Manual – 3D Lattice-Boltzmann Parallel code

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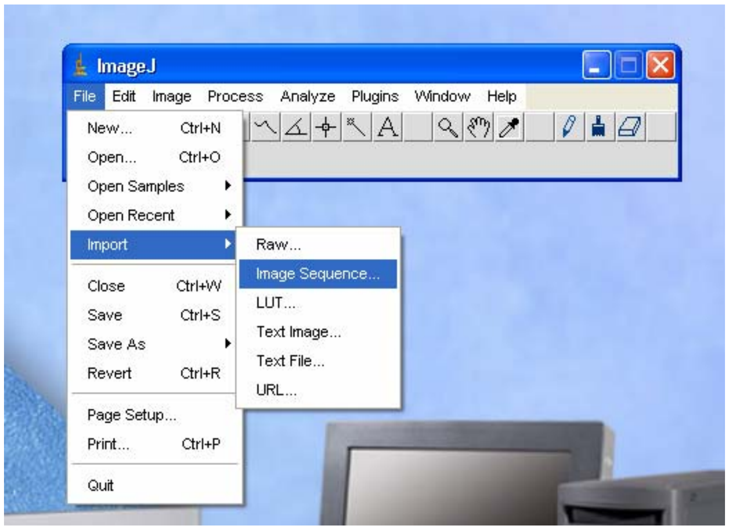
1. Pre-processing (create the '.raw' format)

1.1. Creating Simple Domains

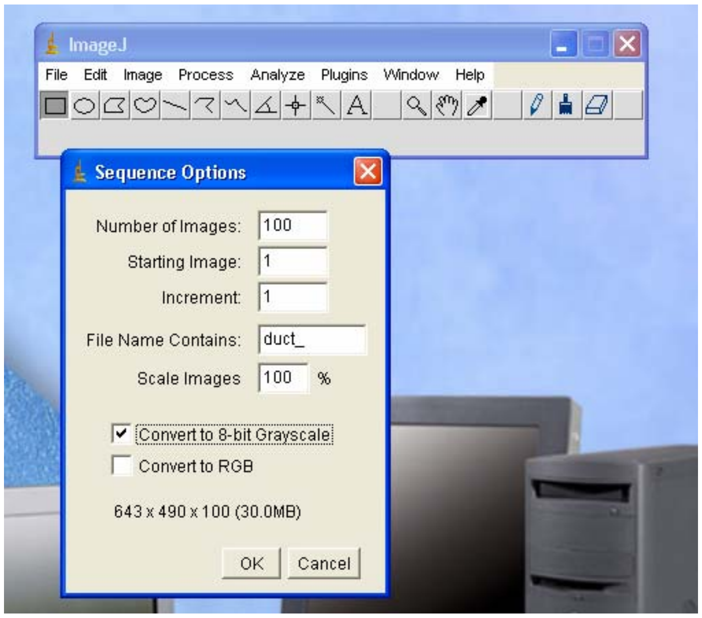
For simple geometry, first we can begin by opening Microsoft Paint or another similar program to draw each slice and using ImageJ to put all slices together and create a raw file as a input geometry for LBM 3D simulations. For example, we create a 83x83 slice with wall (with lines, Notice: in all of our 3D geometries, white is solid, black is pore space) surrounded and then run Matlab "duct.m", then after Matlab run "duct", 100 bmp's named "duct_0001" to "duct_0100" are created.

duct.bmp

content of "duct.m"
"
```
slice = 0
   a=imread(sprintf('duct','.bmp'),'bmp');
for i=1:100
      imwrite(a,sprintf('duct_%04d%s',i,'.bmp'),'bmp');
   end
```
"
After the above 100 slices are created, we using the ImageJ to import all these slices as following figures illustrated:



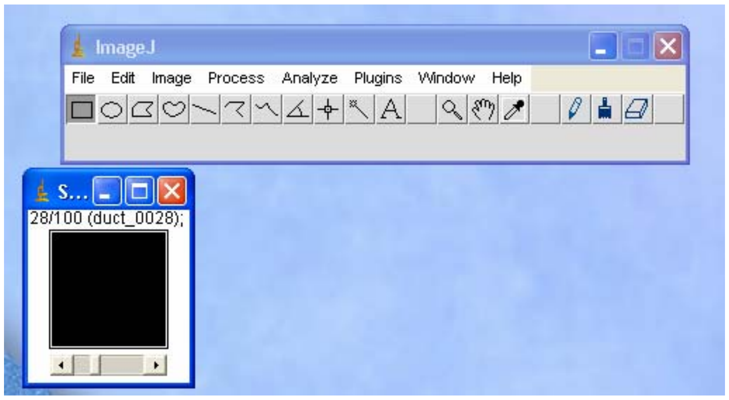
then browse for the created slices, choosing the first file "duct_0001.bmp", then the next step if filling a form :



Number of Images: 100
Starting Image: 1
Increment: 1
File Name Contains: duct_
Scale Images 100 %
[✓] Convert to 8-bit Grayscale
[ ] Convert to RGB
643 x 490 x 100 (30.0MB)

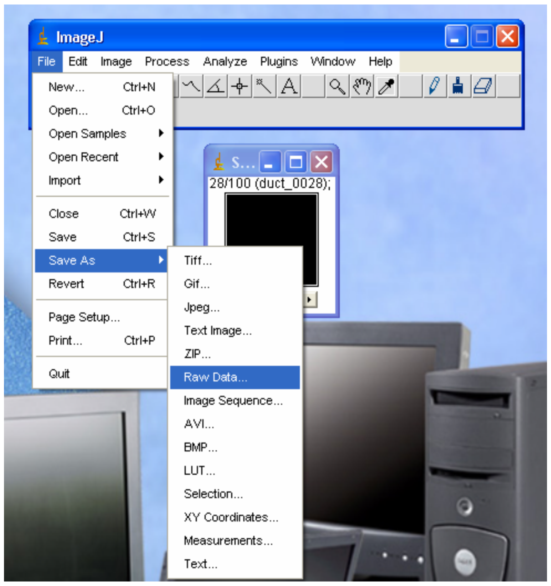
The above steps can be described as: File ->Import ->Image Sequence -> Browse for one file ->Enter number of slices ->Enter unique part of file name

after click “ok”, it will looks like as followin:



28/100 (duct_0028);

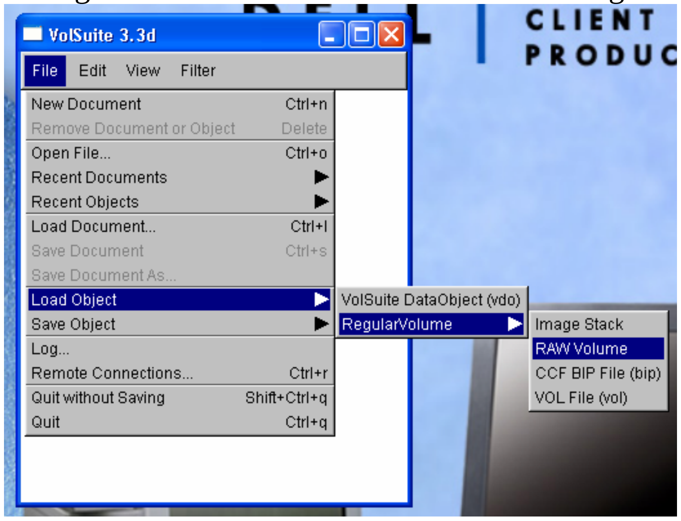
That means our import is successful and all of 100 slices are imported. Then we can export a file as “83x83x100.raw” in the following way.



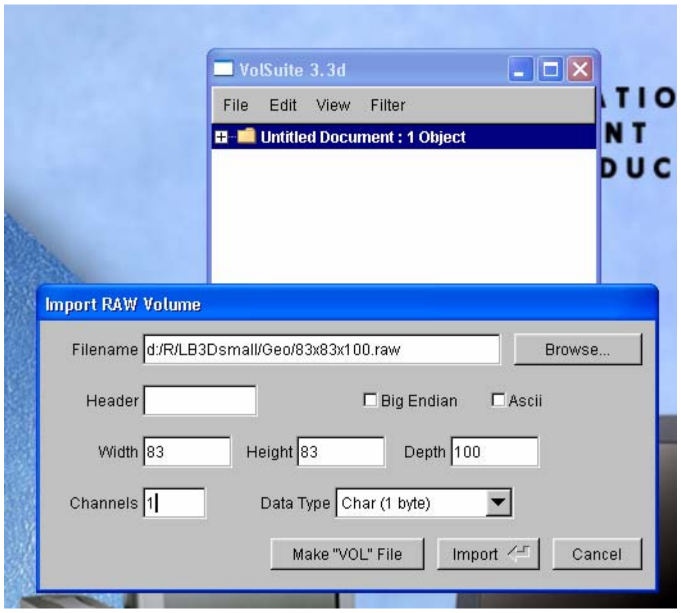
As the "save as 83x83x100.raw", a 3D duct of "83x83x100.raw" is successfully created. The next step is to view the 3D duct using the Volsuite or 3D view,

For example, using Volsuite,

File->Load Object ->Regular Volume-> Raw Volume as following:



Browse file name, Header 0, Enter width, height, depth, input 1 channel as the following:



Filename d:/R/LB3Dsmall/Geo/83x83x100.raw

Header

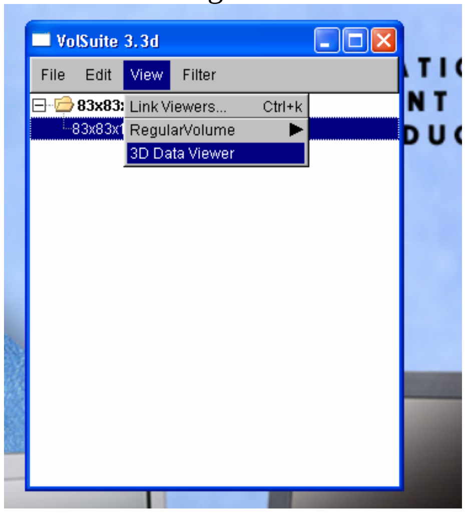
Big Endian

Ascii

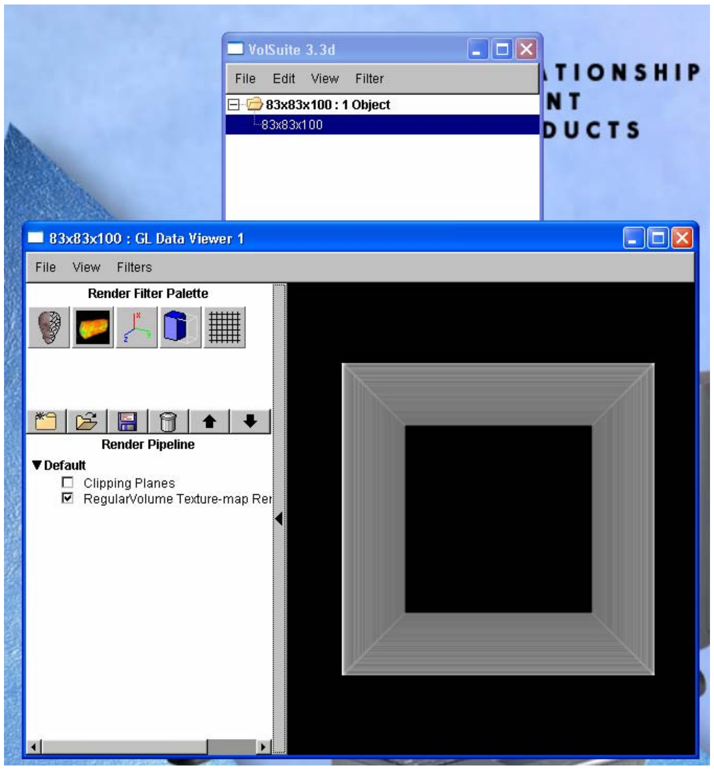
Width 83 Height 83 Depth 100

Channels 1 Data Type Char (1 byte)

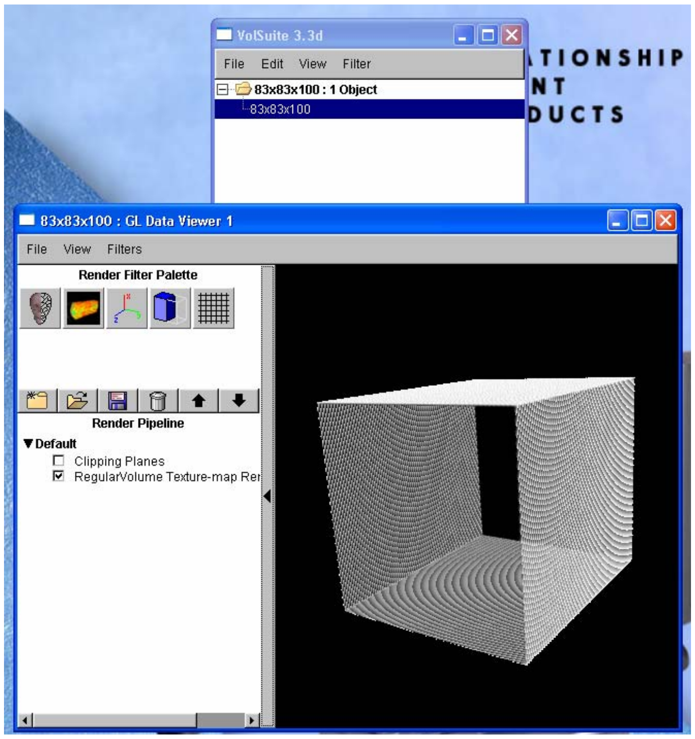
Then click “Import”, it appears as following and we click “view->3D Data Viewer”:



The we can view the 83x83x100 duct as following. The “white” is the ‘solid’ object.



Use the mouse, left-click and moving mouse in the geometry area, we can have a better view.



1.2. Some useful Matlab files and how to create complex domain

Some useful "*.m" file are listed in the following part.
File "**read.m**", the function of this Matlab file can duplicate each of a series frames.

```
clear('all')
close('all')
%     A(:,:,i)=imread(['ML-01_',sprintf('%04d',i),'.jpg']);

w_or_b=0; %white = 255, black = 0

i=1
for slice=1:128

    a=imread(sprintf('del%04d%s',slice,'.bmp'),'bmp');

    for r=1:2
        imwrite(a,sprintf('new256_%04d%s',i,'.bmp'),'bmp');
        i=i+1;
    end
slice
end
```

"**fence2.m**" Matlab file's function is adding walls (white lattice node) to each slice.
Notice: the raw files have data scaled to integers in a range from 0 to 255.

```
X=81;
LY=81;
LX1=LX+2;
LY1=LY+2;
w_or_b=255; %white = 255, black = 0

i=1
for slice=1:81

    a=imread(sprintf('newlay%04d%s',slice,'.bmp'),'bmp');
    b(1:LX1,1:LY1)= 0;

    b(:,1) = w_or_b;
    b(:,LY1) = w_or_b;
    b(1,:) = w_or_b;
    b(LX1,:) = w_or_b;
    for col=1:LX;
    for row=1:LY;
        b(1+col,1+row)=a(col,row);
    end
    end

        imwrite(b,sprintf('fence_%04d%s',slice,'.bmp'),'bmp');
slice
end
```

