CECAM Flagship School, October 2, 2023

First steps with SIESTA: from zero to hero

Analysis I: plotting data on grid

Miguel Pruneda

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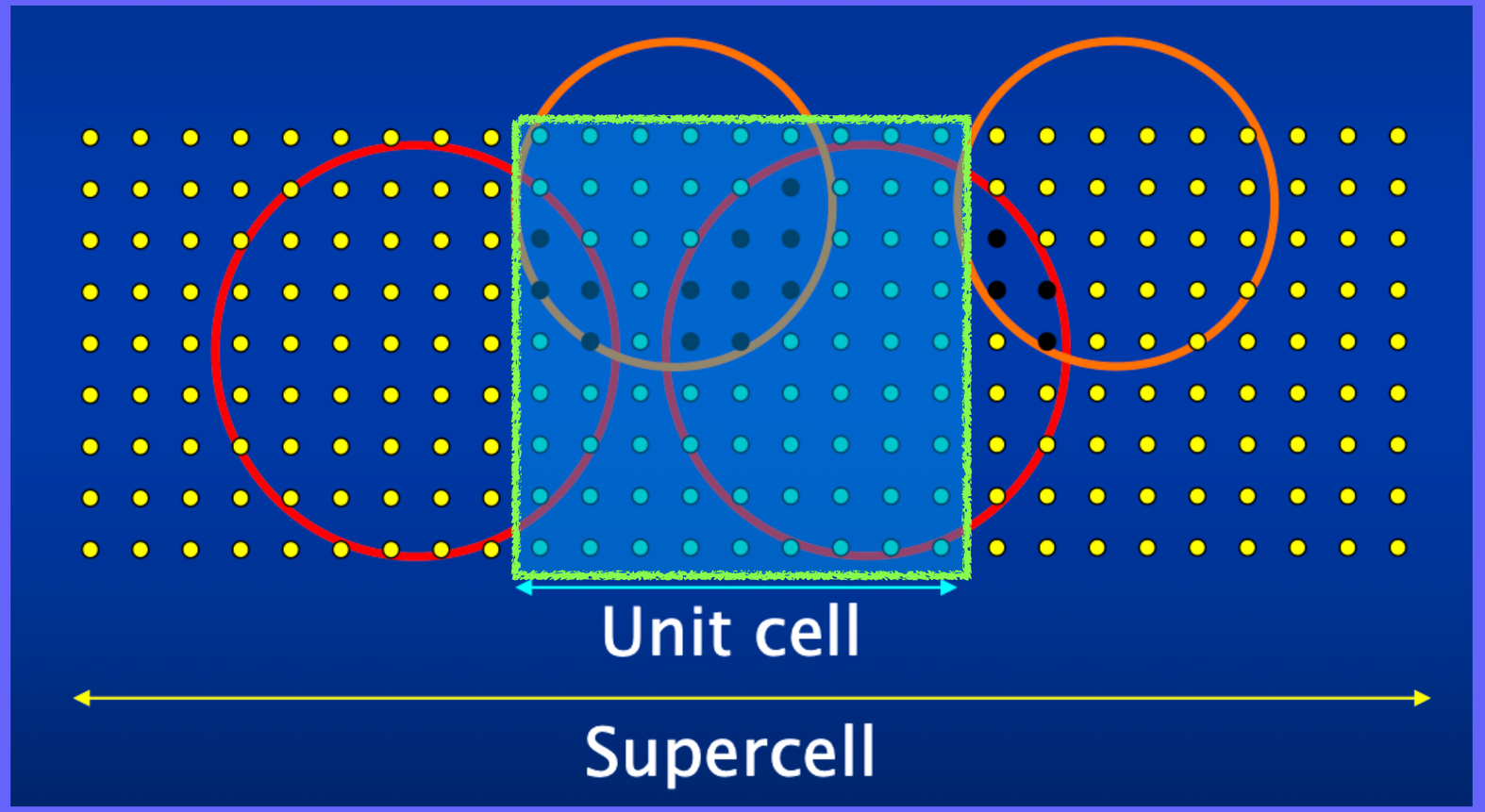
Charge densities and potentials on grid

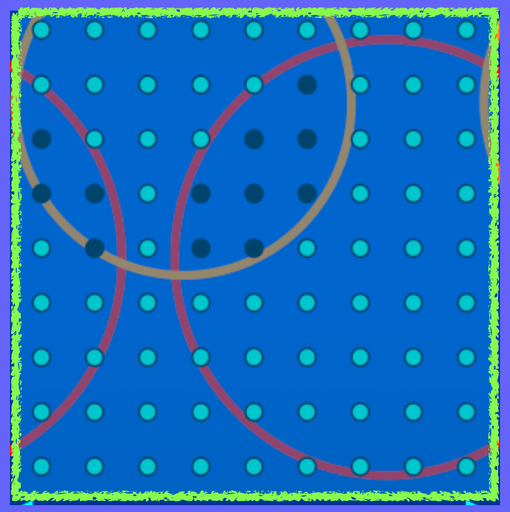


$N_1 \times N_2 \times N_3$ mesh points... $F(i,j,k) \longrightarrow F(n)$

Charge densities and potentials on grid

Possible F(n)?

- RHO $\rho(r) = \sum_{\mu,\nu} \rho_{\mu\nu}\phi_\mu(r)\phi_\nu(r)$
- DRHO $\delta\rho(r) = \rho_{SCF}(r) - \rho_{atom}(r)$
- VT $V_{SCF}(r)$
- VH $\delta V_H(r)$



- SaveRho
- SaveDeltaRho
- SaveTotalPotential
- SaveElectrostaticPotential

$N_1 \times N_2 \times N_3$ mesh points... F(i,j,k) $\longrightarrow$ F(n)

Charge densities and potentials on grid

Possible F(n)?

- LDOS $n(\epsilon, r) = \sum_n |\psi_n(r)|^2 \delta(\epsilon - \epsilon_n)$

$$LDOS(r) = \int_{\epsilon_1}^{\epsilon_2} n(\epsilon, r)$$

```
%block LocalDensityOfStates
   EF  -3.50   0.00  eV
%endblock LocalDensityOfStates
```

- Wavefunctions $|\psi_n(r)|^2$ $\psi_n(r)$ Real, Imag, Mod, Phase

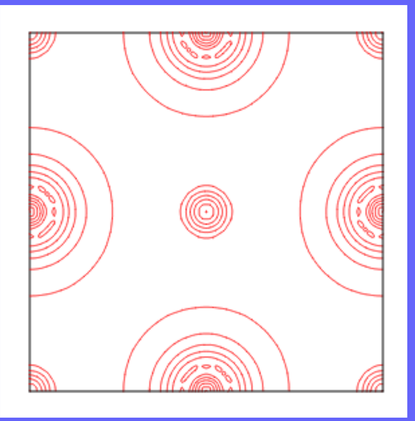
$N_1 \times N_2 \times N_3$ mesh points... F(i,j,k) $\longrightarrow$ F(n)

Charge densities and potentials on grid

Utils that might be useful

- Util/Grid/
  - grid2cdf, cdf2grid
  - cdf2xsf
  - cdf_diff
  - cdf_laplacian
  - grid2val
  - grid2cube
  - grid_rotate

- Util/Contour
  - grid1d (?)
  - grid2d



- Util/Plrho

- Util/Denchar/

https://docs.siesta-project.org/projects/siesta/en/school-2021/reference/denchar.html#reference-denchar

- SISL (wait until Thursday!)

Charge densities and potentials on grid

Utils that might be useful

- `Util/Contrib/FElMellouhi`
  - `Conversion to openDX format`
- `Util/Contrib/APostnikov`
  - `rho2xsf`
  - `(+ eig2bxsf + vib2xsf + etc)`

Visualisation GUI tools

XCrySDen

X-window CRYstalline Structures and DENsities

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XCrySDen

XCrySDen is a **crystalline and molecular structure visualisation program** aiming at display of isosurfaces and contours, which can be superimposed on crystalline structures and interactively rotated and manipulated. It runs on GNU/Linux.

XCrySDen has been also ported to Mac OS (requires X11) and Windows (requires either CYGWIN or WSL).

The name of the program stands for *Crystalline Structures and Densities* and *X* because it runs under the X-Window environment.

Read more... | See screenshots ...

Latest version: 1.6.2

XCrySDen mailing list

XCrySDen mailing list is an open mailing list where XCrySDen related issues can be discussed among users.

