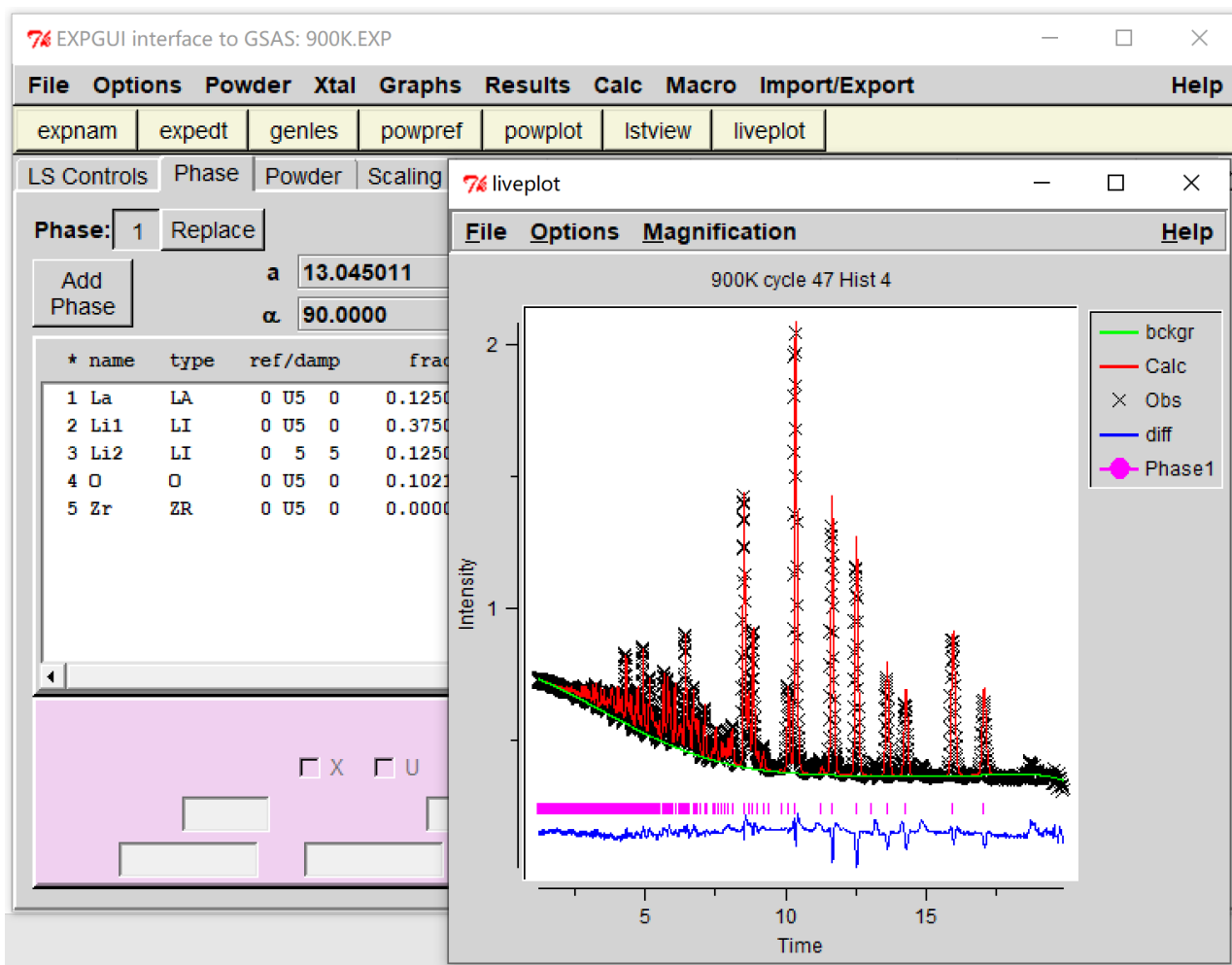


RMCPProfile使用流程

准备NPDF数据文件

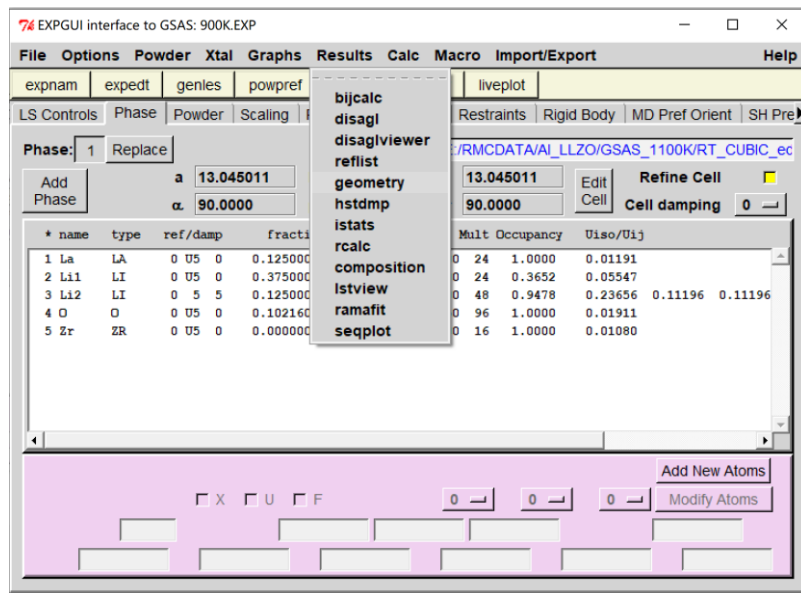
```
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZ0_RMC6_template/LLZ0_RMC6_900K.orig$ cp ../../Dove/PDF/GEM87467.mint01 .
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZ0_RMC6_template/LLZ0_RMC6_900K.orig$ cp ../../Dove/PDF/GEM87467.mdor01 .
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZ0_RMC6_template/LLZ0_RMC6_900K.orig$ ls
GEM87467.mdor01  GEM87467.mint01
```

准备GSAS数据文件



准备GSAS-LST文件

- Result=>hstdmp
- 向LST文件中写入histogram



```
C:\WINDOWS\system32\cmd.exe - C:/Users/blues/OneDrive/tianhl/usr/GSAS/expgui/gsastcl.bat C:\Users\blues\OneDrive\tianhl\usr\GSAS...

C:\Users\blues\Desktop\Dove\gsas\900k>REM a batch file to a DOS command and pause

C:\Users\blues\Desktop\Dove\gsas\900k>if "C:\Users\blues\OneDrive\tianhl\usr\GSAS" == "" set gsas=c:\gsas

C:\Users\blues\Desktop\Dove\gsas\900k>set PGPLOT_FONT=C:\Users\blues\OneDrive\tianhl\usr\GSAS\pgl\grfont.dat

C:\Users\blues\Desktop\Dove\gsas\900k>set SYMOP=C:\Users\blues\OneDrive\tianhl\usr\GSAS\data\symop.dat

C:\Users\blues\Desktop\Dove\gsas\900k>C:\Users\blues\OneDrive\tianhl\usr\GSAS\exe\hstdmp.exe 900K

Program HSTDMP Version Win32
Program for listing contents of the .Pnn files
Distributed on Fri Apr 18 16:12:00 2014

Allen C. Larson and Robert B. Von Dreele
Manuel Lujan, Jr. Neutron Scattering Center, MS-H805
Los Alamos National Laboratory, Los Alamos, NM 87545

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Select an output option (L,0,<?>)? >1
Give number of the histogram to be dumped >3
Give number of the next histogram to be dumped (0 to exit) >4
Give number of the next histogram to be dumped (0 to exit) >5
Give number of the next histogram to be dumped (0 to exit) >0
```

```
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZO_RMC6_template/LLZO_RMC6_900K.orig$ cp ../../Dove/gsas/900k/900K.LST LLZO_RMC6_900K.LST
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZO_RMC6_template/LLZO_RMC6_900K.orig$ ls
GEM87467.mdor01  GEM87467.mint01  LLZO_RMC6_900K.LST
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZO_RMC6_template/LLZO_RMC6_900K.orig$
```