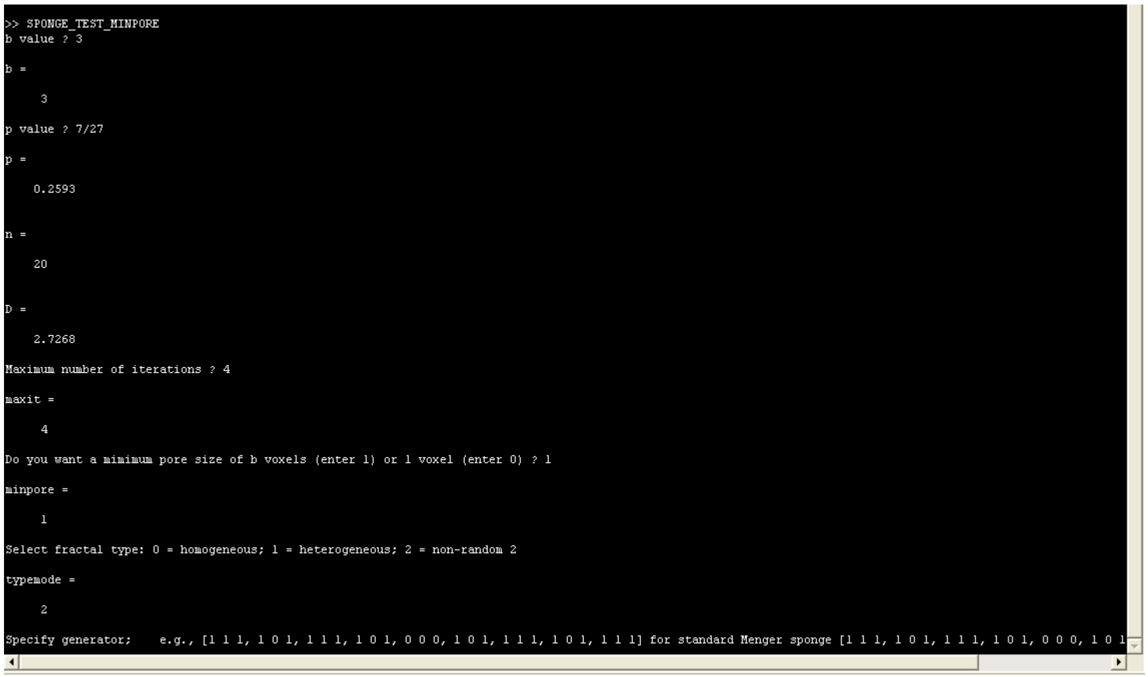
The following file “**construct_fence.m**”, the function of this Matlab file is make several additional slices of pore space at the inlet and outlet end (top and bottom of the object) to accommodate simulation pressure boundary conditions in LBM simulations. Notice, in the following description, the file “newlay0000.bmp” was created by Microsoft Paint, filled with whole slice area with “black” which means pore space.

```
clear('all')
close('all')
i1=7
slice = 0
    a=imread(sprintf('fence_%04d%s',slice,'.bmp'),'bmp');
for i=1:i1
        imwrite(a,sprintf('del_%04d%s',i,'.bmp'),'bmp');
    end
    for i=1:8
    imwrite(a,sprintf('del_%04d%s',i+i1+81,'.bmp'),'bmp');

end

i=i1+1
k=0;
for slice=1:81

    a=imread(sprintf('fence_%04d%s',slice,'.bmp'),'bmp');

     for row=2:82
     for col=2:82
     if( a(row,col) == 0)
         k=k+1;
     end
     end
 end
```

```
        imwrite(a,sprintf('del_%04d%s',i,'.bmp'),'bmp');
        i=i+1;
slice
end

     k
     m=k/81/81/81
```

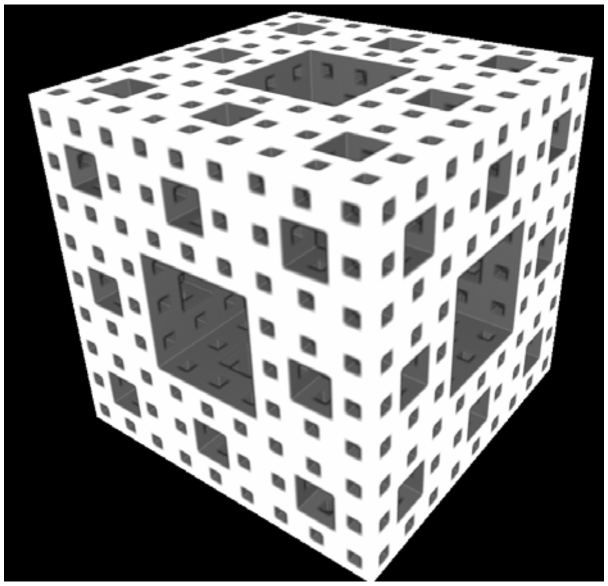
Mike's menger sponge generation Matlab code "SPONGE_TEST_MINPORE.m" can generate a series bmp files of all slices, homogeneously, heterogeneously or regularly. Here we give an example of how to create a regular menger sponge 81cube with minimum pore size b=3 and prepare a 81x81x96 raw file (with 7 and 8 appended pore slices to the top and bottom to accommodate the boundary conditions).

In the Matlab screen, we input the following parameter: b=3, p=7/27, iteration=4, minimum pore size =b, non-random generate method [1 1 1, 1 0 1, 1 1 1, 1 0 1, 0 0 0, 1 0 1, 1 1 1, 1 0 1, 1 1 1], where 1 means solid and 0 means pore. As shows in the following:



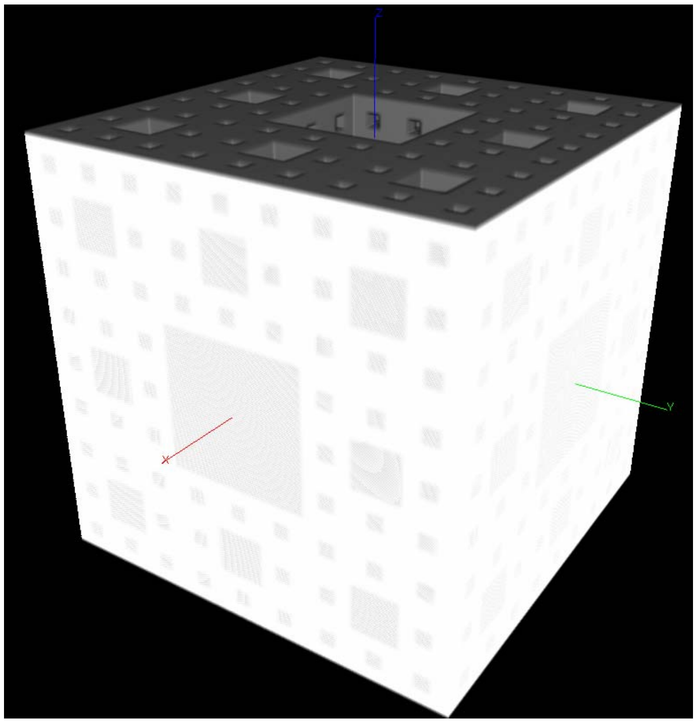
```
>> SPONGE_TEST_MINPORE
b value ? 3

b =

     3

p value ? 7/27

p =

    0.2593


n =

    20


D =

    2.7268

Maximum number of iterations ? 4

maxit =

     4

Do you want a mimimum pore size of b voxels (enter 1) or 1 voxel (enter 0) ? 1

minpore =

     1

Select fractal type: 0 = homogeneous; 1 = heterogeneous; 2 = non-random 2

typemode =

     2

Specify generator;    e.g., [1 1 1, 1 0 1, 1 1 1, 1 0 1, 0 0 0, 1 0 1, 1 1 1, 1 0 1, 1 1 1] for standard Menger sponge [1 1 1, 1 0 1, 1 1 1, 1 0 1, 0 0 0, 1 0 1
```

Then 81 slices from newlay0001 to newlay0081 are generated in the same work folder, we can use ImageJ to make them together and see the 3D view in Volsuite or 3Dview. Use ImageJ we create a 81x81x81.raw file and using Volsuite, we can see the figures as following:



Then we'd like to introduce how to create a 81x81x96 raw file with 7 and 8 appended pore slices to the top and bottom to accommodate the boundary conditions.
The procedure is illustrated as following step by step:

1. on the same work directory, run "fence2" (the file "fence2.m" is illustrated in above section), as a result, we obtained a series fence_00** files (** is from 01 to 81)
2. Using Microsoft Paint to create a bmp file named fence_0000.bmp, click the menu: Image->attributes, filling the dialogue, "width 83, height 83", click ok, and in the color board choose the black, and filling the whole area 83x83 with black color and save as fence_0000.bmp
3. run the Matlab file construct_fence.m (illustrated in the above part) with command "construct_fence" and as a results we got the a series del_00**.bmp files (** is from 1 to 96), the porosity m=0.5936 will also output in the screen.
4. Using the ImageJ to put the above 96 bmp files together and obtain the 83x83x96.raw which is the Menger sponge 81 cube bounded with wall in its sides and 7 and 8 pore slices were appended to the top and bottom. It looks like the following picture:



We can also using Mike’s Menger Sponge generation method to generate the randomly porous medium and construct raw files as the above procedure with minor changes in relevant parameters. In the section 4.1 we would give an example to show how to run LB3D program and obtain the permeability of above Menger Sponge Sample.

The alternative way is create the 3D *.raw directly using C or Fortran code. That’s easy and directly.

Here we give an example of mirroring scheme to create a bigger domain from a small domain. The mirroring examples were introduced in Peter’s master’s thesis. The following C++ program is named “mirror.c”

```
#include <stdio.h>
#include <stdlib.h>
#define ROUND floor
#define NCHAR 132
void skip_label( FILE *in);
void main( )
{
  int size,size2, frame, subs, NumNodes, size_read;
  int i,  n, id,  LX, LY, LZ, LX2, LY2, LZ2,j, k, L, BKL;
  int *rho;
  unsigned char *raw, *raw2 ;
  FILE *in, *fd, *fd2;
  char   filename[1024];
  char   filename2[1024];
  char   line[NCHAR];
BKL = 0;
LX= 336;
LY= 336;
LZ= 336;
LX2 = 576;
```

```
LY2 = 576;
LZ2 = 576;
frame = 0;
subs = 0;


 in = fopen("mirror.in","r+");
 if( !in)
 {
   printf(" ERROR: Can't open file \"%s\". (Exiting!)\n",   "param.dat");
   exit(1);
 }
 skip_label( in); fscanf( in, "%d", &( LX)            );
 skip_label( in); fscanf( in, "%d", &( LY)            );
 skip_label( in); fscanf( in, "%d", &( LZ)            );
 skip_label( in); fscanf( in, "%d", &( LX2)            );
 skip_label( in); fscanf( in, "%d", &( LY2)            );
 skip_label( in); fscanf( in, "%d", &( LZ2)            );
 skip_label( in); fscanf( in, "%d", &( BKL)            );


 fclose(in);
 printf("LX=%d\n", LX);
 printf("LY=%d\n", LY);
 printf("LZ=%d\n", LZ);
 printf("LX2=%d\n", LX2);
 printf("LY2=%d\n", LY2);
 printf("LZ2=%d\n", LZ2);
 printf("BKL=%d\n", BKL);

 NumNodes = LX2 *LY2 *LZ2;
 size2 = NumNodes*sizeof(unsigned char);

 if(!(raw2 = (unsigned char  *)malloc(size2)) )
 {
   printf("%s %d  >> ERROR: Can't malloc rho. (Exiting!)\n",       __FILE__,__LINE__);
   exit(1);
 }


 sprintf(filename , "%dx%dx%d.raw", LX,LY,LZ);

 fd = fopen( filename, "r+");
 if( !fd)
 {
   printf("%s %d >> ERROR: Can't open file \"%s\". (Exiting!)\n",       __FILE__,__LINE__,  filename);
   exit(1);
 }

 size = LX*LY*LZ*sizeof(unsigned char);

 if( !( raw = (unsigned char *)malloc(size)))
 {
   printf("%s %d >> read_solids() -- "
       "ERROR: Can't malloc image buffer. (Exiting!)\n", __FILE__, __LINE__);     exit(1);
 }

 printf("%s %d  >> Reading %d bytes from file \"%s\".\n",        __FILE__, __LINE__,  size, filename);

 size_read = fread( raw, 1, size, fd);
 fclose(fd);
 sprintf(filename2, "./%dx%dx%d.raw",
      LX2,LY2,LZ2 );
 printf("%s %d >> Writting data from file \"%s\"\n", __FILE__,__LINE__,      filename2);


 fd2 = fopen( filename2, "w");


 n = 0;
```

```
  for(k=0; k<BKL; k++)
  {
  for(j=0; j<LY2; j++)
  {
  for(i=0; i<LX2; i++)
  {
    raw2[n]=0;
    n++;
  }

  }
  }
/*
  #define N2X(N,NX,NY,NZ) (N)%(NX)
#define N2Y(N,NX,NY,NZ) (int)floor((double)((N)%((NX)*(NY)))/(double)(NX))
#define N2Z(N,NX,NY,NZ) (int)floor((double)(N)/(double)((NX)*(NY)))
 */

  for(k=BKL; k<BKL+LZ; k++)
  {
  for(j=0; j<LY2; j++)
  {
  for(i=0; i<LX2; i++)
  {
    if(i==0 || i==LX2-1 || j==0 || j==LY2-1) raw2[n]=255;
    else
    {  L = (k-BKL)*LX * LY + (j-1)*LX + (i-1) ;
       if(i<=LX && j<=LY ) raw2[n] = raw[L];
       if(i>LX && j<=LY) raw2[n] = raw[(k-BKL)*LX * LY + (j-1)*LX + ((LX*2-i)-1)];
       if(i<=LX && j>LY) raw2[n] = raw[(k-BKL)*LX * LY + ((LY*2-j)-1)*LX + (i-1)];
       if(i>LX && j>LY)  raw2[n] = raw[(k-BKL)*LX * LY + ((LY*2-j)-1)*LX + ((LX*2-i)-1)];
    }
    n++;
  }

  }
  }

  for(k=BKL+LZ; k<LZ2-BKL; k++)
  {
  for(j=0; j<LY2; j++)
  {
  for(i=0; i<LX2; i++)
  {
     L = (2*(BKL+LZ-1)-k) * LX2 * LY2 + j * LX2 + i ;
     raw2[n] = raw2[L];
     n++;
  }

  }
  }


  for(k=LZ2-BKL; k<LZ2; k++)
  {
  for(j=0; j<LY2; j++)
  {
  for(i=0; i<LX2; i++)
  {
    raw2[n]=0;
    n++;
  }

  }
  }

  printf("n=%d,  LX2*LY2*LZ2=%d \n", n, LX2*LY2*LZ2);

  fwrite( raw2, 1, size2, fd2);
  fclose(fd2);
```

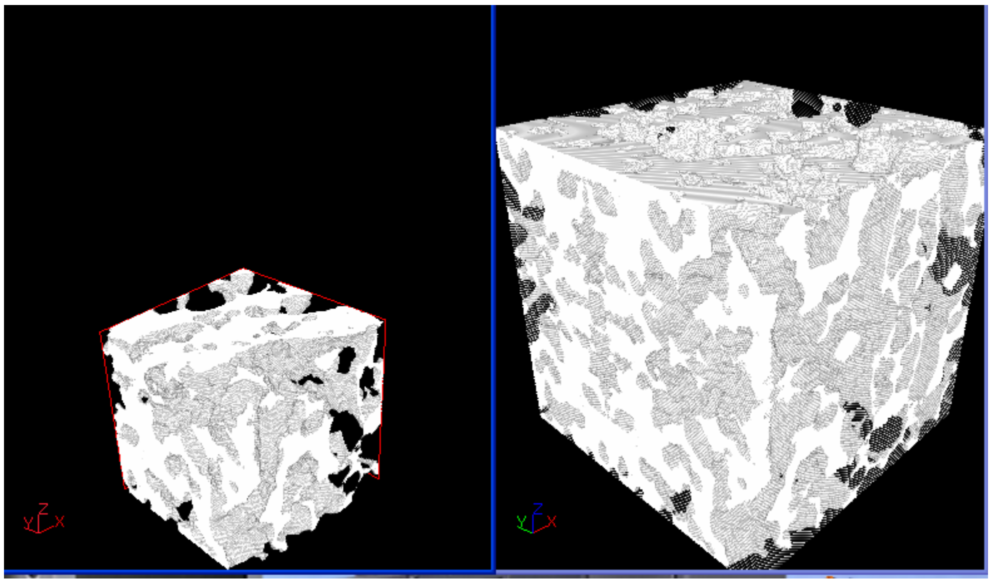
```
} /* void main( ) */


void skip_label( FILE *in)
{
  char c;
  int  done;

  c = fgetc( in);

  if( ( c >= '0' && c <='9') || c == '-' || c == '.')
  {
    // Digit or Sign or Decimal
    ungetc( c, in);
  }
  else
  {
    while( ( c = fgetc( in)) != ' ');
    while( ( c = fgetc( in)) == ' ');
    ungetc( c, in);
  }

} /* void skip_label( FILE *in) */
```

The content of input file “mirror.in” is given in the following:

```
LX       336
LY       336
LZ       336
LX2      576
LY2      576
LZ2      576
BLK      0
```

The parameter “BLK” is useless.