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VESTA

Visualization for Electronic and STructural Analysis

Software > VESTA

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Chibaite
Kinichilite
Topaz

1. Introduction

VESTA is a 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies. Some of the novel features of VESTA are listed below.

- Deal with multiple structural models, volumetric data, and crystal morphologies in the same window.
- Support multiple tabs corresponding to files.
- Support multiple windows with more than two tabs in the same process.
- Deal with virtually unlimited number of objects such as atoms, bonds polyhedra, and polygons on isosurfaces (theoretical limit on 32bit operating system is 1,073,741,823)
- Support lattice transformation from conventional to non-conventional lattice by using matrix. The transformation matrix is also used to create superlattice and sublattice.
- Visualize interatomic distances and bond angles that are restrained in Rietveld analysis with RIETAN-FP.
- Transparent isosurfaces can be overlap with structural models.

The GDIS Home Page

GDIS
Modelling Interface

Snapshot 1
Snapshot 2
Snapshot 3
Snapshot 4
Download

Author:
Sean Fleming

Introduction

GDIS is a GTK based program for the display and manipulation of isolated molecules and periodic systems. It is in development, but is nonetheless fairly functional. It has the following features:

- Support for several file types (CIF, BIOSYM, XYZ, XTL, MARVIN, and GULP)
- OpenGL rendering (requires gtkglarea)
- Assorted tools for visualization (measurements, ribbons, polyhedral display)
- Useful manipulation tools, including matrix transformations and periodic image display.
- Powerful surface generation and crystal morphology tools.
- Animation of BIOSYM and GULP trajectory files

GDIS also allows you to perform the following functions through other packages:

- Model rendering (courtesy of POVRay)
- Energy minimization (courtesy of GULP)
- Morphology calculation (courtesy of cdd)
- Space group processing (courtesy of SeInfo)
- View the Periodic Table (courtesy of GPeriodic)
- Load additional filetypes, such as PDB (courtesy of Babel)

Although developed on a RedHat Linux platform, GDIS has been successfully compiled under IRIX, Solaris, OpenBSD, and OS-X. I've even built a Window's executable using the mingw32 cross-compiler!

The source code is released under the GPL.

Molekel

Molecular visualization

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OpenBabel

Citing

Molekel

Molekel is an open-source multi-platform molecular visualization program.

(citation info)

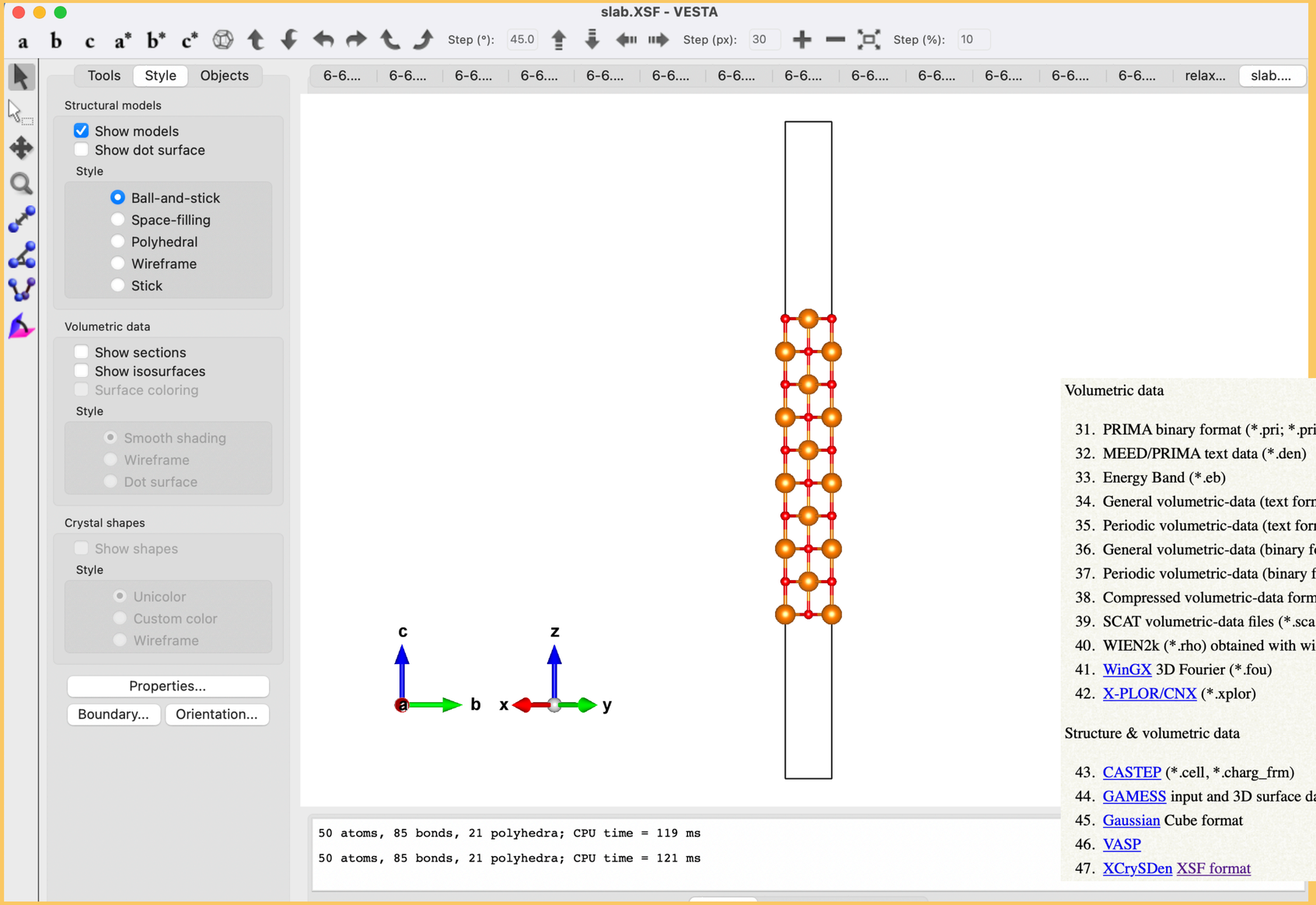
Some of the features available in the new version are:

- Multiplatform: Mac OS X, Windows, Linux
- Different methods to speed-up rendering of molecules with support for billboards and view-dependent level of detail techniques
- Programmable shaders; standard shaders to enhance rendering quality, outline contours and perform sketch-like renderings are provided
- Visualization of residues (ribbon or schematic)

Click on image to enlarge

Grid visualisation with VESTA

https://jp-minerals.org/vesta/en/



Volumetric data

31. PRIMA binary format (*.pri; *.prim)
32. MEED/PRIMA text data (*.den)
33. Energy Band (*.eb)
34. General volumetric-data (text format) (*.?ed)
35. Periodic volumetric-data (text format) (*.grd)
36. General volumetric-data (binary format) (*.ggrid)
37. Periodic volumetric-data (binary format) (*.pgrid)
38. Compressed volumetric-data format (*.m3d)
39. SCAT volumetric-data files (*.sca, *.scat)
40. WIEN2k (*.rho) obtained with wien2venus.py
41. WinGX 3D Fourier (*.fou)
42. X-PLOR/CNX (*.xplor)