准备GSAS-EXP文件

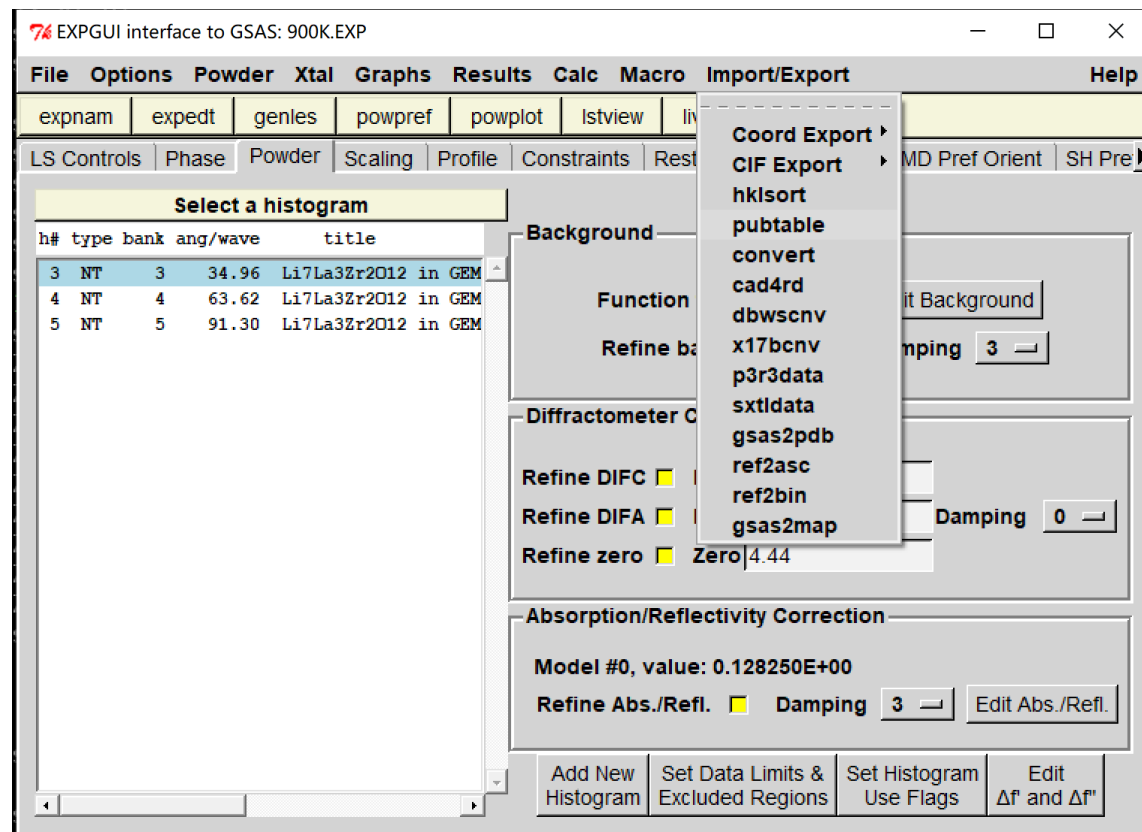
- 拷贝EXP文件

```
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZO_RMC6_template/LLZO_RMC6_900K.orig$ cp ../../Dove/gsas/900k/900K.EXP LLZO_RMC6_900K.EXP
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZO_RMC6_template/LLZO_RMC6_900K.orig$ ls
GEM87467.mdor01  GEM87467.mint01  LLZO_RMC6_900K.EXP  LLZO_RMC6_900K.LST
```

准备GSAS-TBL文件

- Import/export=>pubtable

```
C:\WINDOWS\system32\cmd.exe - C:/Users/blues/OneDrive/tianhl/usr/GSAS/expgui/gsastcl.bat C:\Users\blues\OneDrive\tianhl\usr\GSAS...  
C:\Users\blues\Desktop\Dove\gsas\900k>REM a batch file to a DOS command and pause  
C:\Users\blues\Desktop\Dove\gsas\900k>if "C:\Users\blues\OneDrive\tianhl\usr\GSAS" == "" set gsas=c:\gsas  
C:\Users\blues\Desktop\Dove\gsas\900k>set PGPLOT_FONT=C:\Users\blues\OneDrive\tianhl\usr\GSAS\pgl\grfont.dat  
C:\Users\blues\Desktop\Dove\gsas\900k>set SYMOP=C:\Users\blues\OneDrive\tianhl\usr\GSAS\data\symop.dat  
C:\Users\blues\Desktop\Dove\gsas\900k>C:\Users\blues\OneDrive\tianhl\usr\GSAS\exe\pubtable.exe 900K  
  
Program PUBTABLES Version Win32  
Generate crystal structure data tables  
Distributed on Fri Apr 18 16:12:00 2014  
  
Allen C. Larson and Robert B. Von Dreele  
Manuel Lujan, Jr. Neutron Scattering Center, MS-H805  
Los Alamos National Laboratory, Los Alamos, NM 87545  
  
Copyright, 2000, The Regents of the University of California.  
  
The tables will be written to 900K.TBL  
STOP PUBTABLES successful completion statement executed  
C:\Users\blues\Desktop\Dove\gsas\900k>pause  
请按任意键继续. . .
```



```
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZO_RMC6_template/LLZO_RMC6_900K.orig$ cp ../../Dove/gsas/900k/900K.TBL LLZO_RMC6_900K.TBL  
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZO_RMC6_template/LLZO_RMC6_900K.orig$ ls  
GEM87467.mdor01 GEM87467.mint01 LLZO_RMC6_900K.EXP LLZO_RMC6_900K.LST LLZO_RMC6_900K.TBL
```