Firstly we should compile “mirror.c” with command “gcc mirror.c –o mirror.exe” in the Cygwin command window, after the executable file “mirror.exe” are created, we can execute the file in the Cygwin command window.
Notice, in the above parameter file we want to create a 576 cube from a 336 cube by mirroring scheme. The source raw file 336x336x336.raw should be in the same the folder of the executable file, after the executable file executed, file 576x576x576.raw appears in the same folder.
The source raw file 336x336x336.raw (left) and output 576x576x576.raw (right) are looks like the following picture, it clear that the 576x576x576.raw obtained from mirroring through the top surface and the red sides labeled in the left image.



2. Post-processing (Brief introduction of Tecplot)

2.1 Introduction of Tecplot

Tecplot 360 and Tecplot 10 are CFD & Numerical Simulation Visualization Software. It combines vital engineering plotting with advanced data visualization in one tool.

With one tool you can:

* Analyze and explore complex datasets
* Arrange multiple XY, 2- and 3-D plots
* Create animations
* Communicate your results with brilliant, high-quality output.

For more information, you can view Tecplot website :
http://www.tecplot.com/products/360/360_main.htm

Download of Tecplot User's Manual and Tecplot Reference Manual is also available in the above website : http://www.tecplot.com/support/360_documentation.htm

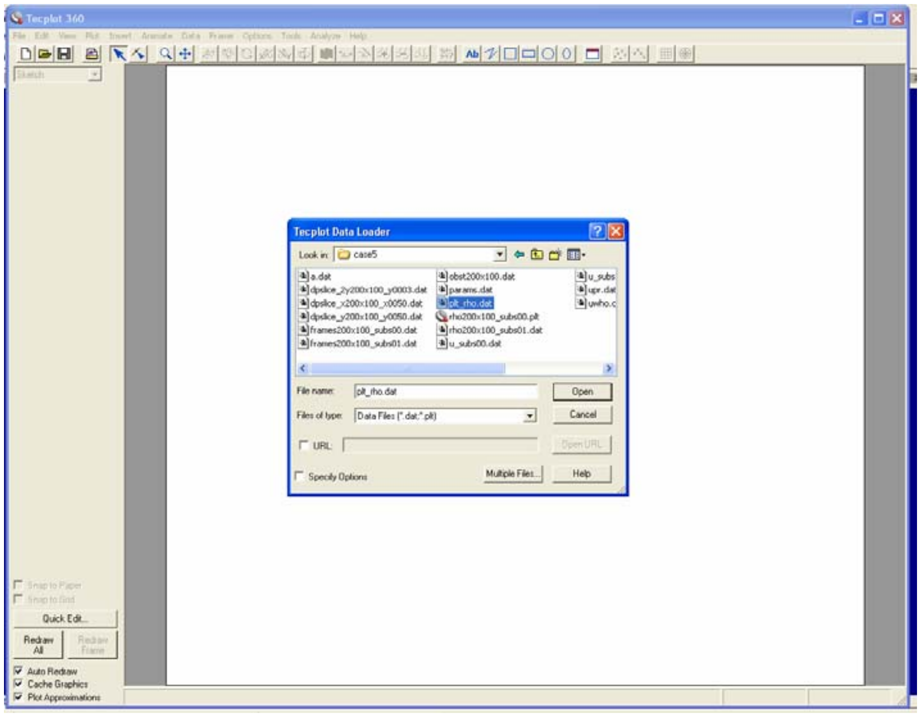
2.2 How to view 2D data files using Tecplot

The Tecplot for 2D flow field should including the Tecplot title, zone, etc.
To output a data file according to the Tecplot format, we should add some code into the source code to output a file as following:

```
variables =x, y, rho1, u1, v1, rho2, u2, v2, upx, upy, uwx, uwy
zone i=200, j=100,  f=point
 0    0 -1.0000  0.0000 -0.0676 -1.0000   0.0000 -0.0362  0.0000 -0.0236  0.0000 -0.0236
 1    0 -1.0000 -0.0000 -0.0677 -1.0000  -0.0000 -0.0363 -0.0000 -0.0236 -0.0000 -0.0236
 2    0 -1.0000  0.0000 -0.0677 -1.0000   0.0000 -0.0363  0.0000 -0.0236  0.0000 -0.0236
…………….
…………….
```

There are 200x100 lines

Click “file->load data file(s)”, then choose the “Tecplot data loader”, then choose the correct folder and the data file (usually we name the data file with appendix name “dat” or “plt”) as following

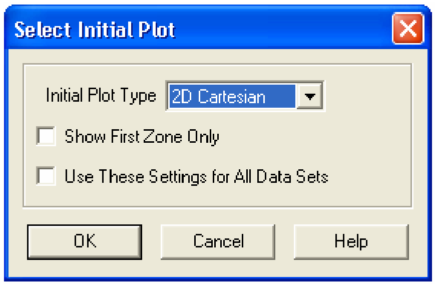


Look in: case5

a.dat
dpslice_2y200x100_y0003.dat
dpslice_x200x100_x0050.dat
dpslice_y200x100_y0050.dat
frames200x100_subs00.dat
frames200x100_subs01.dat
obst200x100.dat
params.dat
plt_rho.dat
rho200x100_subs00.plt
rho200x100_subs01.dat
u_subs00.dat

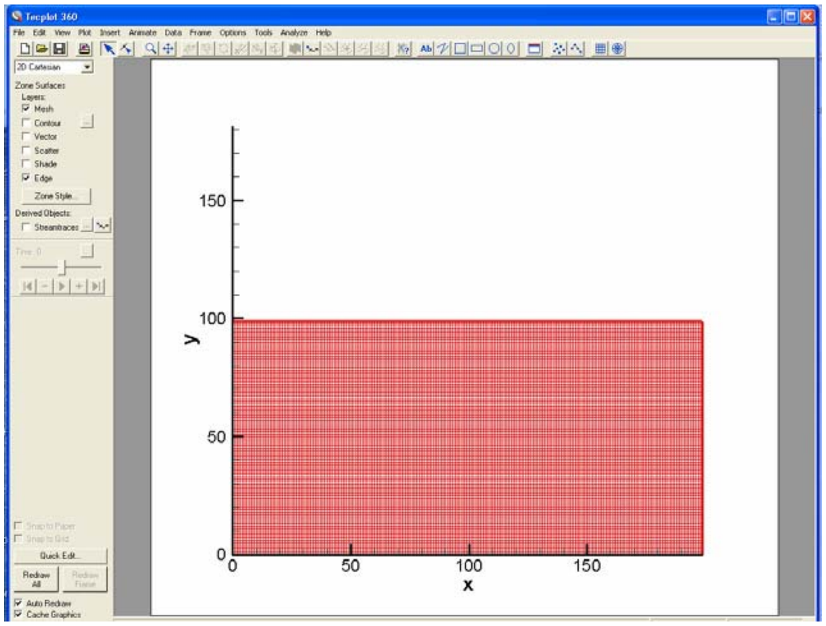
File name: plt_rho.dat
Files of type: Data Files (*.dat;*.plt)
URL: ☐
Specify Options: ☐
Snap to Paper: ☐
Snap to Grid: ☐
Auto Redraw: ☑
Cache Graphics: ☑
Plot Approximations: ☑

After open the file, a pop-up dialogue would appear, usually it can detect the data dimension automatically, here our data is “2D Cartesian”, so click “ok”.

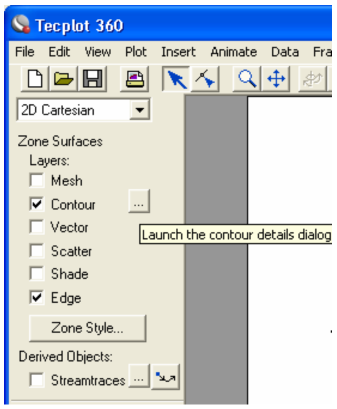


Initial Plot Type: 2D Cartesian
Show First Zone Only: ☐
Use These Settings for All Data Sets: ☐

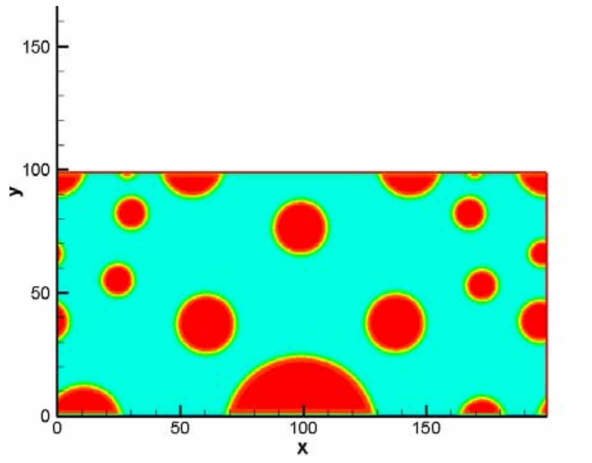
Then there appears the mesh domain x[0,199] and y[0,99] as following:



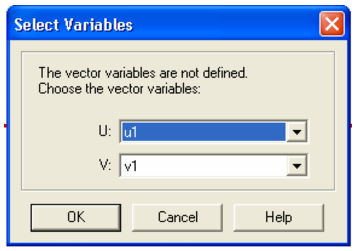
If we want to see the density contours, we should check the “contour” in the upper-left area of the GUI (Graphic User Interface) as following figure. To set the contour levels etc. , please click the box just on the right of “contour”, put mouse here it appears “launch the contour details dialogue”.



The n we can see the contours looks like the following:



To view the vectors, check the item "Vector", then select the vector component variables as following:



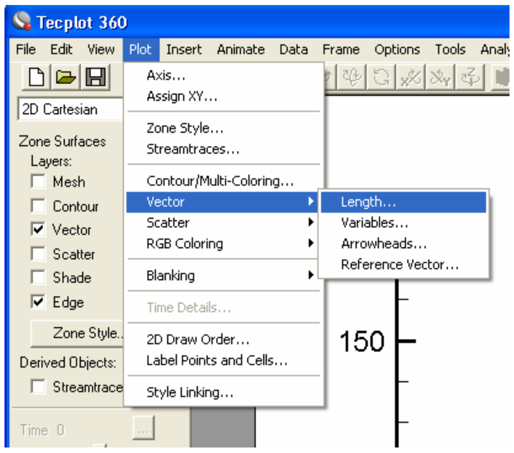
Select Variables

The vector variables are not defined.
Choose the vector variables:

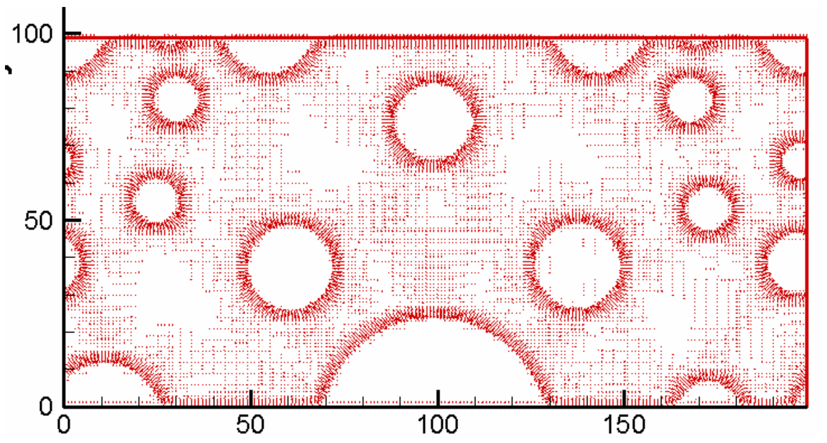
U: u1

V: v1

we can also change the vector relative "length" or "variables", etc. as following:



Then we get the vector plot of the flow field, in the following we can see that in the interface area of the two components, there are spurious velocities.



2.2 Source code to output above 2D data files in Tecplot Format

The following source code segment is about how to output Tecplot-format data using C code. This function is serving for NUM_FLUID_COMPONENTS==2 cases. For single component flow, it is much simpler.

```
void write_plt( /*{{{*/
       struct lattice_struct *lattice,
       double *a, double *b,
       char   *filename)
{
  int size;
  int n, ni, nj;
  FILE *infile;

  ni = lattice->param.LX;
  nj = lattice->param.LY;

  size = ni*nj*sizeof(double);

  if (!(infile = fopen(filename,"w")))
  {
    printf("Can't creat file\n");    exit(-1);
  }
  fprintf( infile, "variables =x, y, rho1, u1, v1, rho2, u2, v2, upx,upy, uwx, uwy\n"  );
  fprintf( infile, "zone i=%d, j=%d,  f=point\n", ni,  nj );

 for( n=0; n<ni*nj; n++)
  {
   if( lattice->bc[0][n].bc_type & BC_SOLID_NODE)
     {
      a[3*n] = -1.;
      lattice->macro_vars[1][n].rho = -1.;
    }
  fprintf( infile, " %4d %4d %7.4f %7.4f %7.4f %7.4f  %7.4f %7.4f %7.4f %7.4f %7.4f
%7.4f\n",  n%ni, n/ni,  a[/*stride*/ 3*n], a[3*n+1], a[3*n+2], b[/*stride*/ 3*n], b[3*n+1],
b[3*n+2],  lattice->upr[n].u[0],  lattice->upr[n].u[1],
                lattice->uwho[n].u[0],  lattice->uwho[n].u[1]          );
  }

  fclose(infile);

  printf(" write_tecplot_file() -- Wrote to file \"%s\".\n", filename);

} /* void write_plt( lattice_ptr lattice, double *a,  ... *//*}}}*/
```

2.3 How to view 3D data files using Tecplot

Here we give an example to show how to use Tecplot to view the velocity vectors, streamlines, etc. This 3D data file obtained from a LB3D simulation of domain 338x338x336, which originally come from the USGS aquifer data sample ML-01 in Miami area.

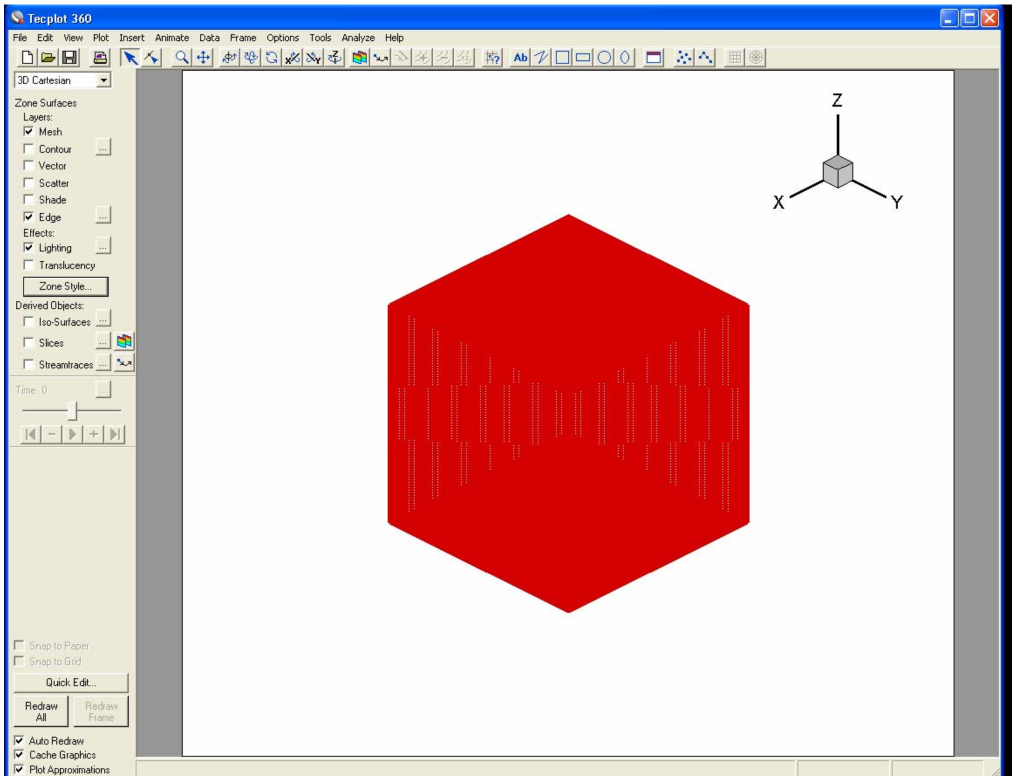
The data file is about 256M, the content in the file is :

```
variables = x, y, z, rho, u, v, w, solid
zone i=169, j=169, k=168,  f=point
   1    1    1   0.9910  -0.00011 -0.00001 -0.00043  0
   3    1    1   0.9910  -0.00003 -0.00025 -0.00147  0
   5    1    1   0.9909   0.00005 -0.00043 -0.00242  0
…………….
…………….
```

There are totally 169x169x168 lines, noticed here to make output data file as small as 256M, in x,y,z direction, index skip is 2. If we do not skip, the output-file of totally 338x338x336 lines is about 256x2x2x2=1,024M, it may be too big to open using Tecplot.