Structure & volumetric data

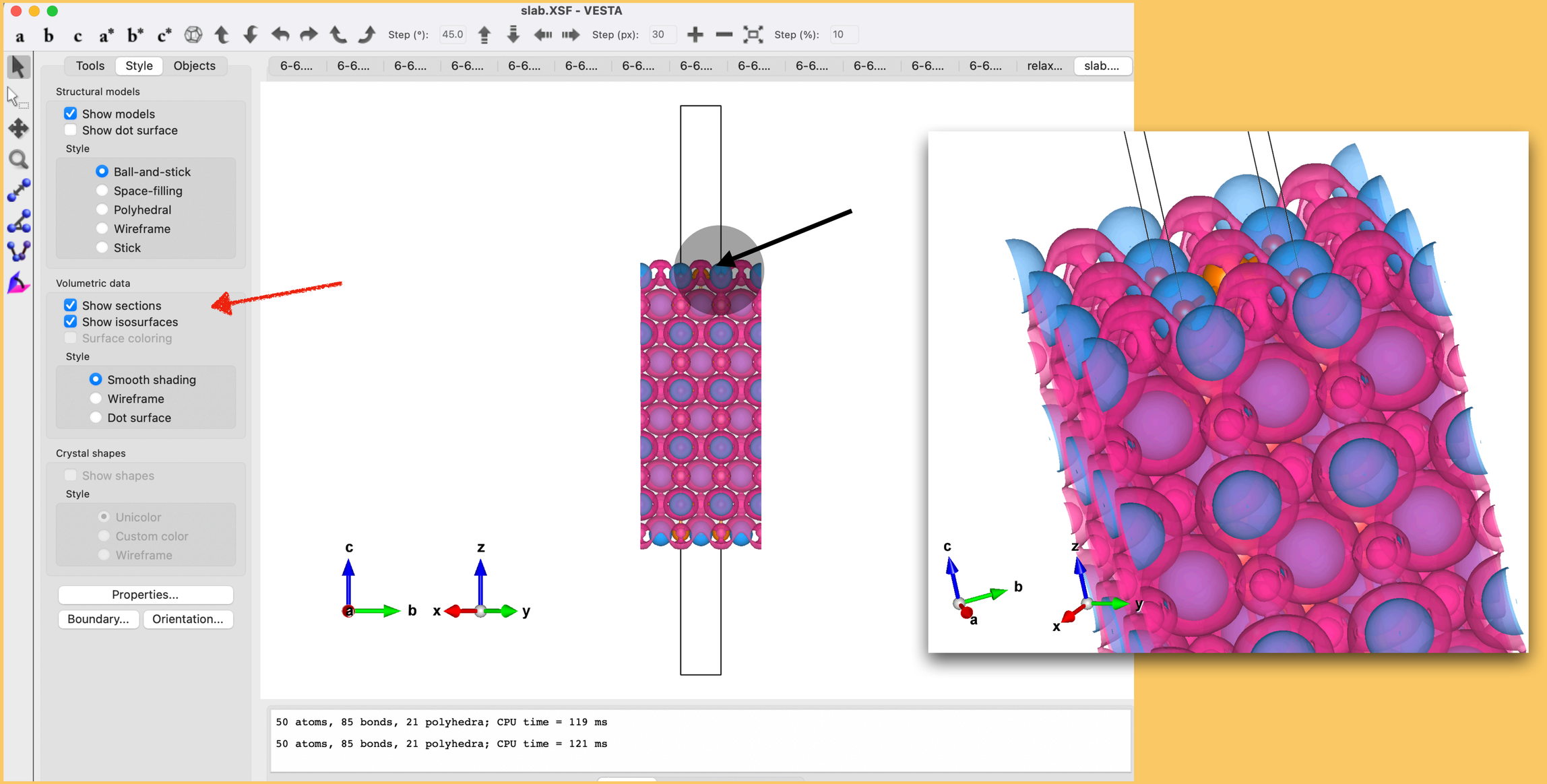
43. CASTEP (*.cell, *.charg_frm)
44. GAMESS input and 3D surface data files output by MacMolPlt
45. Gaussian Cube format
46. VASP
47. XCrySDen XSF format

Input

Structure data

1. VESTA format (*.vesta)
2. VICS format (*.vcs)
3. American Mineralogist Crystal Structure Database (*.amc)
4. asse (*.asse)
5. Chem3D
6. CIF (Crystallographic Information File)
7. CrystalMaker text file (*.cmt)
8. CSSR (Crystal Structure Search and Retrieval)
9. CSD/FDAT
10. DL_POLY CONFIG
11. FEFF input file (feff.inp)
12. FHI-AIMS input file (*.in)
13. GEOMETRY.OUT output by the Elk FP-LAPW Code
14. GSAS format (*.EXP)
15. ICSD (Inorganic Crystal Structure Database)
16. ICSD-CRYSTIN
17. MDL Molfile
18. MINCRYST (Crystallographic Database for Minerals)
19. MOLDA
20. PDB (Protein Data Bank)
21. Input file of RIETAN-FP (*.ins)
22. Output file of RIETAN-FP (*.lst)
23. Input file of SHELXL (*.ins, *.res)
24. Output files of STRUCTURE TIDY (*.sto)
25. Structure data files output by USPEX.
26. WIEN2k (*.struct)
27. XMol XYZ (*.xyz)
28. F01 for SCAT and C04D for contrd
29. MXDORTO/MXDTRICL FILE06.DAT, FILE07.DAT
30. XTL file (*.xtl)

Grid visualisation with VESTA



Grid visualisation with Xcrysden

http://www.xcrysden.org/

Terms of use

XCrySDen is released under the GNU General Public License.

Whenever graphics generated by ***XCrySDen*** are used in scientific publications, it shall be greatly appreciated to include an explicit reference. The preferred form is the following:

[ref] A. Kokalj, *J. Mol. Graphics Modelling*, **1999**, *17*, 176--179. Code available from http://www.xcrysden.org/.

XCrySDen reference

XCrySDen has been described in the following papers:

- A. Kokalj, Computer graphics and graphical user interfaces as tools in simulations of matter at the atomic scale, *Comp. Mater. Sci.*, **2003**, *28*, 155--168.
- A. Kokalj, XCrySDen--a new program for displaying crystalline structures and electron densities, *J. Mol. Graphics Modelling*, **1999**, *17*, 176--179.
- A. Kokalj and M. Causà, Scientific Visualization in Computational Quantum Chemistry, *Proceedings of High Performance Graphics Systems and Applications European Workshop*, Bologna, Italy, **2000**, 51--54.

Open XSF (XCrySDen Structure File)
Open AXSF (Animation XCrySDen Structure File)
Open BXSF (i.e. Fermi Surface Files)

