich offset', 'az', 'I\_mag', 'vrxy', 'u lum den', 'J lum den', 'k mag', 'v\_mag', 'U\_mag', 'v\_mean', 'h lum den', 'v lum den', 'theta', 'b\_mag', 'j mag', 'B lum den', 'jz', 'j\_lum\_den', 'K\_mag', 'V\_mag', 'v2', 'J mag', 'rho', 'H\_mag', 'h\_mag', 'B\_mag', 'aform', 'k\_lum\_den', 'te', 'b\_lum\_den', 'ke', 'age', 'j', 'smooth', 'rxy', 'r', 'R\_lum\_den', 'vphi', 'r\_lum\_den', 'tform', 'R\_mag',

```
'v_disp',
 'mask',
 'smooth',
 'metal',
 'pos',
 'p',
 'rho',
 'vel',
 'turb']
In [94]:
np.shape(M)
Out[94]:
(1291634,)
In [95]:
np.shape(Z)
Out[95]:
(1291634,)
In [96]:
np.shape(n_H)
Out[96]:
(1291634,)
In [97]:
np.shape(rho)
Out[97]:
(1291634,)
In [98]:
np.shape(X_H2)
Out[98]:
(1291634,)
In [99]:
len(n_H)
Out[99]:
1291634
```