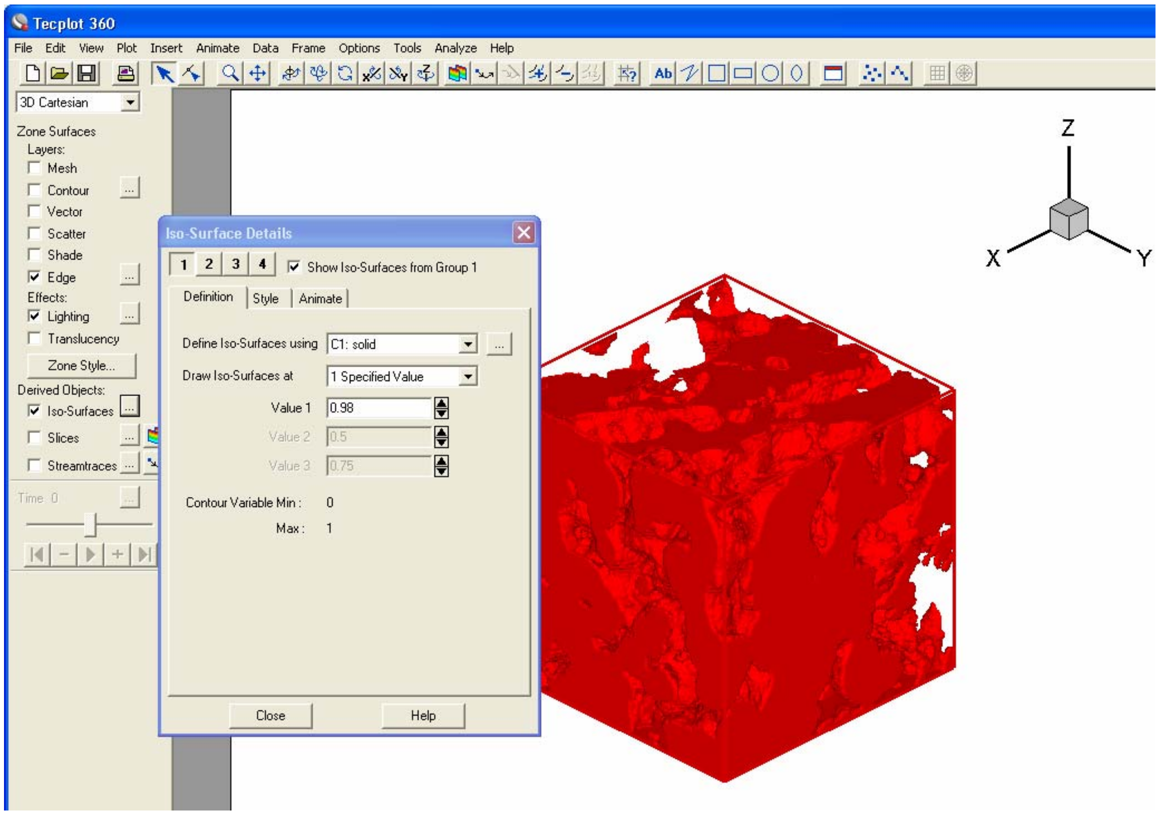
Notice that in the data file, the variable “solid=1” for solid node and “solid=0” for pore node.

After we import the data, it looks like the following 3D huge mesh.



Then uncheck the item “mesh”, click the right button of “Contour”, change the contour variable to the “solid”, then,
Check the item “Iso-Surface”, and click the right button and do a setting in the dialogue. Then we can see the image of the aquifer sample.

Since in the source code, the variable “rho” set as -1 for solid node, while for pore nodes the “rho” is the fluid density at that point, we can also view the image of the sample through set Contour variable as “rho” and “Iso-Surface” contour value as -1.



Show Iso-Surfaces from Group 1 [✓]

Define Iso-Surfaces using: C1: solid

Draw Iso-Surfaces at: 1 Specified Value

Value 1: 0.98

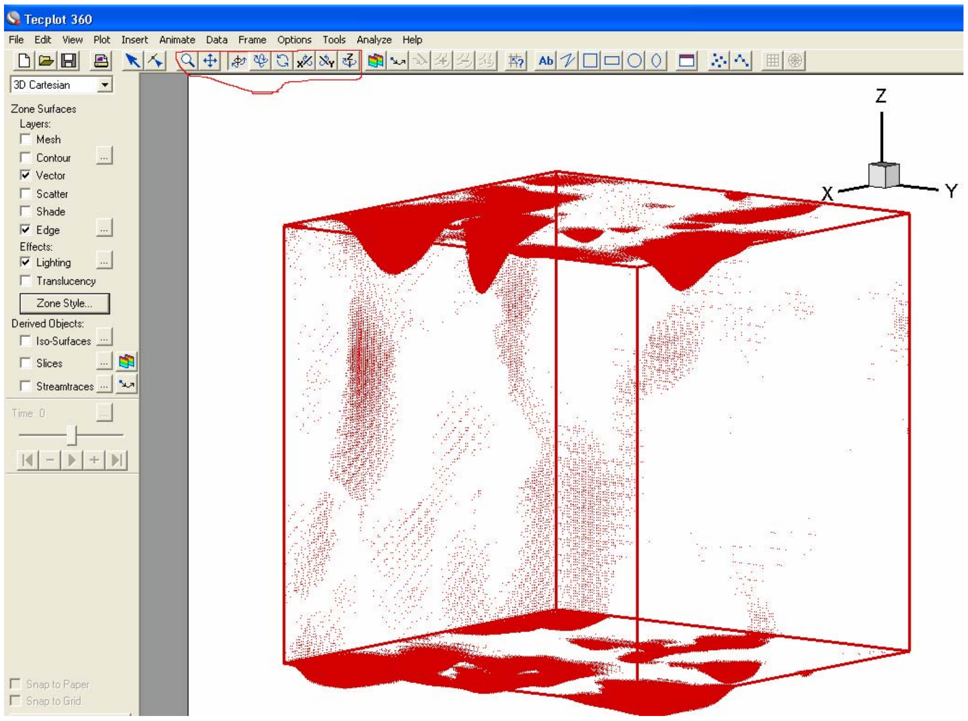
Value 2: 0.5

Value 3: 0.75

Contour Variable Min : 0

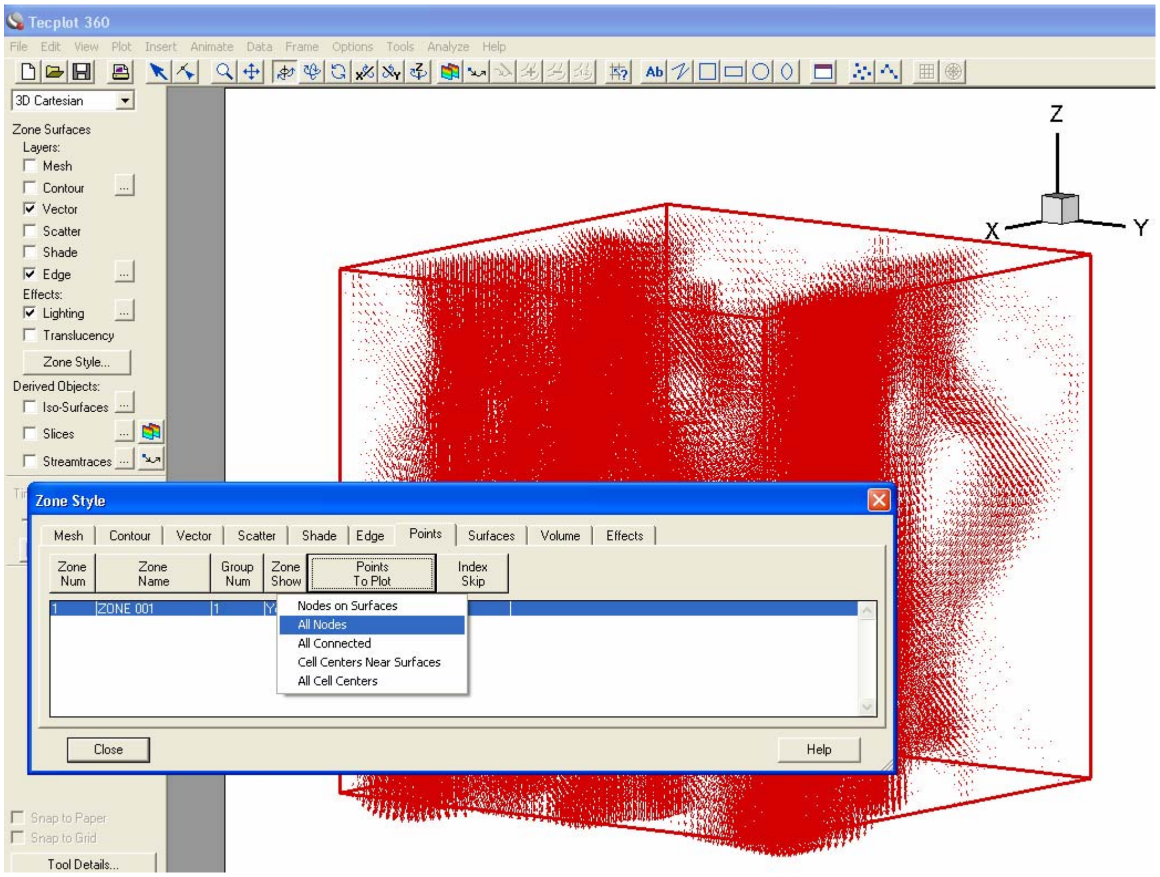
Max : 1

Then we may like to view the flow field, the velocity vector plot. We uncheck the "Iso-Surface", and check the "vector" item in the panel.



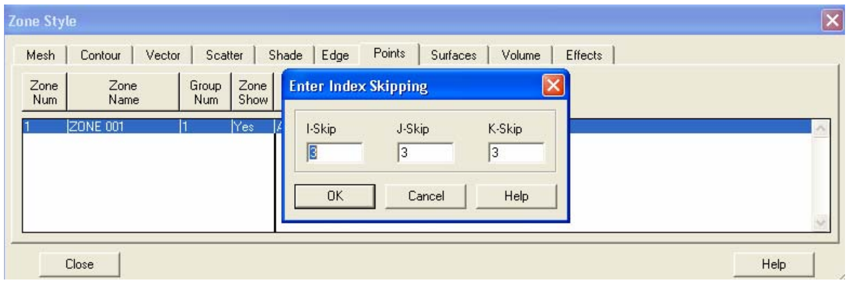
When we have a view, we can use the tools in the top which was circled by red pens to zoom in, zoom out, move or to rotate.

However, it is obvious that the above view is not so good, it seem that only the velocity vectors in top and bottom area shows. To show all the velocity vectors, we click the button "Zone Style", then "Zone Style" appear, click the item "Points", change the option of "Points To Plot" "Nodes on surfaces" to "All nodes", and then click "Index Skip" and filling the skip as following figure.



Zone Num	Zone Name	Group Num	Zone Show	Points To Plot	Index Skip
1	ZONE 001	1	Y	All Nodes	

Nodes on Surfaces
All Nodes
All Connected
Cell Centers Near Surfaces
All Cell Centers

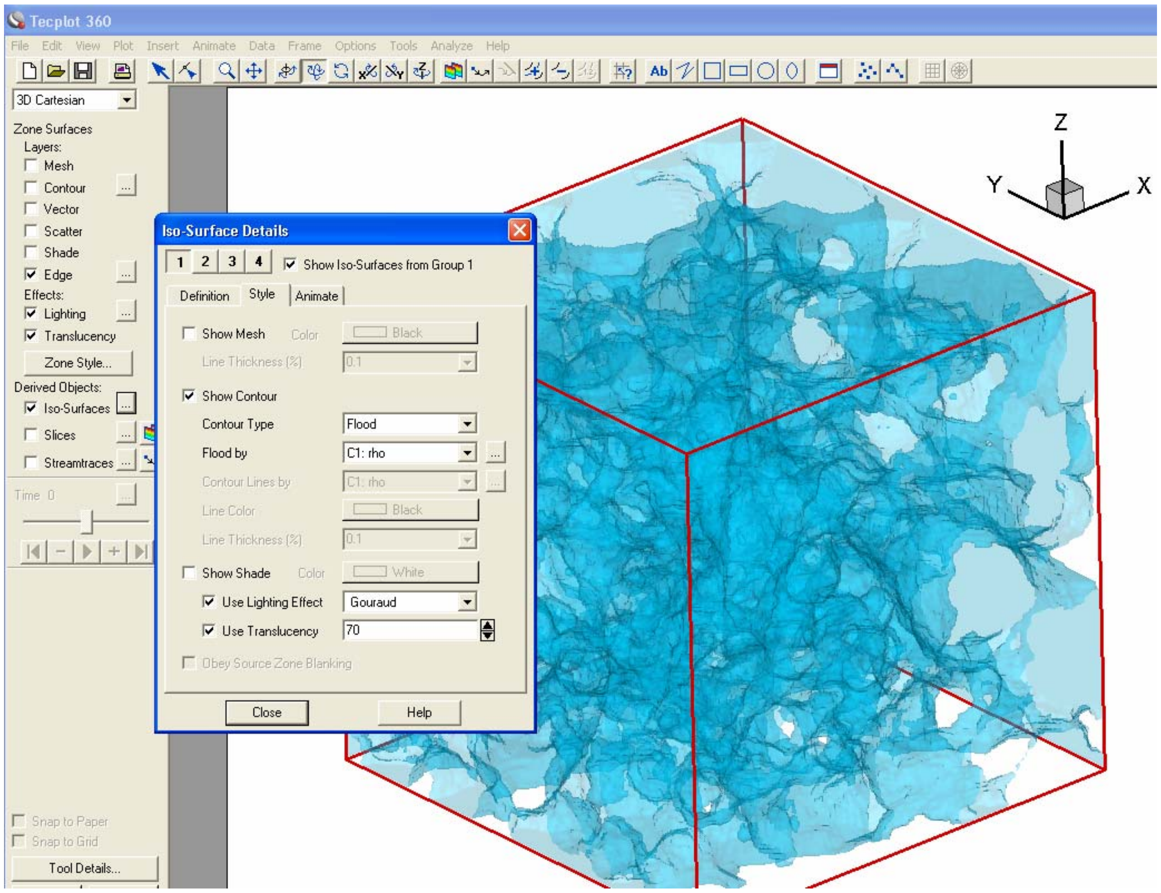


Zone Num	Zone Name	Group Num	Zone Show
1	ZONE 001	1	Yes

I-Skip	J-Skip	K-Skip
3	3	3

Change the vector length and k-skip value (for example k-skip=7) and rotate the object, we can enjoy the view.

Then we'd like to introduce how to view the streamlines using the Tecplot.
Uncheck the "vector", firstly we'd like to use the almost the same method introduce just above to show the solid background, as following, it should be noticed that the "Translucency" =70, which means 70% transparency are used in the following figure.


Tecplot 360
File Edit View Plot Insert Animate Data Frame Options Tools Analyze Help
Z
Y
X
Zone Style...
Close
Help
Tool Details...