Open XCrySDen Scripting File

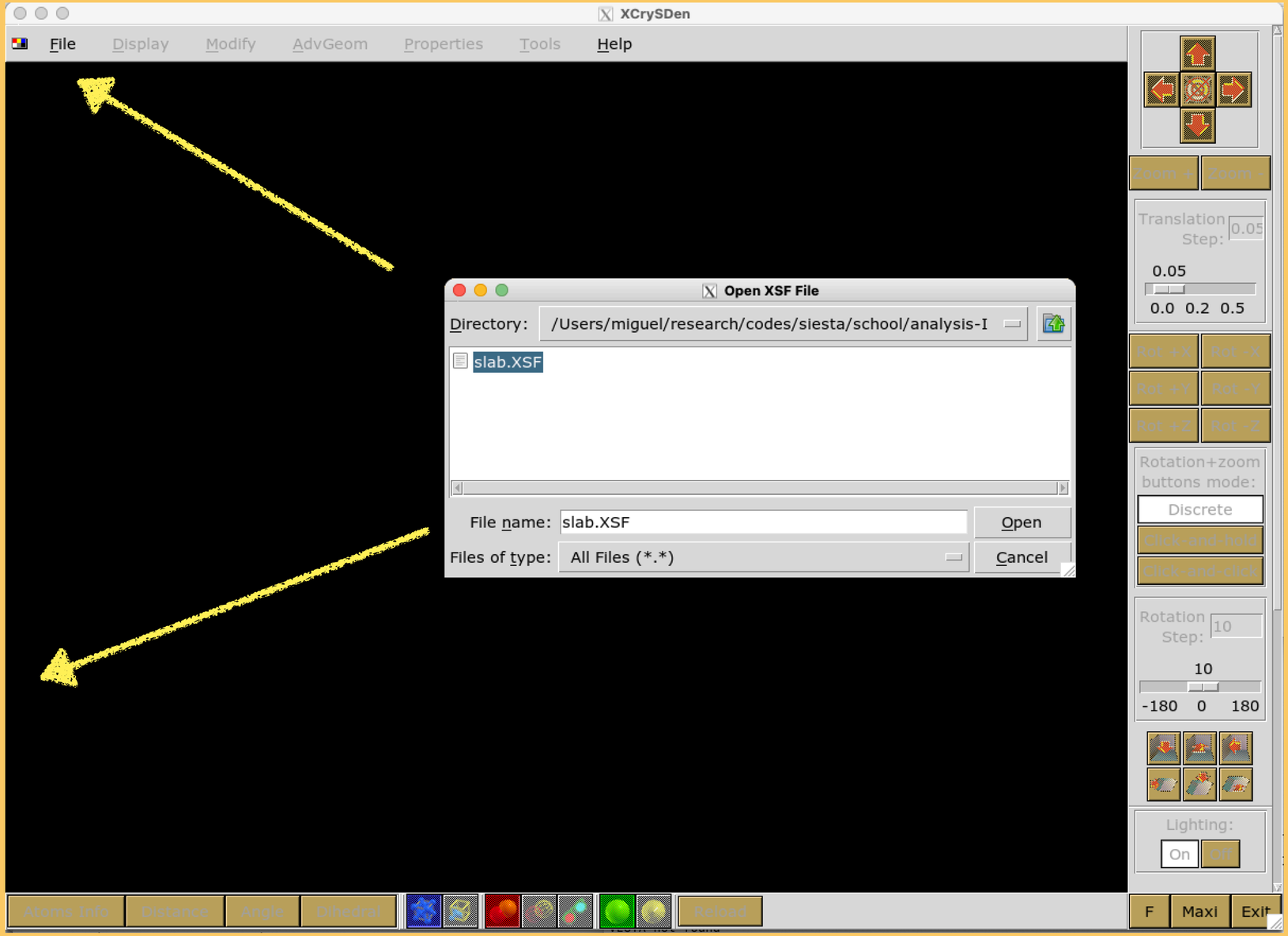
Open XYZ
Open PDB

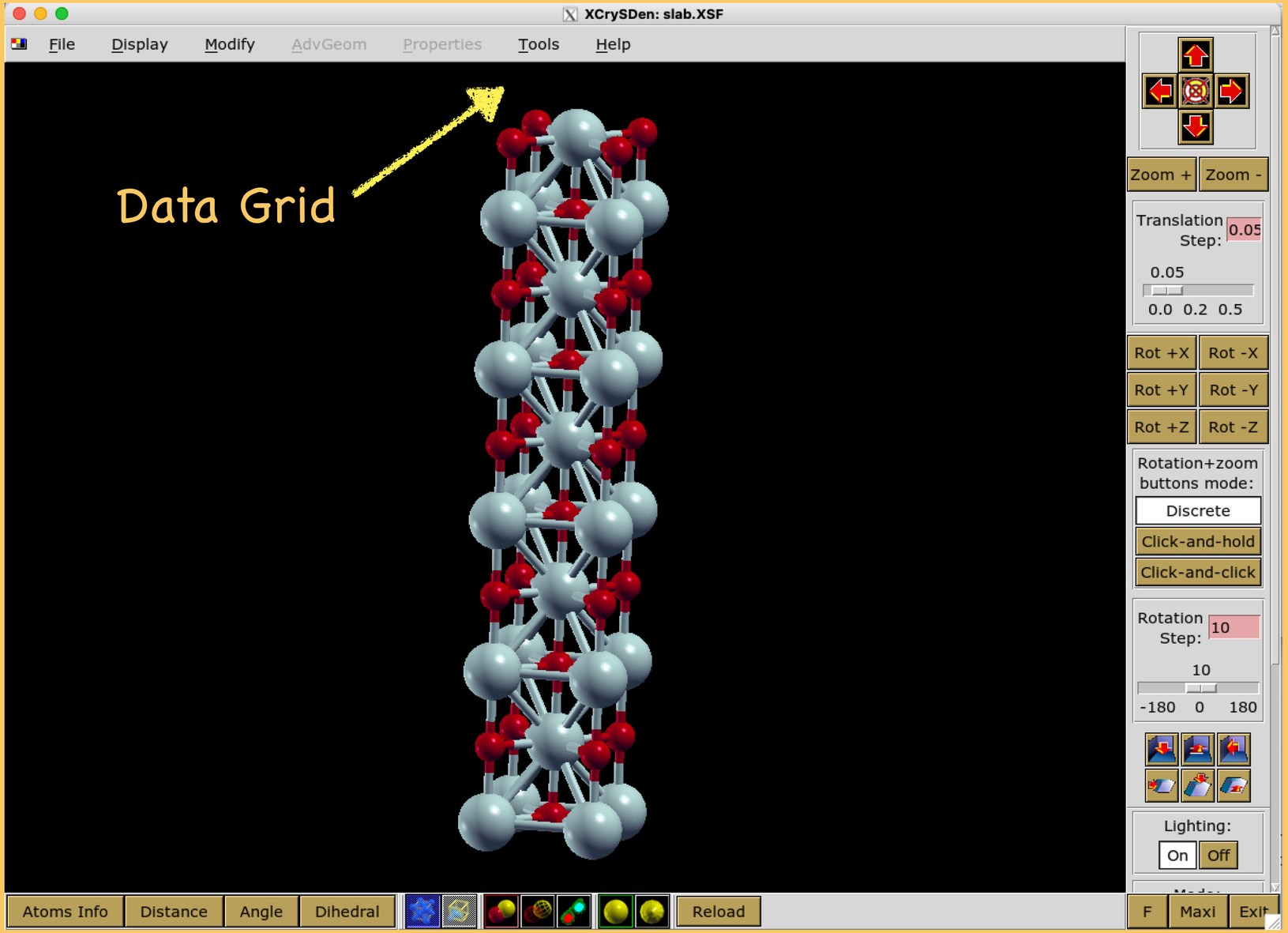
Open Gaussian Z-Matrix File
Open Gaussian Output File
Open Gaussian Cube File