修改TBL文件，产生rmc6f文件

- 把占位比Fraction都改为1.0000
- 执行data2config，产生rmc6f的配置文件

```
The equivalent positions are:
( 1)   X       Y       Z ( 2)   Z       X       Y ( 3)   Y       Z       X
( 4) 1/2+X     Y 1/2-Z ( 5) 1/2-Z     1/2+X     Y ( 6)   Y 1/2-Z 1/2+X
( 7)   -Z 1/2+X 1/2-Y ( 8) 1/2-Y     -Z 1/2+X ( 9) 1/2+Y 1/2-Z  -X
(10)   -X 1/2+Y 1/2-Z (11) 1/2-Z     -X 1/2+Y (12) 1/2+X 1/2-Y  -Z
(13) 1/4+Y 1/4+X 1/4+Z (14) 1/4+Z     1/4+Y 1/4+X (15) 1/4+X 1/4+Z 1/4+Y
(16) 3/4+Y 1/4+X 1/4-Z (17) 1/4-Z     3/4+Y 1/4+X (18) 1/4+X 1/4-Z 3/4+Y
(19) 3/4-Z 3/4+Y 1/4-X (20) 1/4-X     3/4-Z 3/4+Y (21) 3/4+X 1/4-Z 3/4-Y
(22) 3/4-Y 3/4+X 1/4-Z (23) 1/4-Z     3/4-Y 3/4+X (24) 3/4+Y 1/4-X 3/4-Z

Lattice constants are
a = 13.04501(10) b = A c = A
Alpha = 90 Beta = 90 Gamma = 90
Cell volume = 2219.899(28)

Name      X      Y      Z      Ui/Ui+100  Site sym Mult Type Seq Fractn
La        0.125000  0.000000  0.250000  1.191(24)  222(100) 24  LA  1 1.0000
Li1       0.375000  0.000000  0.250000  5.5(6)     -4(100) 24  LI  2 1.0000
Li2       0.125000  0.187500  0.437500  15.35*     2(011) 48  LI  3 1.0000
O         0.102160  0.197170  0.281250  1.911(23)  1       96  O   4 1.0000
Zr        0.000000  0.000000  0.000000  1.079(32)  -3(111) 16  ZR  5 1.0000
CUBIC_900K
PUBTABLE Version Win32 Jul 25 15:29:19 2019 Page 2
```

```
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZO_RMC6_template/LLZO_RMC6_900K.orig$ data2config -rmc6f -supercell [4 4 4] LLZO_RMC6_900K.TBL
Request for metadata for configuration
Blank replies are acceptable (if foolish); they just cancel the request
... Name of material: LLZO
... Name of configuration owner: tianhl
... Source of structure: LLZO
... Additional notes: 900K
Job done by data2config. Enjoy your RMC journey!
```

数据文件整理

- 由于rmcprofile只能处理一个bank的文件，所以要选择bank
- Rmcprofile只能读四行inst文件，所以要删除一行

```
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZ0_RMC6_template/LLZ0_RMC6_900K.orig$ cp LLZ0_RMC6_900K_4.back LLZ0_RMC6_900K.back
k
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZ0_RMC6_template/LLZ0_RMC6_900K.orig$ cp LLZ0_RMC6_900K_4.bragg LLZ0_RMC6_900K.bragg
agg
tianhl@tianhl-surface4:/mnt/c/Users/blues/Desktop/LLZ0_RMC6_template/LLZ0_RMC6_900K.orig$ ls
GEM87467.mdor01      LLZ0_RMC6_900K_3.bragg  LLZ0_RMC6_900K_5.back  LLZ0_RMC6_900K.bragg  LLZ0_RMC6_900K.LST
GEM87467.mint01      LLZ0_RMC6_900K_4.back  LLZ0_RMC6_900K_5.bragg  LLZ0_RMC6_900K.EXP   LLZ0_RMC6_900K.rmc6f
LLZ0_RMC6_900K_3.back LLZ0_RMC6_900K_4.bragg LLZ0_RMC6_900K.back    LLZ0_RMC6_900K.inst  LLZ0_RMC6_900K.TBL
```

```
3
3
2802.8200000000002      0.9899999999999999      4.4400000000000004      34.960000000000001
0.000000E+00  0.200000E+00  0.312302E+02  0.567270E+02
0.000000E+00  0.303210E+03  0.469337E+01
0.000000E+00  0.598124E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.128250E+00
4
4891.4700000000003      -2.0099999999999998      -1.8000000000000000      63.619999999999997
0.000000E+00  0.200000E+00  0.312302E+02  0.567270E+02
0.000000E+00  0.199267E+03  0.621466E+01
0.000000E+00  0.440716E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.100340E+00
5
6677.8000000000002      -4.0300000000000002      -2.0699999999999998      91.370000000000005
0.000000E+00  0.200000E+00  0.312302E+02  0.567270E+02
0.000000E+00  0.939882E+02  0.595873E+00
0.000000E+00  0.301958E+01  0.000000E+00  0.000000E+00  0.000000E+00
0.701146E-01
```


运行文件

- 拷贝一个dat运行文件，做一些修改
- 执行rmcprofile LLZO_RMC6_900K 前缀要一致

查看运行结果

- 执行rmcplot LLZO_RMC6_900K
- 点击5, 查看Bragg精修结果
- 点击3, 点击1, 查看PDF拟合结果