3D Cartesian

Zone Surfaces
Layers:
- [ ] Mesh
- [ ] Contour
- [ ] Vector
- [ ] Scatter
- [ ] Shade
- [✓] Edge

Effects:
- [✓] Lighting
- [✓] Translucency

Derived Objects:
- [✓] Iso-Surfaces
- [ ] Slices
- [ ] Streamtraces

Time 0

- [ ] Snap to Paper
- [ ] Snap to Grid

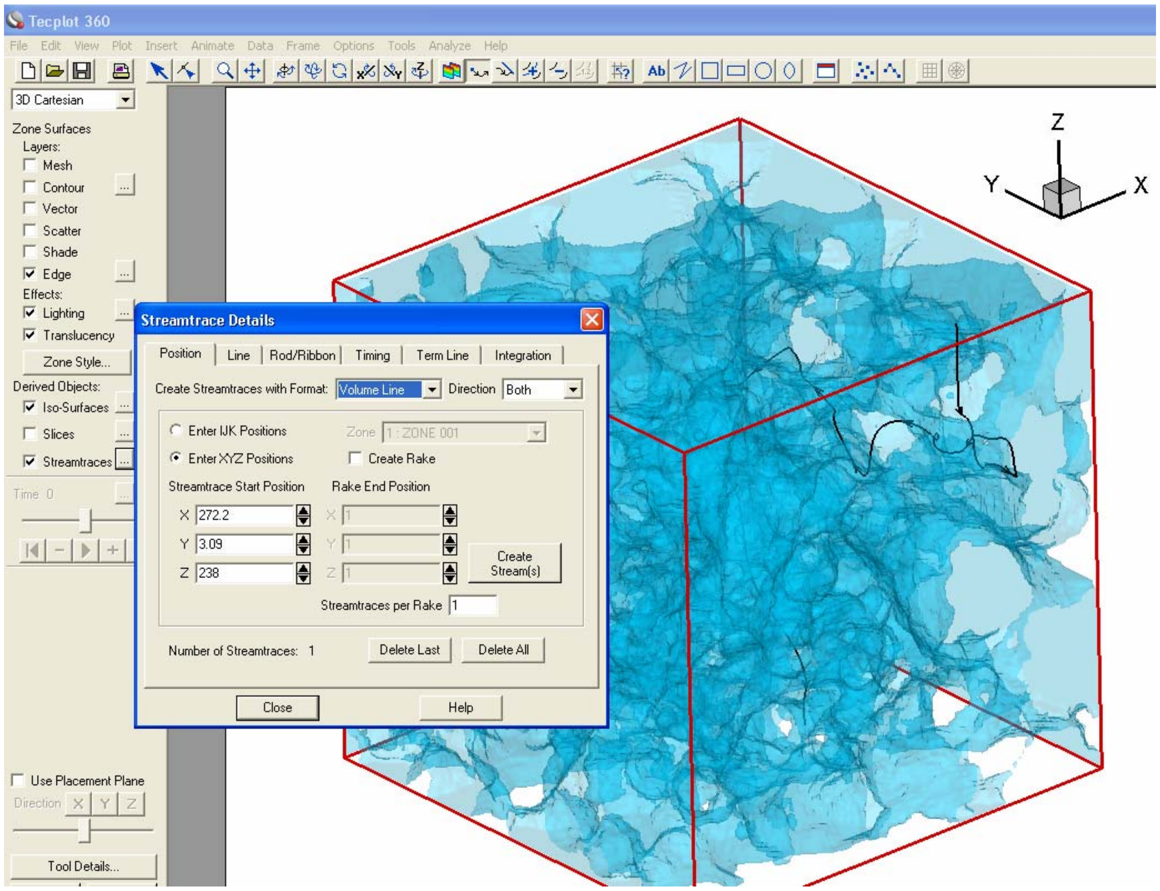
Iso-Surface Details

1 2 3 4 — [✓] Show Iso-Surfaces from Group 1

Definition | Style | Animate

- [ ] Show Mesh — Color: Black
- Line Thickness (%): 0.1
- [✓] Show Contour
- Contour Type: Flood
- Flood by: C1: rho
- Contour Lines by: C1: rho
- Line Color: Black
- Line Thickness (%): 0.1
- [ ] Show Shade — Color: White
- [✓] Use Lighting Effect: Gouraud
- [✓] Use Translucency: 70
- [ ] Obey Source Zone Blanking

Then we check the item "Streamtraces" in the left panel and click the right button, then Dialogue of "Streamtrace Details" appear, to make the streamline more obvious, we change the "Line" -> "Line thickness" to 0.3%, and if we want to create a streamline which passing through point (272.2, 3.09, 238), we just fill up the "Streamtrace Starting point" and click the button of "Create Streams". Then the streamline(s) are created.


Tecplot 360
File Edit View Plot Insert Animate Data Frame Options Tools Analyze Help
Z
Y
X

3D Cartesian

Zone Surfaces
Layers:
- ☐ Mesh
- ☐ Contour
- ☐ Vector
- ☐ Scatter
- ☐ Shade
- ☑ Edge

Effects:
- ☑ Lighting
- ☑ Translucency

Zone Style...

Derived Objects:
- ☑ Iso-Surfaces
- ☐ Slices
- ☑ Streamtraces

Time 0

☐ Use Placement Plane
Direction X Y Z

Tool Details...

Streamtrace Details

Position | Line | Rod/Ribbon | Timing | Term Line | Integration

Create Streamtraces with Format: Volume Line Direction: Both

○ Enter IJK Positions Zone: 1 : ZONE 001
● Enter XYZ Positions ☐ Create Rake

Streamtrace Start Position	Rake End Position
X 272.2	X 1
Y 3.09	Y 1
Z 238	Z 1

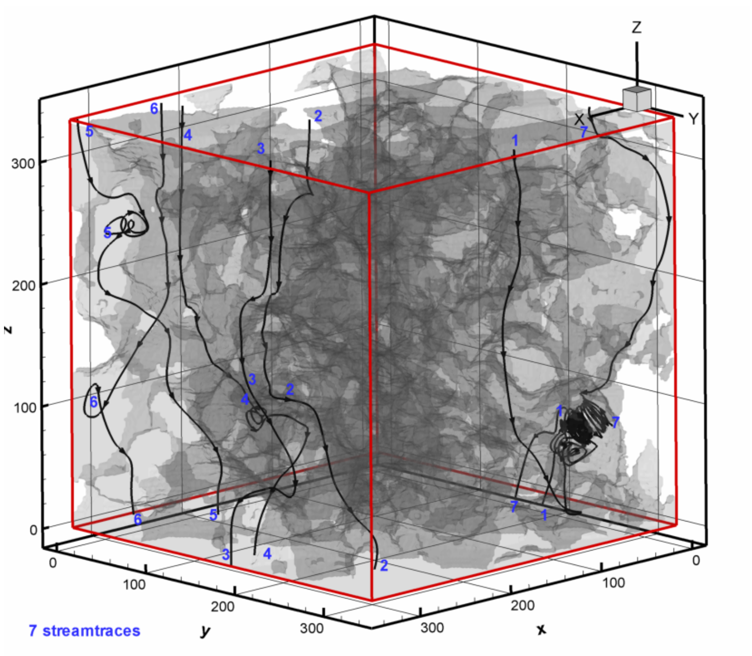
Create Stream(s)

Streamtraces per Rake 1

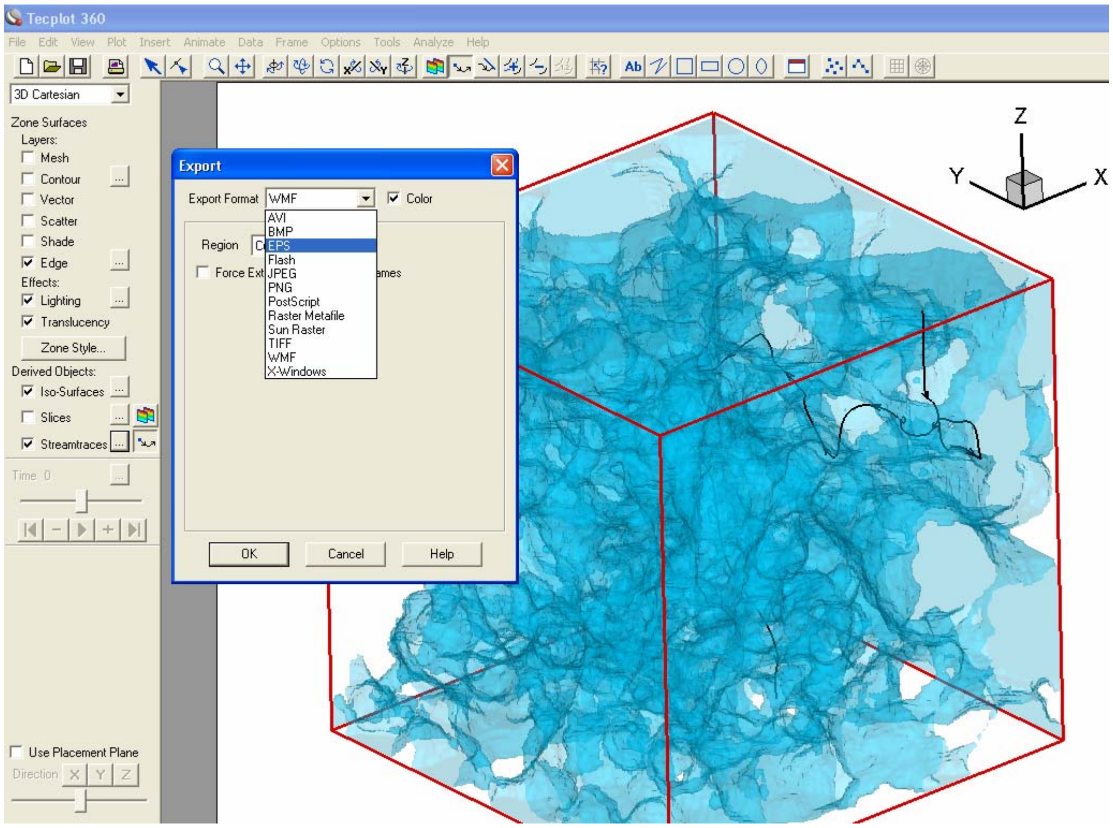
Number of Streamtraces: 1 Delete Last Delete All

Close Help

In this way, we can create more streamlines, the following figure is a good example.



If we want to save the view we obtained, just click "File->Export", then in the Dialogue, we can choose in what format to save the view.



2.4 Source code to output above 3D data files in Tecplot Format

The following source code segment is about how to output 3D Tecplot-format data using C code. This function is serving for NUM_FLUID_COMPONENTS==1 case for single component flow.

```
void write_plt_single(
       lattice_ptr lattice,
       double *a,
       char   *filename)
{
  int size;
  int n, ni, nj, nk, basek;
  double v_in, v_out;
  FILE *infile, *FL1, *FL2;

  ni = lattice->param.LX;
  nj = lattice->param.LY;
  nk = lattice->param.LZ;
  basek = 0;
#if PARALLEL
  basek = get_g_SZ( lattice);
#endif

  size = ni*nj*nk*sizeof(double);
   printf("get_num_proc=%d", get_num_procs(lattice));

  if(lattice->time==0 && get_proc_id(lattice) == get_num_procs(lattice)-1)
  {
    if (!(FL1 = fopen("./out/in_vels.dat","w+")))
  {
    printf("Can't creat file\n");
    exit(-1);
  }
  fprintf(FL1, "time  integration in \n" );

  }//endif   if(get_proc_id(lattice) == get_num_procs(lattice)-1)
  if(lattice->time!=0 && get_proc_id(lattice) == get_num_procs(lattice)-1)
  {
  if (!(FL1 = fopen("./out/in_vels.dat","a+")))
  {
    printf("Can't creat file\n");
    exit(-1);
  }
  }//endif   if(get_proc_id(lattice) == get_num_procs(lattice)-1)

  if (lattice->time==0 && get_proc_id(lattice) == 0)
  {
  if (!(FL2 = fopen("./out/out_vels.dat","w+")))
  {
    printf("Can't creat file\n");
    exit(-1);
  }
  fprintf(FL2, "time  integration in \n" );

  }
  if (lattice->time!=0 && get_proc_id(lattice) == 0)
  {
  if (!(FL2 = fopen("./out/out_vels.dat","a+")))
  {
    printf("Can't creat file\n");
    exit(-1);
  }
  }
  if (!(infile = fopen(filename,"w")))
  {
    printf("Can't creat file\n");
    exit(-1);
  }
  fprintf( infile, "variables = x, y, z, rho1, u, v, w, solid\n"  );
  fprintf( infile, "zone i=%d, j=%d, k=%d,  f=point\n", ni,  nj, nk );

  v_in = 0.;
  v_out = 0.;
 for( n=0; n<ni*nj*nk; n++)
  {
   if( lattice->solids[0][n].is_solid)
     {
      a[4*n] = -1.;
     }
   else
     {
               if(  (get_proc_id(lattice) == get_num_procs(lattice)-1) &&
                                N2Z(n,ni,nj,nk)+basek == get_num_procs(lattice) *lattice-
>param.LZ-1) v_in= v_in + a[4*n+3];
               if(  (get_proc_id(lattice) == 0) && N2Z(n,ni,nj,nk)+basek ==1) v_out= v_out
+ a[4*n+3];
     }
  fprintf( infile, "%4d  %4d %4d  %7.4f  %8.5f %8.5f %8.5f %2d\n",
N2X(n,ni,nj,nk),N2Y(n,ni,nj,nk), N2Z(n,ni,nj,nk)+basek,
  a[/*stride*/ 4*n], a[/*stride*/ 4*n+1], a[/*stride*/ 4*n+2], a[/*stride*/ 4*n+3], lattice-
>solids[0][n].is_solid/255  );
  }

  if(get_proc_id(lattice) == get_num_procs(lattice)-1)
  {
  fprintf(FL1, "%8d  %12.7f\n", lattice->time, v_in );
  fclose(FL1);
  }

  if(get_proc_id(lattice) == 0)
  {
  fprintf(FL2, "%8d  %12.7f\n", lattice->time, v_out );
  fclose(FL2);
  }

  fclose(infile);

  printf("%s %d %04d >> write_tecplot_file() -- Wrote to file \"%s\".\n",
      __FILE__, __LINE__, get_proc_id(lattice), filename);
```

```
} /* void write_plt( lattice_ptr lattice, double *a,  ... */
```

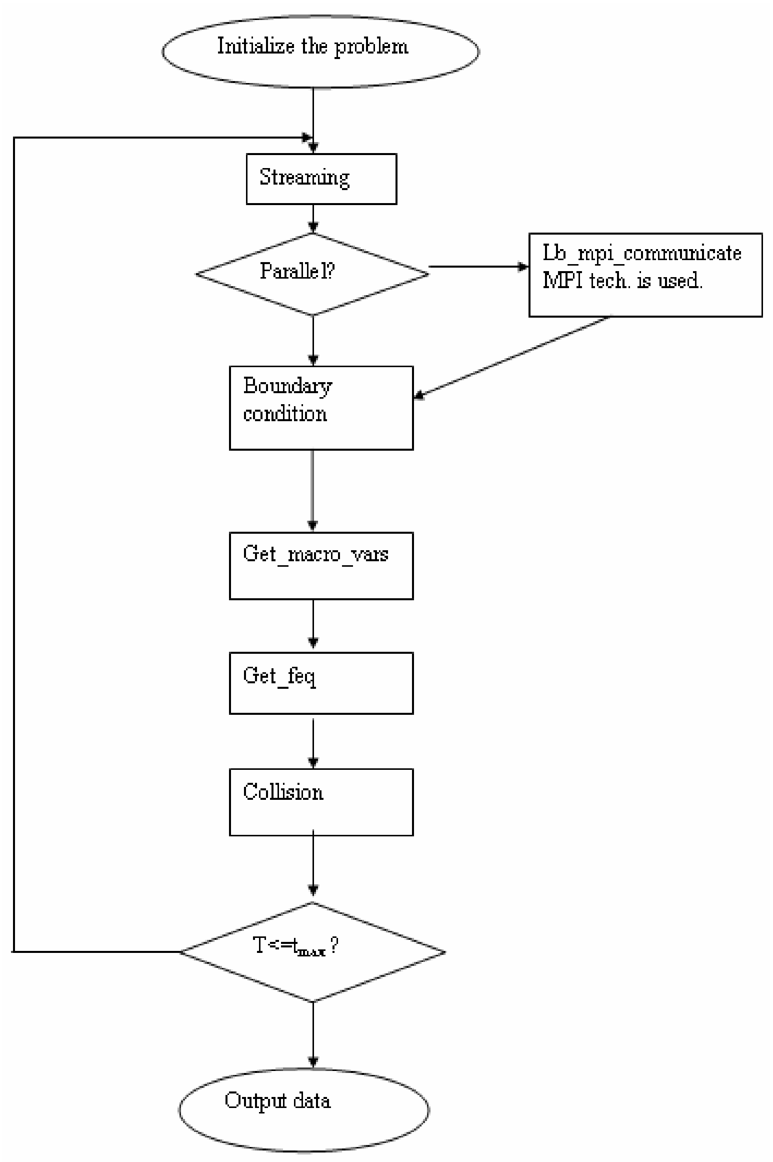
3. Structure and functions in the LB3D program

3.1 Basic flowchart of LB3D program

Overall procedure of the lb_3D code is: (lb3d_prime.c)

```
------------------------------------------------------------------------------------------------
  construct_lattice( &lattice, argc, argv);

  init_problem( lattice);

  output_frame( lattice);

  for( frames = 0, time=1; time<=lattice->NumTimeSteps; time++)
  {
    lattice->time = time;

    stream( lattice);

    if( !lattice->param.GZL && (!lattice->param.AllBoundaryPeriodic)) bcs( lattice);

    compute_macro_vars( lattice);

#if SAVE_MEMO
//feq was calculated in collide_save(lattice)
#else
    compute_feq( lattice);
#endif

    collide( lattice);

    if( lattice->param.GZL && (!lattice->param.AllBoundaryPeriodic)) bcs( lattice);
//compute_feq( lattice);

    if( !(time%lattice->param.FrameRate)) { output_frame( lattice); frames++;}

  } /* for( time=1; time<=lattice->NumTimeSteps; time++) */

  destruct_lattice( lattice);

---------------------------------------------------------------------------------------------------
```

The above procedure can be illustrated in the following flowchart.