Open Orca Output File

Open PWscf Input File
Open PWscf Output File

Open FHI98MD "inp.ini" File
Open FHI98MD "coord.out" File

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File
Display
Modify
AdvGeom
Properties
Tools
Help
Data Grid
Zoom +
Zoom -
Translation Step:
0.05
0.05
0.0 0.2 0.5
Rot +X
Rot -X
Rot +Y
Rot -Y
Rot +Z
Rot -Z
Rotation+zoom buttons mode:
Discrete
Click-and-hold
Click-and-click
Rotation Step:
10
10
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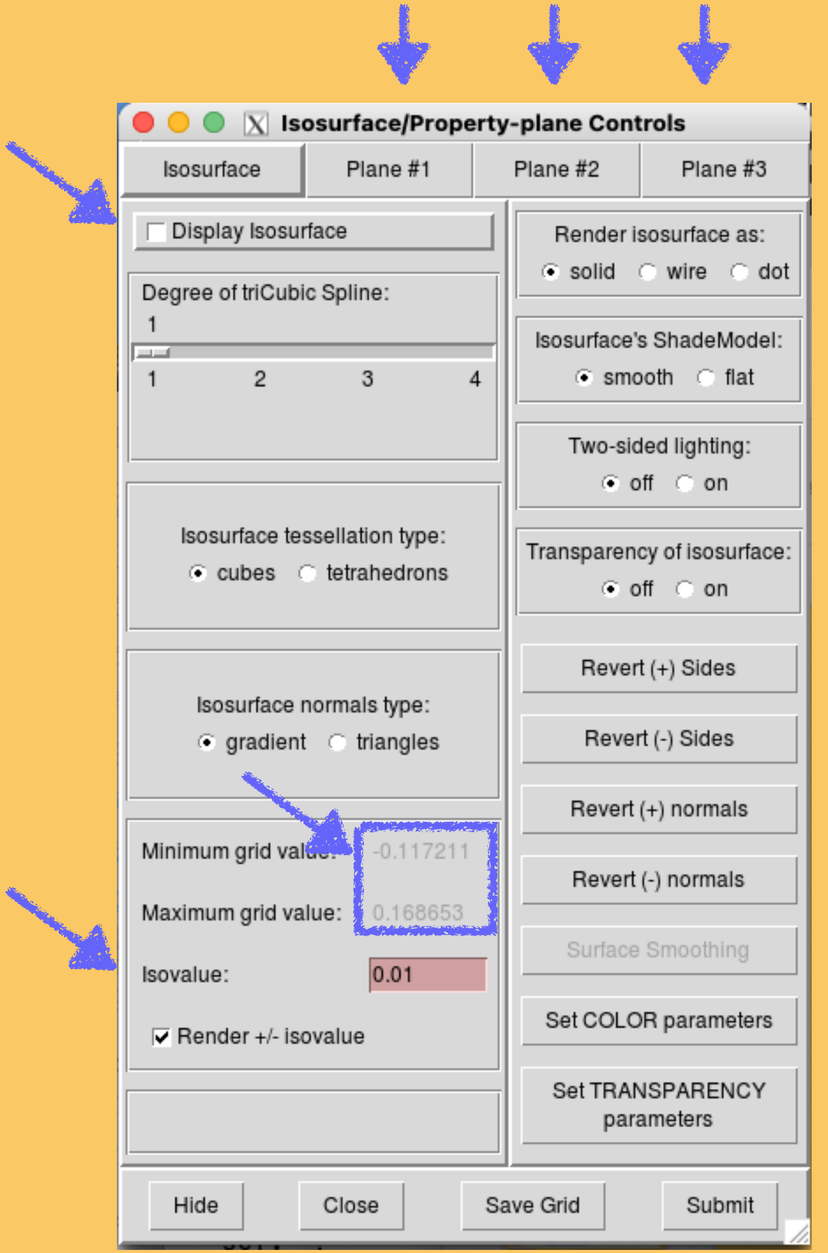
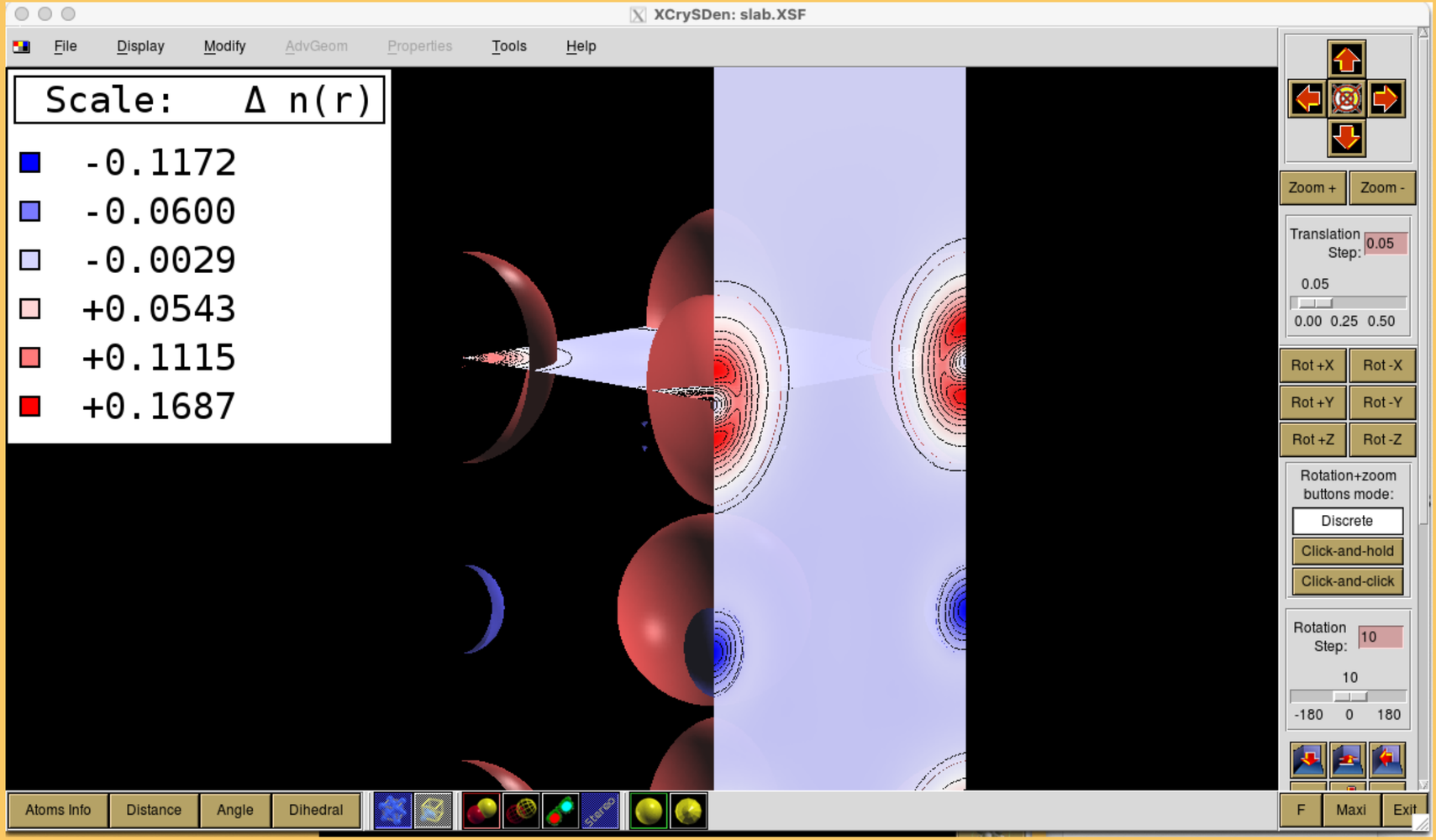
Lighting:
On
Off
Atoms Info
Distance
Angle
Dihedral
Reload
F
Maxi
Exit


Isosurface/Property-plane Controls
Isosurface
Plane #1
Plane #2
Plane #3
Display Isosurface
Degree of triCubic Spline:
1
1 2 3 4
Isosurface tessellation type:
cubes
tetrahedrons
Isosurface normals type:
gradient
triangles
Minimum grid value:
-0.117211
Maximum grid value:
0.168653
Isovalue:
0.01
Render +/- isovalue
Render isosurface as:
solid
wire
dot
Isosurface's ShadeModel:
smooth
flat
Two-sided lighting:
off
on
Transparency of isosurface:
off
on
Revert (+) Sides
Revert (-) Sides
Revert (+) normals
Revert (-) normals
Surface Smoothing
Set COLOR parameters
Set TRANSPARENCY parameters
Hide
Close
Save Grid
Submit