3.2 Data structure and main functions of each source file

Our LB3D program package including 9 C source file

lb3d_prime.c, lbio.c, latman.c, compute.c, bcs.c, collide.c, process.c, stream.c, lattice.c
and 6 head files
lattice.h, params.h, flags.h, lb3d_prime.h, forward_declarations.h, process.h.

The other files under *./src/* are junk files can be discarded when do compile.

----
lattice.c is not important, it introduced some minor functions:

```
int get_LX( lattice_ptr lattice)
int get_LY( lattice_ptr lattice)
int get_LZ( lattice_ptr lattice)
void set_LX( lattice_ptr lattice, const int arg_LX)
void set_LY( lattice_ptr lattice, const int arg_LY)
void set_LZ( lattice_ptr lattice, const int arg_LZ)
int get_NumNodes( lattice_ptr lattice)
void set_NumNodes( lattice_ptr lattice)
int is_solid( lattice_ptr lattice, const int n)
int is_not_solid( lattice_ptr lattice, const int n)
double get_rho( lattice_ptr lattice, const int subs, const int n)
double get_ux( lattice_ptr lattice, const int subs, const int n)
double get_uy( lattice_ptr lattice, const int subs, const int n)
double get_uz( lattice_ptr lattice, const int subs, const int n)
```

----
lbio.c is important, the main functions are:

```
void dump_frame_summary( struct lattice_struct *lattice)
```

void dump_macro_vars(struct lattice_struct *lattice, int time)
The most important part in this function is writing TECPLOT file in the following way for single component and two-component flows.

```
#if WRITE_PLOT_FILE
    if(NUM_FLUID_COMPONENTS == 2)
    {
    sprintf( filename, "./out/plt_%dx%dx%d_frame%04d_proc%04d.dat",
        ni, nj, nk, frame, get_proc_id( lattice));
    sprintf( filename2, "./out/R2_%dx%dx%d_frame%04d_proc%04d.dat",
        ni, nj, nk, frame, get_proc_id( lattice));
    printf("Huang tecplot 2 component\n");
    write_plt(
      lattice,
      &(lattice->macro_vars[0][0].rho),
      &(lattice->macro_vars[1][0].rho),
      filename, filename2);

    //get saturation
   basek = 0;
#if PARALLEL
  basek = get_g_SZ( lattice);
#endif
        sprintf( fn3, "./out/saturation_proc%04d.dat",      get_proc_id( lattice));
  if(frame ==0)
  {
```

```
  if(  !( sat = fopen(fn3, "w+")))
   {
    printf(" %04d>> ERROR: "   "fopen(\"%s\",\"r\") = NULL.  Bye, bye!\n",
__FILE__, __LINE__,  get_proc_id( lattice),      fn3);
    exit(1);
   }
  }
  if(frame !=0)
  {
  if(  !( sat = fopen(fn3, "a+")))
   {
    printf(" %04d>> ERROR: "   "fopen(\"%s\",\"r\") = NULL.  Bye, bye!\n",
      __FILE__, __LINE__,     get_proc_id( lattice),       fn3);
    exit(1);
   }
  }
  count =0;
  count1 =0;
  count2 =0;

 for( n=0; n<ni*nj*nk; n++)
  {

     if( (N2Z(n,ni,nj,nk)+basek >lattice->param.z1 &&
                     N2Z(n,ni,nj,nk)+basek <lattice->param.z2
                                    ) )
     {
                 count++;
      if ( lattice->macro_vars[0][n].rho> (lattice->param.rho_A[0]+lattice-
>param.rho_A[1])/2.) count1 ++;
      if ( lattice->solids[0][n].is_solid) count2++;
     }
  }
  fprintf( sat, " %7d, %7d, %7d, %7d\n",   count, count2, count-count2, count1  );


fclose(sat);
    }

    else
    {
    sprintf( filename, "./out/plt_%dx%dx%d_frame%04d_proc%04d.dat",
       ni, nj, nk, frame, get_proc_id( lattice));
    printf("Huang tecplot 1 component\n");
    write_plt_single(
      lattice,
      &(lattice->macro_vars[0][0].rho),
      filename);
    }
#endif
```

In the function void write_raw, the most important formula is Xpix1[n] = (unsigned char)ROUND(1.+254.*(rho-a_min)/(a_max-a_min)); which is prepared for two component flows. Normalize the density of fluid. Raw file, integer [0,255].

----

void write_plt_single, the most important segment:

```
  fprintf( infile, "variables = x, y, z, u, v, w\n"  );
  fprintf( infile, "zone i=%d, j=%d, k=%d,  f=point\n", ni,  nj, nk );

fprintf( infile, "%4d  %4d %4d  %7.4f  %8.5f %8.5f %8.5f %2d\n",
N2X(n,ni,nj,nk),N2Y(n,ni,nj,nk), N2Z(n,ni,nj,nk)+basek,
  a[/*stride*/ 4*n], a[/*stride*/ 4*n+1], a[/*stride*/ 4*n+2], a[/*stride*/ 4*n+3], lattice->solids[0][n].is_solid/255  );
```

3.3 Flags.h File for Compiler Directives

A very important file is flags.h. To use this LBM 3D code efficiently a comprehensive knowledge of this file is required.

Flags.h is best explained as an include file that contains compile-time switches for various options of LB3D. Thus, if any changes are made to flags.h, the program *must* be recompiled (type 'make' in cygwin for PC version or "make mpi" for parallel version).

The first option is "save_memo", if save_memo=0, then in the program, then the most memory consuming mode was set. Three set of distribution functions "f", "feq", "ftemp" would all be used in simulation, the advantage of this mode is that it is very easy to realize the "streaming step" which is one of the two most important steps (steaming and collision step) in LBM. Using this mode, the "ftemp" value used to calculate the macro variables so as to perform next collision step in a lattice node can be easily obtained from the "f" value which is record for the "post-collision" state. While if save_memo=1, then in this lb3d program, the most memory-saving mode was set. "feq" of all lattice nodes would not be remembered in simulation procedure. "f" would also be discard. The "post-collision" state of each node record in "ftemp" array in whole procedure, here performing "streaming step" is somewhat complex than mode of save_memo=0, because we must ensure $ftemp(\mathbf{x}+\mathbf{e}_i)=ftemp(\mathbf{x})$ is implemented correctly. Obviously, some intermediate variables must used to finish this task. For more information please refer to the following section "*memory issure*".

'verbosity level'. This option is mainly for troubleshooting. It controls how much output is given or 'printed' during program execution. For example if it is set at 0 nothing will be printed, if it is set to 1 only items outside of loops will be displayed, if it is set to 2, items inside the first level of loops will be printed, and so on.

Another method of troubleshooting is the 'say hi' function. If this is on, some routines will display "hi" and "bye" messages. If there is a problem with the simulation this toggle allows the user to see how far the program has run before it failed.

Flags.h needs to be told how many components are involved in a particular simulation. This number can be either 1 or 2, and is set in the 'num_fluid_components' setting.

"SPONGE" is only meaningful for two component fluid flows. If define SPONGE (1 && NUM_FLUID_COMPONENTS==2), the total computational domain firstly initiallized

as randomly distributed fluid1 and fluid2 (volume ration “cut” was set in file *./in/params.in*) , however, the upper and lower computational domain controlled by lattice->param.z1 (<), and lattice->param.z2 (>) will be re-initiallized as uniform fluid1 (Wetting). SPONGE==1 usually used for measure the relative permeability.
If define SPONGE (0 && NUM_FLUID_COMPONENTS==2), the upper and lower computational domain would not be re-initiallized.

Presently, ‘inamuro_sigma_component’ is always set =0, it’s not used in our LB3D program. It is useless.

Presently “porous media=0” , it’s not used in the LB3D program.

The ‘store_ueq’ is set to 1 when there is a multiphase and multicomponent system. Therefore, if this is to be used, not only does it need to be on, but also there must be two components.

If your flow area is small compared to the total size of the area, it would be beneficial to have ‘do_not_store_solids’ option on. This will reduce the storage requirements. However this option is not yet functional in the main distribution.

Usually we define COMPUTE_ON_SOLIDS 1
If COMPUTE_ON_SOLIDS is on, macroscopic variables and feq will be computed on solid nodes, even though they are not conceptually meaningful there. This can be helpful for debugging purposes.

‘Non_local_forces’ turns on/off methods for calculating interaction forces, thus it is important when modeling multiphase separation and surface interactions.

‘WM’ and ‘WD’ are weighting factors, for D3Q19 LBM, WM=1/18, WD=1/36. These values should not be changed.

Since we used D3Q19 model, we define Q 19

If the simulation can be analyzed by only *.plt (using Tecplot) (set WRITE_PLOT_FILE=1) and Matlab slice files then is may be useful to turn off write_macro_var_dat_files and write_pdf_dat_files. This will save time and memory.

Another useful tool for debugging is using the write_rho_and_u_to_txt and write_rho_and_u_to_txt. This function should only be used when the simulation requires a very small lattice since it will give density and velocity data at every node of the lattice.

3.4 Memory Issues

In the file of lattice.c,
We need to open the following structures which consuming the memory:

```
  struct pdf_struct        *pdf[        NUM_FLUID_COMPONENTS];
  struct macro_vars_struct   *macro_vars[ NUM_FLUID_COMPONENTS];
  struct solids_struct      *solids[     NUM_FLUID_COMPONENTS];
  struct force_struct       *force[      NUM_FLUID_COMPONENTS];
  struct ueq_struct         *ueq;
```

These above structures are defined as:

```
struct pdf_struct
{
  double feq[   /*NUM_DIRS*/ 19];
  double f[     /*NUM_DIRS*/ 19];
  double ftemp[ /*NUM_DIRS*/ 19];
};

struct macro_vars_struct
{
  double rho;
  double u[   /*NUM_DIMS*/ 3];
};

struct solids_struct
{
  unsigned char is_solid;
};


struct force_struct
{
  double force[  /*NUM_DIMS*/3];
  double sforce[ /*NUM_DIMS*/3];
};

struct ueq_struct
{
  double u[   /*NUM_DIMS*/ 3];
};
```

NOTICE: 1 double occupies 8 bytes while not 4 bytes.

For the pdf_struct, for Single component per lattice node, it occupies	19*3*8 bytes
For the macro_vars_struct, for Single component per lattice node, it need	4*8 bytes
For the solid_struct, for Single component per lattice node, it need	1*8 bytes
For the force_struct, for Single component per lattice node, it need	6*8 bytes

For the ueq_struct, for Multi-component per lattice 3*8 bytes

Hence for a domain 64*64*72, Nonwetting displacing wetting problem, it need
64*64*72*((19*3 +4 +1 +6) *2 (components) +3) *8 = 312M
In our simulation we observed the case need 317M, our calculation is very accurate!

If we using only “ftemp” in our code, and we are able to discard “f ” and “feq”, then in the “pdf_struct”, we only use “ double ftemp[/*NUM_DIRS*/ 19];”, Hence, , for Single component per lattice node, it occupies 19*1*8 bytes
Then for a domain 64*64*72, Nonwetting displacing wetting problem, it only need
64*64*72*((19*1 +4 +1 +6) *2 (components) +3) *8 = 141.1M
In our simulation we observed the case need 142M, our calculation is very accurate!

Table: Memory Usage (2 component 2 phase cases)

Case (domain)	Mode	My calculation (Mb)	Observation in 3D simulation (Mb)
30x30x30	! save_memo mode	30.0	30.8
30x30x30	save_memo mode	13.6	14.78
64x64x72	! save_memo mode	312	317
64x64x72	save_memo mode	141	142

By using our new streaming subroutine , we are able to discard “f” and “feq”,
We can save (317-142)/317= 55% memory!!

For 128x128x128 SAVE_MEMO mode will use memory:
128*128*128*((19*1 +4 +1 +6) *2 (components) +3) *8 =1.05G
For 256x256x256 SAVE_MEMO mode will use memory:
256*256*256*((19*1 +4 +1 +6) *2 (components) +3) *8 =8.4G

CPU time:

Case 64x64x72

PC (1 CPU)	120,000	50hrs		
Parallel 3D 8 CPU	120,000	12hrs		
Parallel 3D 24 CPU	120,000	4.8hrs	10,000	24mins

Case 128x128x144

Parallel 3D 24 CPU	10,000	3hrs30min		
Parallel 3D 36 CPU	10,000	2hrs30min		

Case 256x256x256

Parallel 3D 32 CPU	25,000	35hrs20min	10,000	14.133hr

!save_memo mode (using “feq” , “f”, and “ftemp”)
Hence for a domain 64*64*72, Single component problem, it need
64*64*64*((19*3 +4 +1) *1 (components)) *8 = 130M

maximum cube size:
2G per node, 48 node available.
48*2G=48*2,000,000,000= x^3*(19*3+ 4 +1) *8, we obtain x=578

2G per node, 24 node (48 CPU) available.
24*2G=24*2,000,000,000= x^3*(19*3+ 4 +1) *8, we obtain x=459

2G per node, 64 node (128 CPU) available.
64*2G=64*2,000,000,000= x^3*(19*3+ 4 +1) *8, we obtain x=636

----
save_memo mode (using “ftemp” only)

If we using only “ftemp” in our code, and we are able to discard “f ” and “feq”, then in the “pdf_struct”, we only use “ double ftemp[/*NUM_DIRS*/ 19];”, Hence, , for Single component per lattice node, it occupies 19*1*8 bytes
Then for a domain 64*64*64, Nonwetting displacing wetting problem, it only need
64*64*64*((19*1 +4 +1) *1 (components)) *8 = 50M

maximum cube size:
2G per node, 48 node available.
48*2G=48*2,000,000,000= x^3*(19*1+ 4 +1) *8, we obtain x=793

2G per node, 24 node (48 CPU) available.
24*2G=24*2,000,000,000= x^3*(19*1+ 4 +1) *8, we obtain x=629

2G per node, 64 node (128 CPU) available.
64*2G=64*2,000,000,000= x^3*(19*1+ 4 +1) *8, we obtain x=873

SAVE_MEMO & 2 component fluid flow:
2G per node, 64 node (128 CPU) available.
64*2G=64*2,000,000,000= x^3*((19*1+ 4 +1+6)*2+3) *8,   we obtain x=633

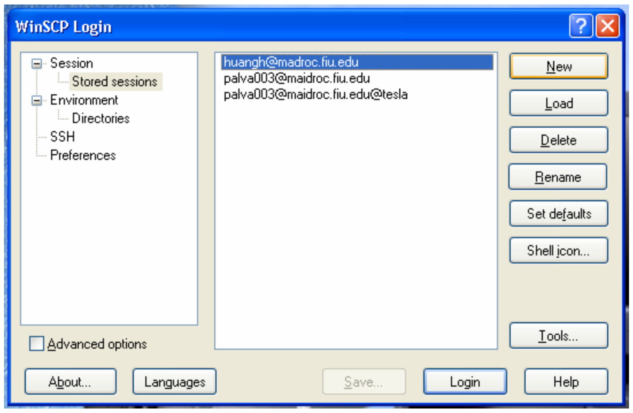
4. Run LB3D parallel version in Tesla-128 CPU parallel supercomputer

4.1. Introduction of Tesla, a 128-CPU parallel supercomputer

Our parallel LBM code made it possible to run a sample as large as 873 pixel cube (SAVE_MEMO==1 and single component flow). This code was run on the MAIDROC cluster “TESLA-128” located at Florida International University’s Applied Engineering Center (http://maidroc.fiu.edu).

The MAIDROC computing laboratory at FIU is equipped with a secure network consisting of one SGI R10000 workstation, six 3.0GHz PCs, two laser printers and a high intensity projector for PowerPoint presentations. The centerpiece of the MAIDROC Lab is the new 128-processor parallel computer. The parallel machine uses a variant of MPI and Linux operating system. The MAIDROC cluster was designed, assembled, and tuned in January of 2004. This machine is composed of 64 nodes that were assembled and tested by Alienware. Each node has a Tyan S2882G3NR (Thunder SK8) motherboard with two AMD Opteron 1.6 GHz CPU's, 80 GB ATA IDE Seagate hard drive and 2GB RAM per node. Each of the nodes has an Intel® 82551QM 10/100 fast Ethernet controller and two Broadcom® BCM5704C Gigabit Ethernet controllers. Two Dell PowerConnect 5224 24-port Gigabit Ethernet switches and one HP ProCurve 5400zl 72-port switch are used to connect the nodes. The ProCurve switch features a 76.8 Gbps switching fabric. All communication within the cluster is on a 1 Gbps network. The Linux operating system (RedHat Taroon 64-bit beta) is used on all nodes. We are currently running kernel 2.4.21-4 compiled for a 64-bit SMP. The MPI message passing library LAM 7.0.4 and 64-bit Portland Group compilers are currently used for all MPI programs. A dual 2.4 GHz Xeon processor based PC is used as the NFS server and DQS queue master. This cluster has a peak performance of more than 288 Gigaflops/sec. However, the largest measured sustained speed achieved was 112 Gigaflops/sec using the high performance Linpack benchmark on 64 processors over the Gigabit network.

You can down load the WinSCP3 from the following website:
http://www.cs.csustan.edu/resources_files/WinSCPDownload-frame.htm
When you open the WinSCP3, if you are the new user and have an account in the MAIDROC cluster “TESLA-128”, you can click “new” as the following figure:

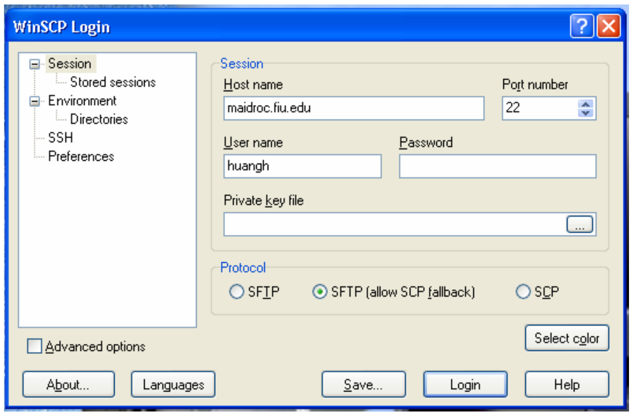


WinSCP Login

Stored sessions:

- huangh@madroc.fiu.edu
- palva003@maidroc.fiu.edu
- palva003@maidroc.fiu.edu@tesla

and then fill up the items in the pop-up dialogue as the following figure, and leave the Private key file as unfilled. Then click the "login" button and input your password,



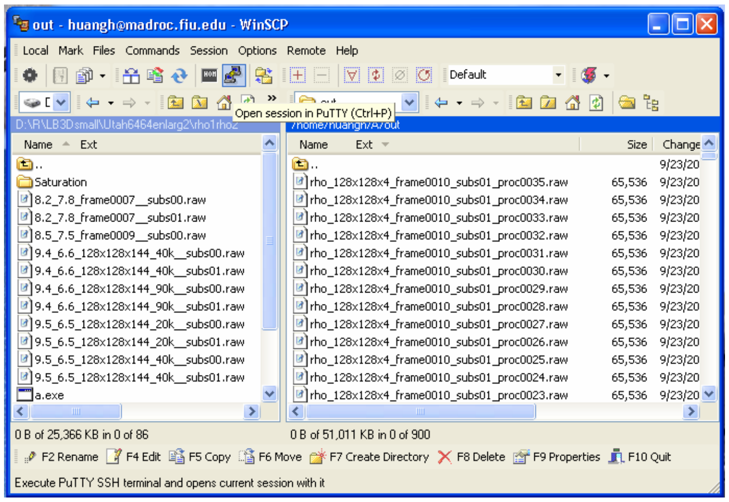
WinSCP Login

Session
Host name: maidroc.fiu.edu
Port number: 22
User name: huangh
Password:
Private key file:

Protocol: ( ) SFTP [✓ SFTP (allow SCP fallback)] ( ) SCP

Advanced options: ☐

Then you can log into the cluster "TESLA-128" and see the interface of WinSCP, left column is the local file system, right column is the file systems in cluster "TESLA-128". Then you can upload and download files to (form) cluster "TESLA-128" easily. If you want to input command to the cluster "TESLA-128", you should click the icon "open session in PuTTY (Ctrl+P)".



out - huangh@madroc.fiu.edu - WinSCP

Open session in PuTTY (Ctrl+P)

Local: D:\R\LB3Dsmall\Utah6464enlarg2\rho1rho2

Name	Ext
..	
Saturation	
8.2_7.8_frame0007__subs00.raw	
8.2_7.8_frame0007__subs01.raw	
8.5_7.5_frame0009__subs00.raw	
9.4_6.6_128x128x144_40k__subs00.raw	
9.4_6.6_128x128x144_40k__subs01.raw	
9.4_6.6_128x128x144_90k__subs00.raw	
9.4_6.6_128x128x144_90k__subs01.raw	
9.5_6.5_128x128x144_20k__subs00.raw	
9.5_6.5_128x128x144_20k__subs01.raw	
9.5_6.5_128x128x144_40k__subs00.raw	
9.5_6.5_128x128x144_40k__subs01.raw	
a.exe	

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Remote: /home/huangh/A/out

Name	Ext	Size	Change
..			9/23/20
rho_128x128x4_frame0010_subs01_proc0035.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0034.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0033.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0032.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0031.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0030.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0029.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0028.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0027.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0026.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0025.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0024.raw		65,536	9/23/20
rho_128x128x4_frame0010_subs01_proc0023.raw		65,536	9/23/20

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Execute PuTTY SSH terminal and opens current session with it

4.2. How to run LB3D in the parallel supercomputer

After you should click the icon “open session in PuTTY (Ctrl+P)” in WinSCP3 and you input your password, then you can input command to edit or compile files in “TESLA-128”.

We should compile the source files in folder ./src, after we make some revision or changes, we should re-compile the source files again to get the executable file ./lb3d. In the “maidroc” screen, we should input “make mpi”, as

```
huangh@maido:~/B> make mpi
```

Notice: the source files in folder ~/B/src
After the executable file “./lb3d” is created, we can execute and perform our parallel LB 3D simulations. If it is using 64 CPUs to do simulation, Just input

```
huangh@maido:~/B> qsub 64.sh
your job 675788 has been submitted
```

We can check whether the job was performed using the command: qstat
The screen may show the information as following:

```
cassian  cass-g1   maido01      675763   0:1   r      RUNNING   09/13/07 07:40: 1
huangh   B_LB3D    maido01      675788   0:1   r      RUNNING   09/14/07 16:27:51
huangh   B_LB3D    maido02      675788   0:1   r      RUNNING   09/14/07 16:27:51
huangh   B_LB3D    maido03      675788   0:1   r      RUNNING   09/14/07 16:27:51
huangh   B_LB3D    maido04      675788   0:1   r      RUNNING   09/14/07 16:27:51
…………………………………….

………………………………………..
```

The displayed information tells us the job who submitted (huangh), the job name (B_LB3D), the node used (maido01), job number (675788) and when the job was submitted.

If we want to kill the submitted job using the command: “qdel 675788”

The 64.sh was written as following:

```
#!/bin/sh
#$ -cwd
#$ -l qty.eq.64                    //number of CPUs requested.
#$ -N B_LB3D                //name of job: B_LB3D
#$ -V
PATH=/usr/local/lam/bin:/usr/lib:$PATH
export PATH
LD_LIBRARY_PATH=/usr/lam/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH
mdo_mpi_fast ./lb3d
```

The above 64.sh is used for the parallel run using 64 CPUs. For example, if we want to use 100 CPUs, we should change the parameter 64 into 100, and we'd better rename the .sh file as 100.sh.

Some useful command may used in Unix system:

Edit a file *.*,	vi *.*
Remove a file *.*,	rm *.*
Remove a folder and all folder and files under it,	rm –R ./folder
Make a copy	cp A/*.* B/**.*
Copy whole folder A to B	cp –R ./A ./B

5. Examples

5.1. Permeability measurement (single-component flow)

When we simulate the permeability of porous media, the single-component should be set in *flags.h* and initial condition==0 (uniformly initialized), the rho_in and rho_out should be set in *./in/params.in*.
The most important parameters should be set are listed as following, the parameter value is depend on different case but their correct values must be set before perform correct simulations:

```
LX                      83
LY                      83
LZ                      96
characteristic_length   81
NumFrames               8
FrameRate               2000
tau[0]                  1.0
rho_A                   8.0
GZL                      0
PressureBC               1
AllBoundaryPeriodic      0
rho_in                  8.05
```

```
rho_out                 7.95
initial_condition       0
```

Notice: the above setting is for mode of SAVE_MEMO==0, if SAVE_MEMO =1 was set in *flags.h*, then here `GZL = 1.`

The simulations use pressure boundaries on the top and bottom that impose a gradient across the fractal domain. In the calculations for *k*, *L* = 81 *lu*. In a convenient form for the LBM, Darcy's law, is

$$q = \frac{k}{\rho c_s^2 (\tau - 0.5)\Delta t} \frac{\Delta p}{L}, \tag{1}$$

where *q* is the Darcy flux (the average velocity of fluid exiting the entire face – including solid areas where the velocity is zero), c_s^2 (τ – 0.5) is the kinematic viscosity, and $\Delta p/L$ is the pressure gradient. Note that the average density is used in the denominator of Eq. (1).

Two cases were simulated. In the first case, the average fluid density was ρ=8 *mu* lu^{-3} with inlet and outlet pressure of $p_{in} = 2.6833$ and $p_{out} = 2.65$ *mu* $lu^{-1}ts^{-2}$, respectively. Under those conditions, the observed flow through the system was 6.87 lu^3 ts^{-1}. The Darcy flux *q* is the flow divided by the cross-sectional area $q = 6.87/(81 \times 81)$. It can be used to determine the permeability via Darcy's Law written in terms of the density gradient: $q = \frac{k}{\rho(\tau - 1/2)\Delta t}\frac{\Delta\rho}{L} = \frac{k}{8 \times (1 - 1/2) \times 1}\frac{8.05 - 7.95}{81}$. Solving for k, we get $k = 3.39\, lu^2$. If we take the mean pore water velocity $\bar{u} = \frac{q}{\phi}$, we can compute an average Reynolds number as $\mathrm{Re} = \frac{\bar{u}L}{\nu} = \frac{\bar{u}L}{c_s^2(\tau - 1/2)\Delta t} = \frac{6.87/(81 \times 81 \times 0.594)}{1/3 \times (1 - 1/2) \times 1} = 0.01$; departures from Darcy's law behavior should be very small at this Re. The second case used ρ=2 *mu lu*$^{-3}$, with $p_{in} = 0.6833$ and $p_{out} = 0.65$ *mu lu*$^{-1}$*ts*$^{-2}$. The observed flow was 27.25 *lu*^{3} *ts*$^{-1}$ and with the Darcy flux $q = 27.25/(81 \times 81) = \dfrac{k}{\rho(\tau - 1/2)\Delta t}\dfrac{\Delta\rho}{L} = \dfrac{k}{2 \times (1.0 - 1/2)}\dfrac{2.05 - 1.95}{81}$, we obtain the permeability as $k = 3.36\,lu^{2}$. In this case, $\mathrm{Re} = \dfrac{\overline{u}L}{\nu} = \dfrac{\overline{u}L}{c_s^2(\tau - 1/2)\delta t} = \dfrac{27.25/(81 \times 81 \times 0.594)}{1/3 \times (1 - 1/2) \times 1} = 0.067$ and some minor deviation from Darcy's law might be observed. This would be expected to lead to a smaller apparent permeability because head is being dissipated through inertial processes.

Thus, the best current LBM estimate of the saturated permeability of the deterministic Menger Sponge is 3.39 *lu*^{2}. Conversion to real units is trivial. To convert '*lu*^{2}' to real permeability units, multiply by the scale conversion factor as follows:

$$k_{sat}^{physical} = k_{sat}^{LBM}\left(\frac{L_{physical}}{L_{LBM}}\right)^{2} \tag{2}$$

where the *L*'s are the length of any comparable feature in physical and LBM units.

More details and more cases simulation can be found in reference of paper2 and paper3.

5.2. Non-wetting fluid displacing wetting fluid and vice-versa

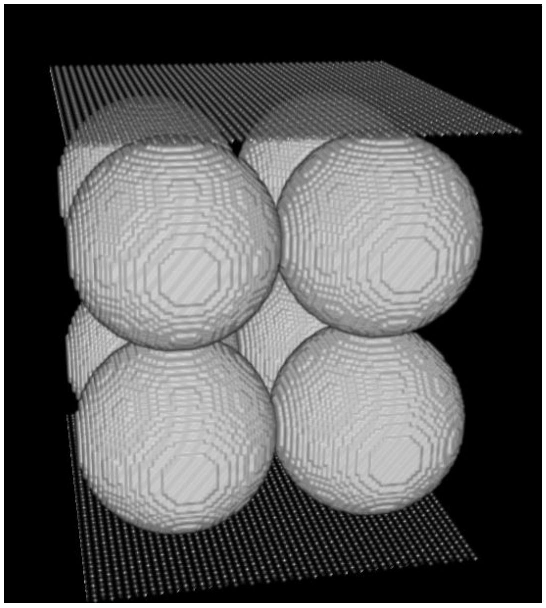
The four packed balls domain 100x100x150 as following, there are two plates with very small pore sizes in the top and bottom of the simulation domain. The 3D raw file is created by the C program directly since it is very convenient. The source code of the C program is also illustrated in the following:

```
#include <stdio.h>
#include <stdlib.h>
#define ROUND floor
#define NCHAR 132
void main( )
```

```
{
  int size,size2, frame, subs, NumNodes, size_read, cons;
  int i,  n, id,  LX, LY, LZ, LX2, LY2, LZ2,j, k, L;
  int LZ3, LY3, LX3, R2, R3, R4, R5,LZ4, LY4, LX4,LZ5, LY5, LX5;
  int LXC[9],LYC[9],LZC[9];
  int *rho;
  unsigned char  *raw2 ;
  FILE *in, *fd, *fd2;
  char   filename[1025 ];
  char   filename2[1025 ];
  char   line[NCHAR];
LX= 100;
LY= 100;
LZ= 150;
cons = 25;

  for(i=1; i<5; i++)
  {
    LZC[i]= 25 +cons;
  }
    LXC[1] = 25 ;
    LYC[1] = 25 ;
    LXC[2] = 25 +50;
    LYC[2] = 25 ;
    LXC[3] = 25 ;
    LYC[3] = 25 +50;
    LXC[4] = 25 +50;
    LYC[4] = 25 +50;

  for(i=5; i<9; i++)
  {
    LZC[i]= 25 +50+cons;
  }
    LXC[5] = 25 ;
    LYC[5] = 25 ;
    LXC[6] = 25 +50;
    LYC[6] = 25 ;
    LXC[7] = 25 ;
    LYC[7] = 25 +50;
    LXC[8] = 25 +50;
    LYC[8] = 25 +50;

R2 = 25;
frame = 0;
subs = 0;
```

```
  printf("LX=%d\n", LX);
  printf("LY=%d\n", LY);
  printf("LZ=%d\n", LZ);
  printf("LX2=%d\n", LX2);
  printf("LY2=%d\n", LY2);
  printf("LZ2=%d\n", LZ2);

  NumNodes = LX *LY *LZ;
  size2 = NumNodes*sizeof(unsigned char);

  if(!(raw2 = (unsigned char  *)malloc(size2)) )
  {
    printf("%s %d  >> ERROR: Can't malloc rho. (Exiting!)\n",      __FILE__,__LINE__);
    exit(1);
  }


  sprintf(filename2, "./%dx%dx%d.raw",  LX,LY,LZ );
  printf("%s %d >> Writting data from file \"%s\"\n", __FILE__,__LINE__,   filename2);

  fd2 = fopen( filename2, "w");

   n = 0;
  for(k=0; k<LZ; k++)
  {
  for(j=0; j<LY; j++)
  {
  for(i=0; i<LX; i++)
  {
    raw2[n] = 0;

    if((k==20 || k==130) && (j%2)==0 && (i%2)==0) raw2[n] =255;
    //create the top bottom plate;

    for(L=1; L<9; L++)
    {
      if((i-LXC[L])*(i-LXC[L])+(j-LYC[L])*(j-LYC[L])+(k-LZC[L])*(k-ZC[L])<R2*R2 )
raw2[n]=255;
    }
    n++;
  }

  }
  }

  printf("n=%d,  LX*LY*LZ=%d \n", n, LX*LY*LZ);
  fwrite( raw2, 1, size2, fd2);
  fclose(fd2);
} /* void main( ) */
```