XCrySDen: slab.XSF
File
Display
Modify
AdvGeom
Properties
Tools
Help
Scale: Δ n(r)
-0.1172
-0.0600
-0.0029
+0.0543
+0.1115
+0.1687
Zoom +
Zoom -
Translation Step:
0.05
0.05
0.00 0.25 0.50
Rot +X
Rot -X
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Rot -Y
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Rot -Z
Rotation+zoom buttons mode:
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Click-and-hold
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Rotation Step:
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Atoms Info
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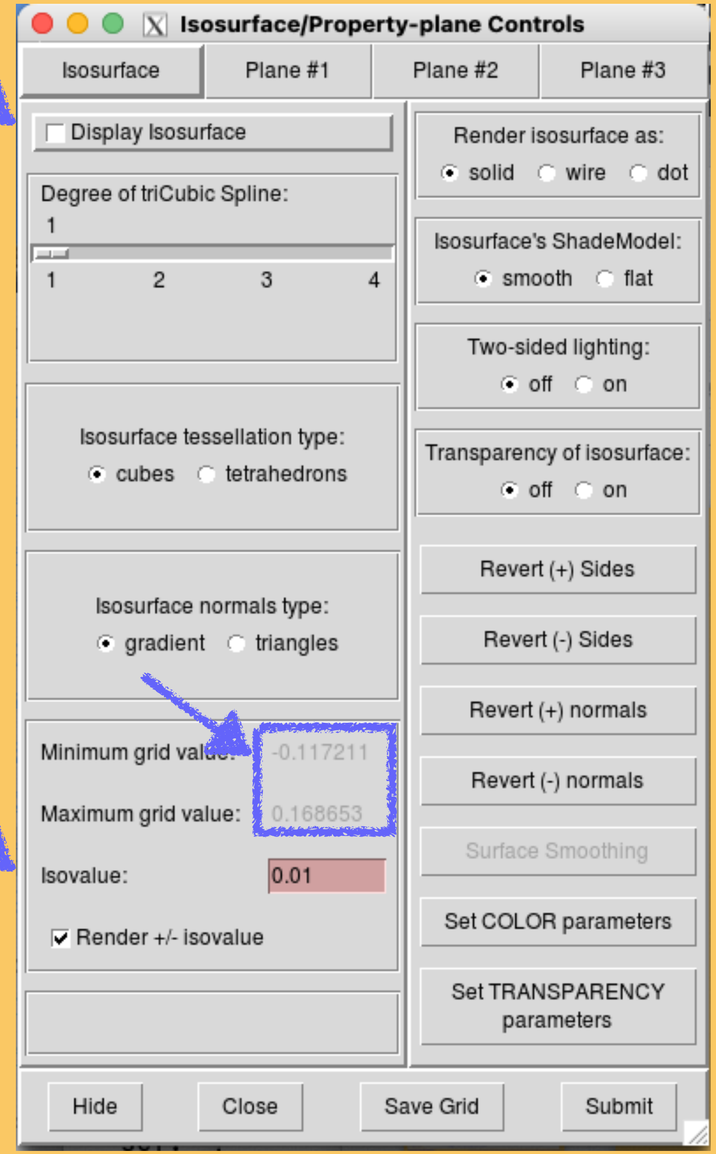
Exit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Isosurface
Plane #1
Plane #2
Plane #3
Display Isosurface
Degree of triCubic Spline:
1
1 2 3 4
Isosurface tessellation type:
cubes
tetrahedrons
Isosurface normals type:
gradient
triangles
Minimum grid value:
-0.117211
Maximum grid value:
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Render +/- isovalue
Render isosurface as:
solid
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Isosurface's ShadeModel:
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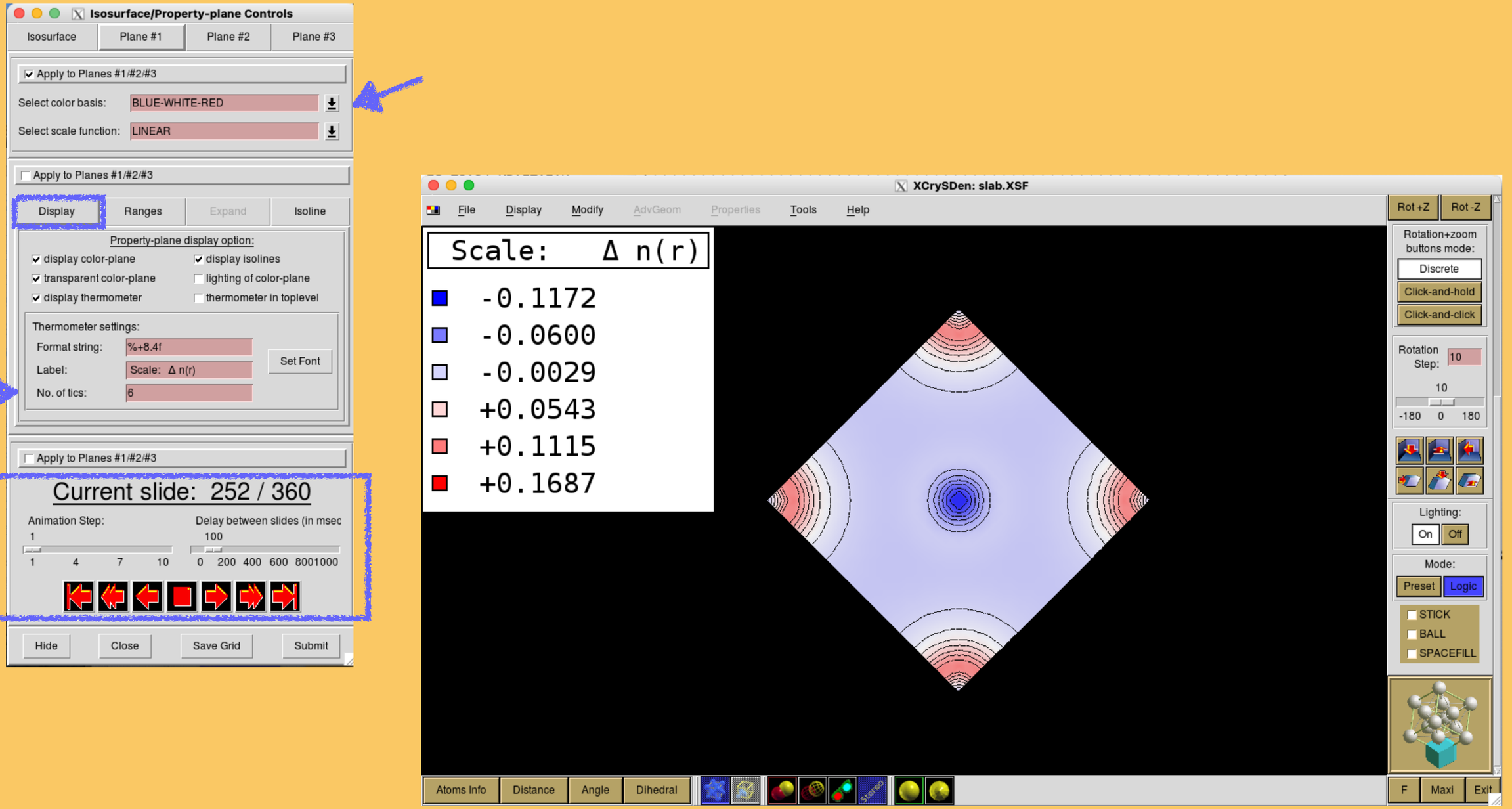
flat
Two-sided lighting:
off
on
Transparency of isosurface:
off
on
Revert (+) Sides
Revert (-) Sides
Revert (+) normals
Revert (-) normals
Surface Smoothing
Set COLOR parameters
Set TRANSPARENCY parameters
Hide
Close
Save Grid
Submit


Isosurface/Property-plane Controls
Isosurface
Plane #1
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Plane #3
Apply to Planes #1/#2/#3
Select color basis:
BLUE-WHITE-RED
Select scale function:
LINEAR
Apply to Planes #1/#2/#3
Display
Ranges
Expand
Isoline
Property-plane display option:
display color-plane
display isolines
transparent color-plane
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display thermometer
thermometer in toplevel
Thermometer settings:
Format string:
%+8.4f
Label:
Scale: Δ n(r)
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6
Set Font
Apply to Planes #1/#2/#3
Current slide: 252 / 360
Animation Step:
Delay between slides (in msec
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XCrySDen: slab.XSF
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Rotation Step:
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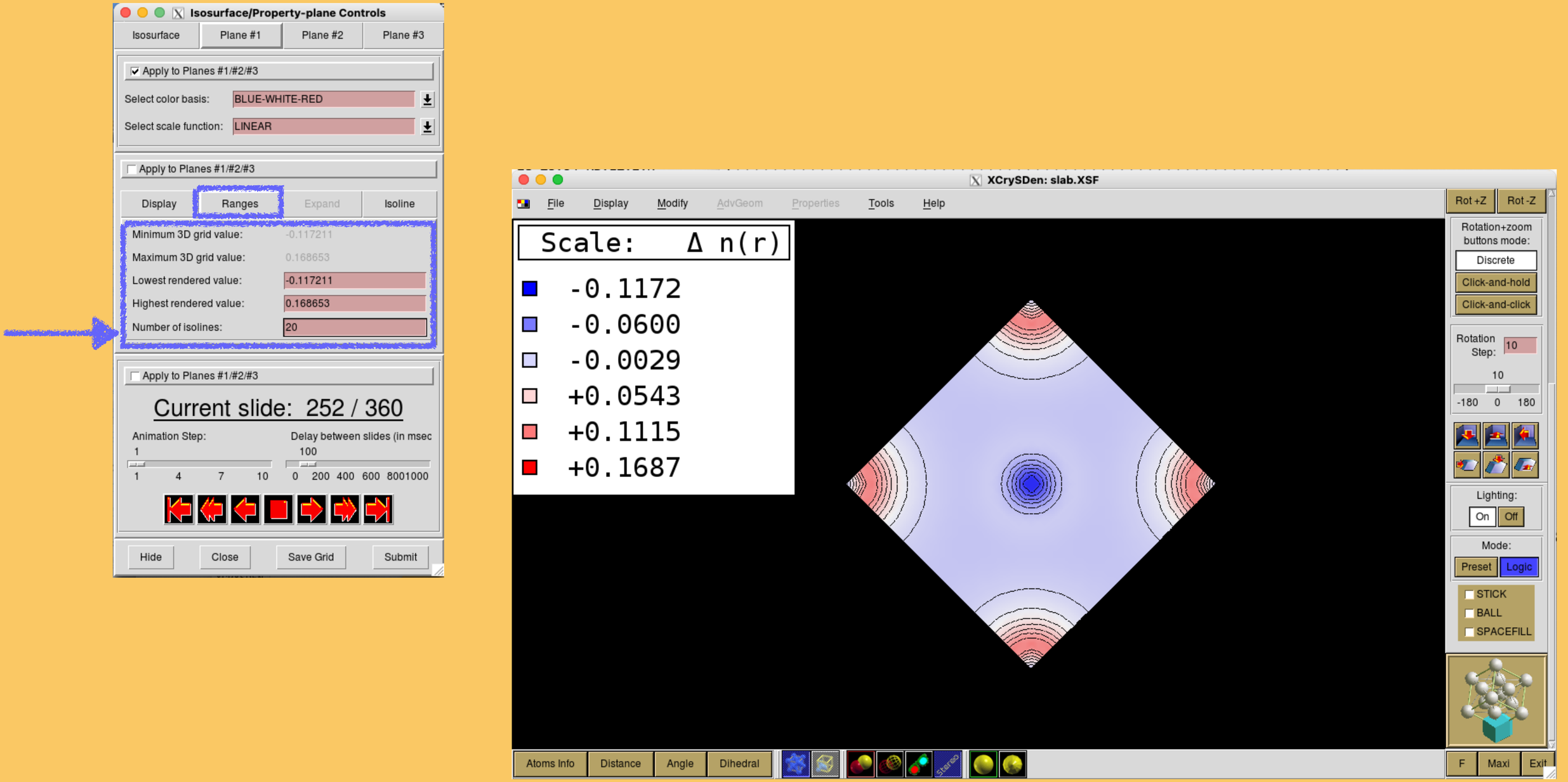
Isosurface/Property-plane Controls
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Plane #3
Apply to Planes #1/#2/#3
Select color basis:
BLUE-WHITE-RED
Select scale function:
LINEAR
Apply to Planes #1/#2/#3
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Ranges
Expand
Isoline
Minimum 3D grid value:
-0.117211
Maximum 3D grid value:
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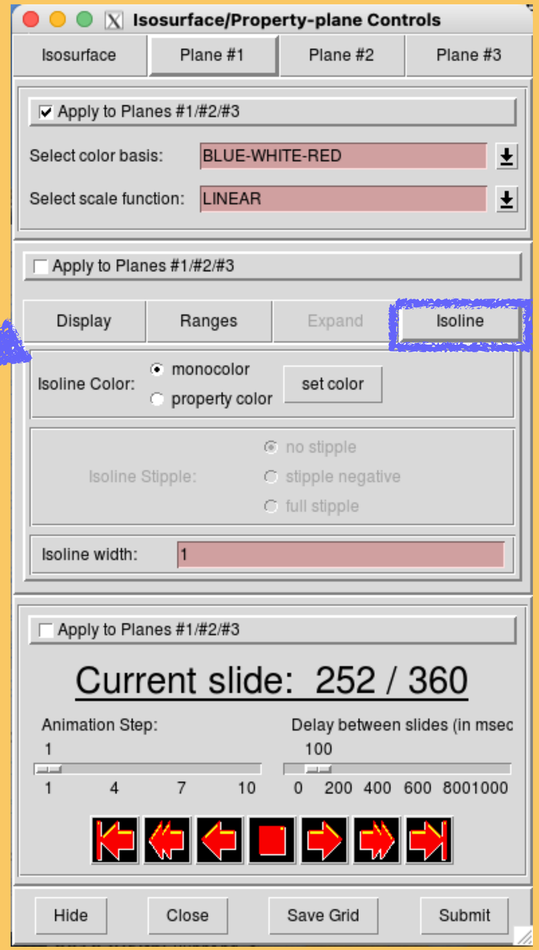
Isosurface/Property-plane Controls
Isosurface
Plane #1
Plane #2
Plane #3
Apply to Planes #1/#2/#3
Select color basis:
BLUE-WHITE-RED
Select scale function:
LINEAR
Apply to Planes #1/#2/#3
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Isoline Color:
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property color
set color
Isoline Stipple:
no stipple
stipple negative
full stipple
Isoline width:
1
Apply to Planes #1/#2/#3
Current slide: 252 / 360
Animation Step:
Delay between slides (in msec
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Save Grid
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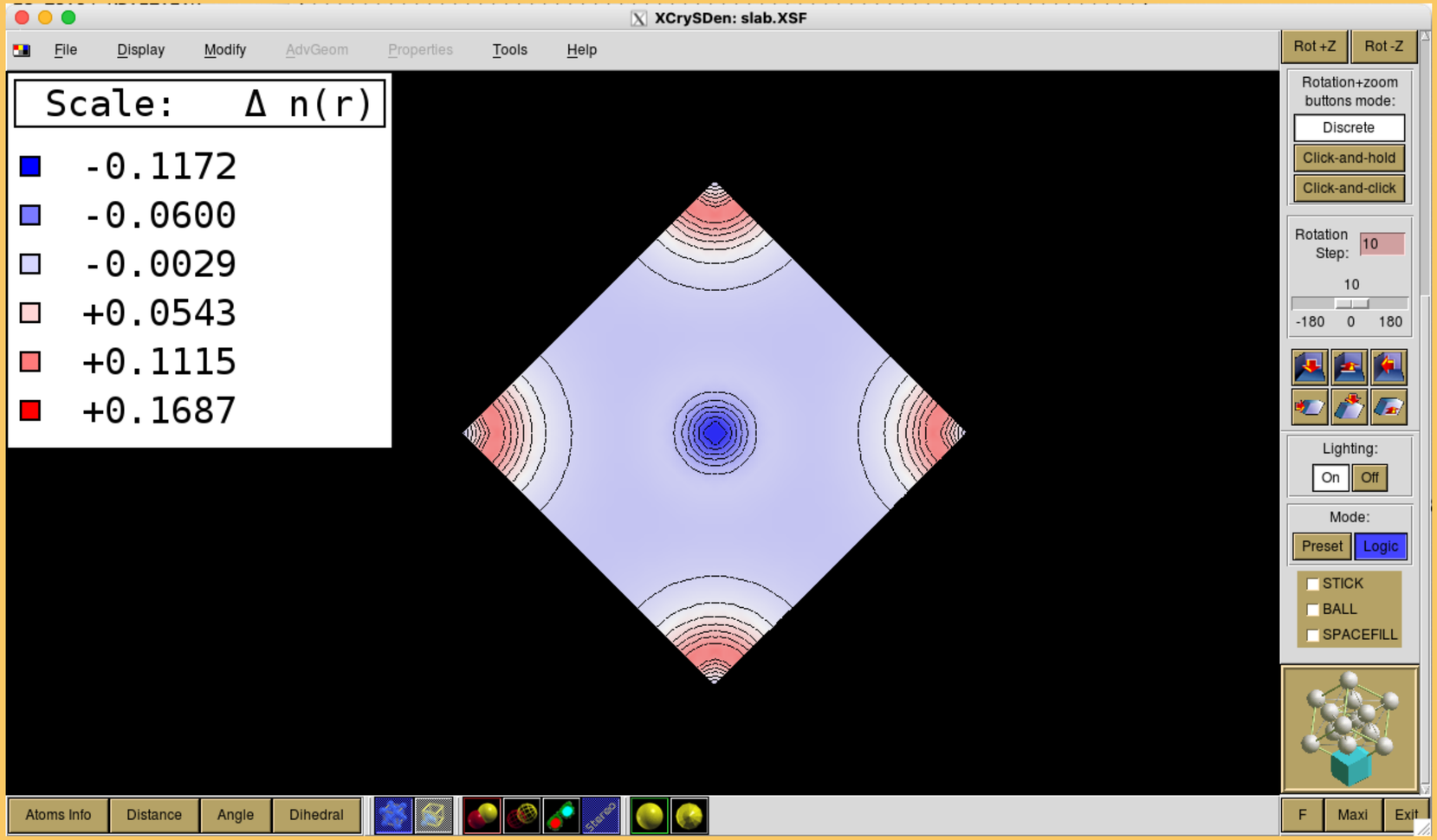
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-0.0029
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Lighting:
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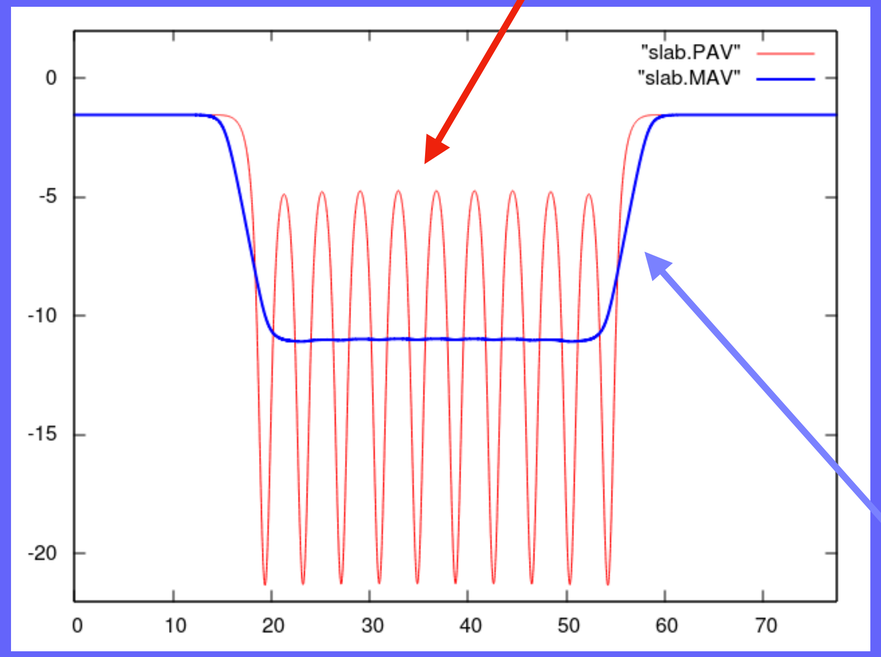
BALL
SPACEFILL
Atoms Info
Distance
Angle
Dihedral
F
Maxi
Exit