The created 100x100x150 is domain looks like the following figure:



When use the LB3D to do simulation, for the case of wetting displacing non_wetting fluid, the main parameters in the params.in should be:

```
LX                       100
LY                       100
LZ                       150
NumFrames                6
FrameRate                2000
tau[0]                   1.0
tau[1]                   1.0
rhow                     4.0
rho_A                    8.0
rho_B                    0.16
GZL                       0
PressureBC                1
AllBoundaryPeriodic       0
rho_in                   8.02
rho_out                  7.98
big_V0                   .30
big_V0_solid[0]          -0.15  //contact angle =0, wetting displacing
big_V0_solid[1]          0.15   // non-wetting
initial_condition        2
cut                      0.9
cut2                     -10000.  //any negative value is ok.
```

```
x1                      0
x2                      100
y1                      0
y2                      100
z1                      130
z2                      150
```

If we simulate the case of non-wetting displacing wetting fluid, some parameters in the params.in should be, here the fluid 0 is the non-wetting fluid.

```
big_V0                  .30
big_V0_solid[0]         0.15  //contact angle =0, non-wetting displacing
big_V0_solid[1]         -0.15   // wetting
```

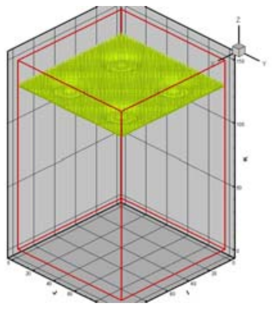
When simulate the nonwetting fluid displacing the wetting fluid or in versa, the contact angle of fluid 0 can be determined by cos(theda)=(G_ads2- G_ads1)/G_c, then “the initial Condition ==2”, and the top area of the domain MUST be initialized as the fluid 0, if the fluid 0 on the top is displacing the fluid 1 under the top area.
The rho_in and rho_out should be set.

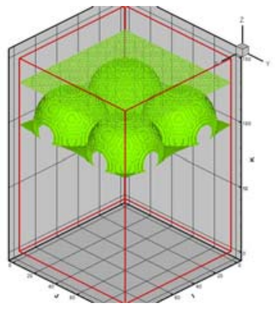
The top area should be initialized as the fluid 0, because in the code:

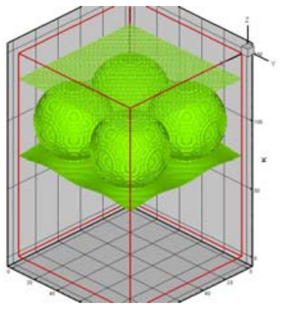
```
#if (SPONGE==0)

        if(subs==0)
        {
                hua   = (lattice->param.rho_in -lattice->param.rho_A[0])/(5000.);
                rho_in =  lattice->param.rho_A[0] + hua *(double)lattice->time;//
                if( lattice->time >5000)  {rho_in = lattice->param.rho_in;}
              }
        if(subs==1) rho_in = 0.001 ;    //lattice->param.uz_in; subs= 1 Wetting
#else
        if(subs==0)
        {
                 rho_in = lattice->param.rho_in;
              }
        if(subs==1) rho_in = lattice->param.rho_A[subs] ;    //lattice->param.uz_in; subs=
1 Wetting
//lattice->param.rho_A[subs]
#endif
```

Notice: The SPONGE should be set as 0.

The wetting fluid displacing non-wetting fluid simulation results are illustrated in the following figure:


2,000steps


4,000 steps,


6,000 steps

5.3. Relative permeability for non-wetting and wetting fluids

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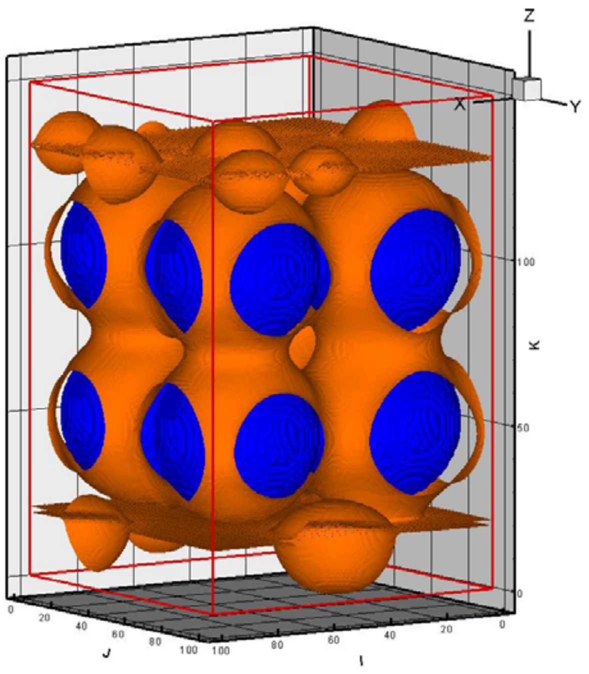
When we simulate the two-phase flow in porous media and measure the relative permeability that depend on fluid saturation, we should set SPONGE==1 and initial condition ==1 (Randomly distributed in an area), z<z1, and z>z2 will be re-initialized as fluid 0 after the initial condition==1 performed.

Notice: SPONGE==1

The input file of this case is :
```
LX                     100
LY                     100
LZ                     150
NumFrames              6
FrameRate              2000
tau[0]                 1.0
tau[1]                 1.0
rhow                   4.0
rho_A                  8.0
rho_B                  0.16
GZL                     0
PressureBC              1
AllBoundaryPeriodic     0
rho_in                 8.02
rho_out                7.98
big_V0                 .30
big_V0_solid[0]        0.15
big_V0_solid[1]        -0.15   //fluid 0 is non-wetting
initial_condition      1
cut                    0.9
cut2                   -10000.  //any negative value is ok.
x1                     0
x2                     100
y1                     0
```

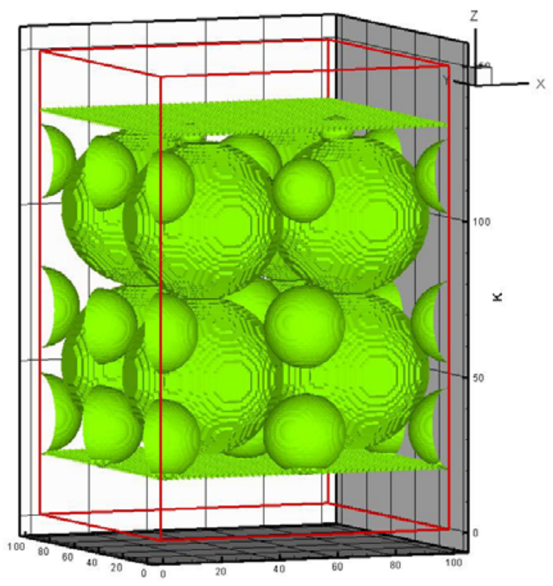
```
y2                      100
z1                      30
z2                      120
```

In this case the fluid 0 is the non-wetting fluid, the domain between z=30 and z=120 is randomly initialized as the fluid 0 occupied 90% volume. Since the SPONGE==1, domain of z<30 and z>120 will be initialized as fluid 0. The 3D isosurfaces of contour rho= 6 may looks like the following Figure, the wetting fluid was attach to the solid wall.



If the fluid 0 is the wetting fluid, the result of 3D isosurfaces of contour rho= 6 may looks like the following, we can see that the some non-wetting bubbles stuck in between the area of the 4 sphere and space between the plates and balls.

```
big_V0_solid[0]         -0.15
big_V0_solid[1]         0.15   //fluid 0 is non-wetting
```



Reference

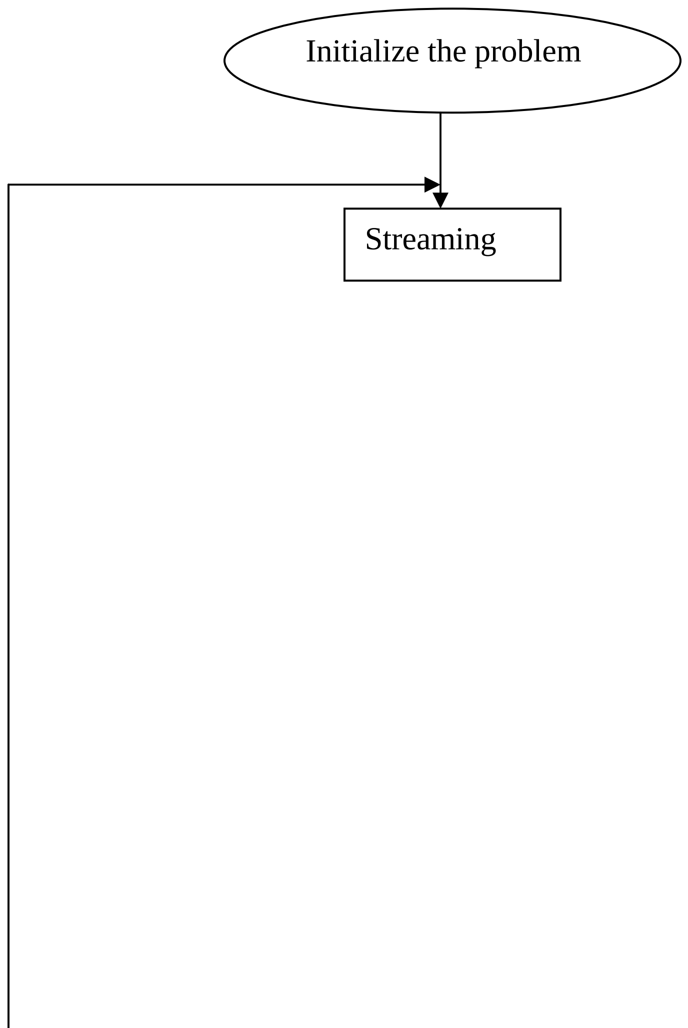
Sukop, M.C. and D.T. Thorne, Jr., 2006. Lattice Boltzmann Modeling: An introduction for geoscientists and engineers. Springer, Heidelberg, Berlin, New York.

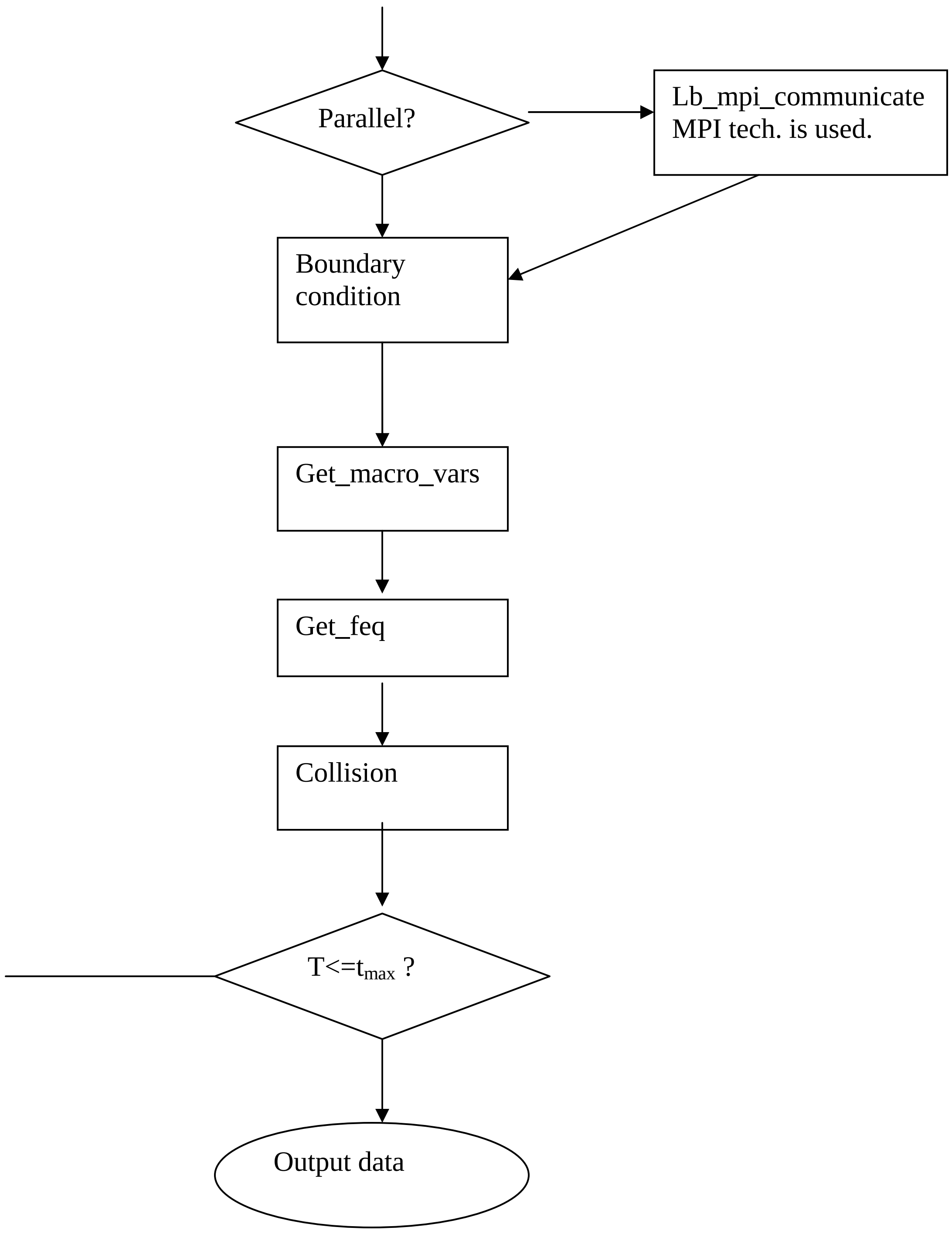
Haibo Huang, Marcel Schaap, Jr. Thorne Daniel T., Michael C. Sukop，
Proposed approximation for contact angles in Shan-and-Chen-type multi-component multiphase lattice Boltzmann models， Physical Review E, in press

Paper1: Michael C. Sukop, Haibo Huang, Chen Luh Lin, Milind D. Deo, Kyeongseok Oh, and Jan D. Miller, Validation of Lattice Boltzmann Modeling of Multiphase Fluids in Porous Media with Micro-X-ray Tomography Data, 2007

Paper2: Michael C. Sukop, Haibo Huang, Pedro F. Alvarez, Kevin J. Cunningham, and Christian D. Langevin, Investigating Non-Darcy Flow in Highly Porous Aquifer Materials with Lattice Boltzmann Methods

Paper3: ANALYTICAL AND LATTICE BOLTZMANN PREDICTIONS OF SATURATED PERMEABILITY FOR RANDOMIZED MENGER SPONGES


Initialize the problem
Streaming


Parallel?
Lb_mpi_communicate MPI tech. is used.
Boundary condition
Get_macro_vars
Get_feq
Collision
T<=t_max ?
Output data