Macroscopic averages of grid functions

MACROAVE (`siesta/Util/Macroave`)

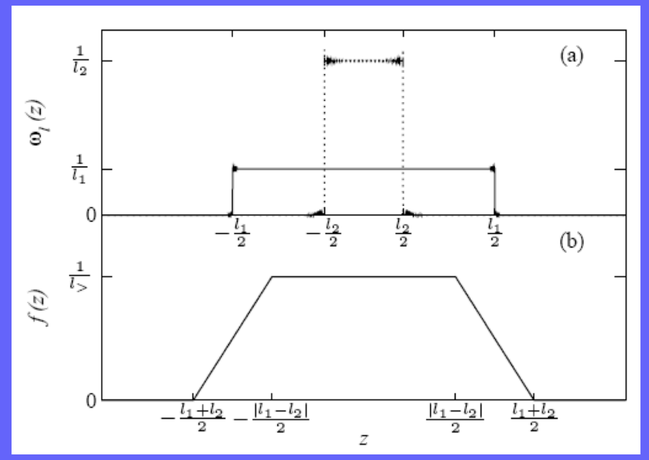
$$\overline{F}(z) = \frac{1}{S}\int_S dxdy\, F(x,y,z)$$



Atomic scale fluctuations can be washed out by convolution with a filter function

$$\Theta(z-z') = \int dz''\omega_{l_1}(z-z'')\,\omega_{l_2}(z''-z')$$

$$\overline{\overline{F}}(z) = \int dz'\Theta(z-z')\overline{F}(z')$$



How to use macroave?

1) Run SIESTA to extract the grid-function you want to analyse.

FDF flags		Output files
SaveRho	.true.	SystemLabel.RHO
SaveDeltaRho	.true.	SystemLabel.DRHO
SaveElectrostaticPotential	.true.	SystemLabel.VH
SaveTotalPotential	.true.	SystemLabel.VT
SaveTotalCharge	.true.	SystemLabel.TOCH
SaveIonicCharge	.true.	SystemLabel.IOCH
…		

2) Edit the input file macroave.in (see next)

3) Execute the code: `$path/to/your/executable/macroave.x`

How to use macroave?

Input file: `macroave.in`

```
siesta                  # Which code have you used to get the input data?
charge                  # Which is the input data used to compute the band offset?
slab                    # Name of the file where the input data is stored
1                       # Number of convolutions required to calculate the macro. ave.
4.200                   # First length for the filter function in macroscopic average
4.000                   # Second length for the filter function in macroscopic average
330                     # Total charge
spline                  # Type of interpolation
```

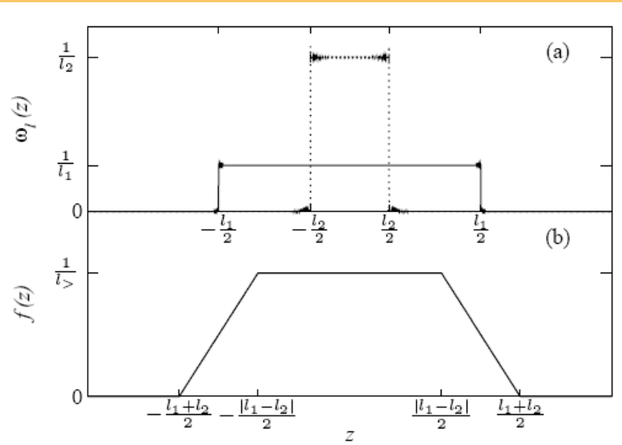
1) siesta / abinit

2) Potential / Charge / TotalCharge

3) 1 for surfaces / 2 for interfaces

4) total number of electrons (used to renormalise charge)

5) Spline / linear



How to use macroave?

Output files:

`SystemLabel.PAV`

Planar average

$$\overline{F}(z) = \frac{1}{S}\int_S dxdy\, F(x,y,z)$$

`SystemLabel.MAV`

Nanosmoothed

$$\overline{\overline{F}}(z) = \int dz' \Theta(z-z')\overline{F}(z')$$

Units:

- Coordinates in Bohr
- Potential in eV
- Charge density in electrons/Bohr^3

Charge analysis

Background

N electronic states

$$n(r) = \sum_{i}^{N} |\psi_i^{KS}(r)|^2$$

Basis Expansion:

M basis functions

$$|\psi_i\rangle = \sum_{\mu=1}^{M} c_{i,\mu} \, |\mu\rangle$$

$$\int_{\Omega} n(r) = N = \sum_{i}^{N} \langle \psi_i | \psi_i \rangle = \sum_{i} \sum_{\mu\nu} c_{i\mu}^{*} c_{i\nu} \langle \mu | \nu \rangle = \sum_{\mu\nu} \rho_{\mu\nu} S_{\mu\nu}$$

Density matrix

$$\rho_{\mu\nu} = \sum_{i} c_{i\mu}^{*} c_{i\nu}$$

Overlap matrix

$$S_{\mu\nu} = \langle \mu | \nu \rangle$$

Charge analysis

N electronic states

$$n(r) = \sum_{i}^{N} |\psi_i^{KS}(r)|^2$$

Basis Expansion:

M basis functions

$$|\psi_i\rangle = \sum_{\mu=1}^{M} c_{i,\mu} \, |\mu\rangle$$

$$\int_{\Omega} n(r) = N = \sum_{i}^{N} \langle \psi_i | \psi_i \rangle = \sum_{i} \sum_{\mu\nu} c_{i\mu}^{*} c_{i\nu} \langle \mu | \nu \rangle = \sum_{\mu\nu} \rho_{\mu\nu} S_{\mu\nu}$$

$$N = \sum_{I} q_I = \sum_{I} \sum_{\mu \in I} \sum_{\nu} \rho_{\mu\nu} S_{\mu\nu}$$

Mulliken charges

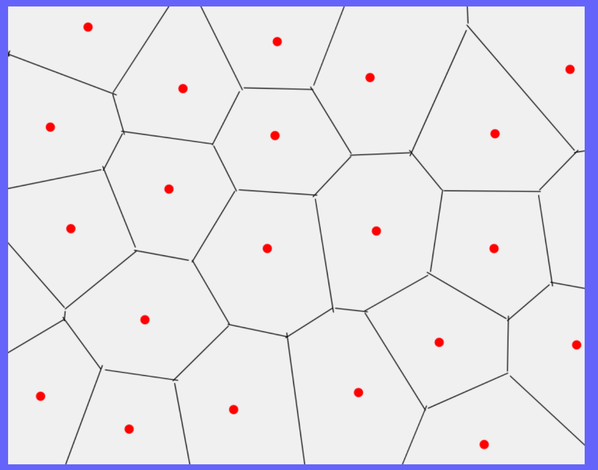
`WriteMullikenPop` 0/ 1 / 2 / 3

Charge analysis

$$\int_{\Omega} n(r) = N = \sum_{I} \int_{\Omega_I} n(r)$$

Voronoi charges

```
Write.VoronoiPop        True
```



$$q_I = \int_{\Omega} dr \frac{\rho^I_{atom}(r)}{\sum_J \rho^J_{atom}(r)} n(r)$$

Hirshfeld charges

```
Write.HirsfeldPop       True
```

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Analysis I: plotting data on grid

Questions?

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