Spin transport in Magnetic Tunnel Junctions

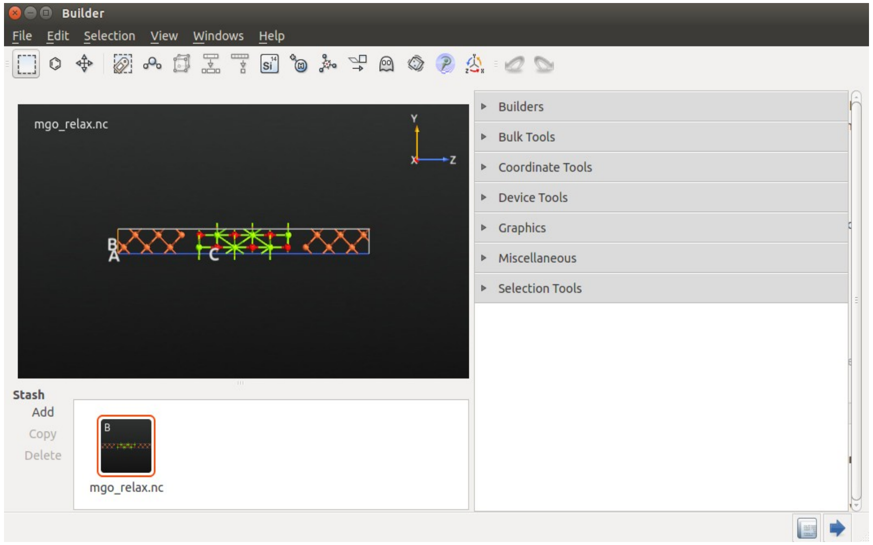
Quantum Wise
When every atom matters

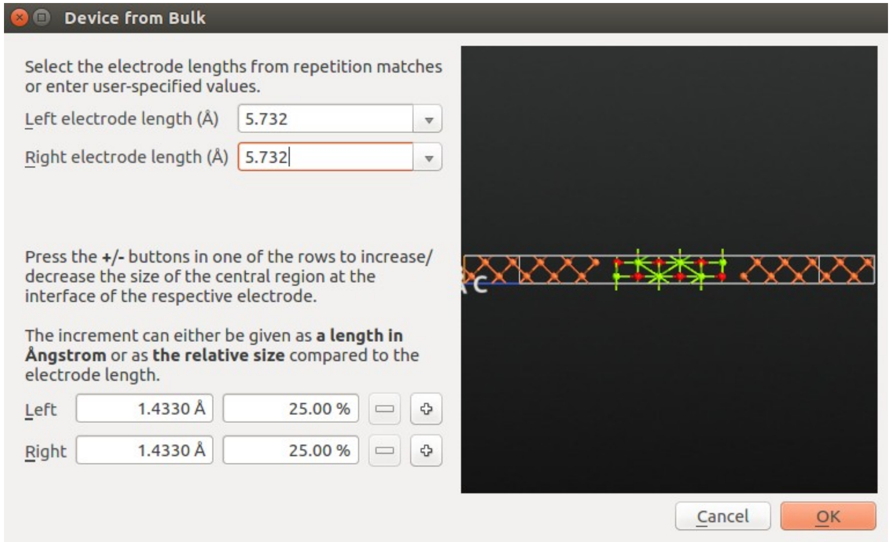
This tutorial shows how to simulate and analyze the electronic transport properties of magnetic tunnel junctions (MTJs). You will study the collinear and non-collinear spin-dependent transport properties of the Fe-MgO-Fe magnetic tunnel junction. In particular you will study the electronic transmission, the tunnel magnetoresistance and the spin-transfer torque.

Setup the MTJ device

Builder

- Download the already relaxed Fe-MgO-Fe geometry and save it in the *Project Folder*.
- Select the bulk configuration and send it to the **Builder**.
- Use **Device Tools → Device From Bulk …** to generate the device structure.
- Send the structure to the **Script Generator**.





Select the electrode lengths from repetition matches or enter user-specified values.

Left electrode length (Å) 5.732

Right electrode length (Å) 5.732

Press the +/- buttons in one of the rows to increase/decrease the size of the central region at the interface of the respective electrode.

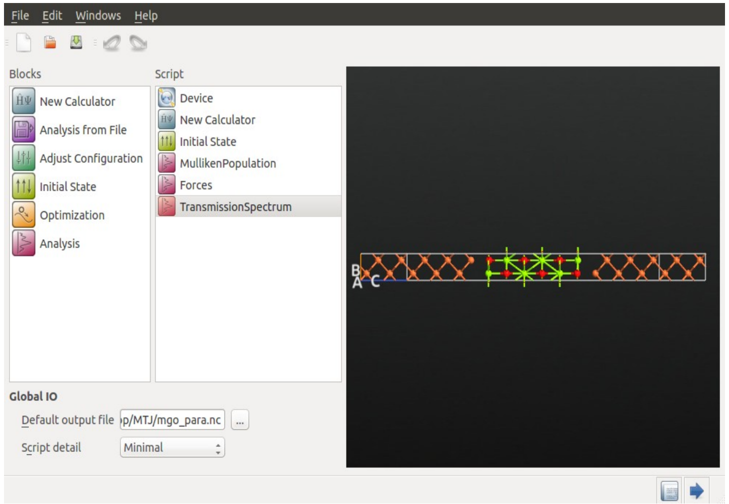
The increment can either be given as **a length in Ångstrom** or as **the relative size** compared to the electrode length.

Left	1.4330 Å	25.00 %
Right	1.4330 Å	25.00 %

Setup the script for transmission calculation: spin parallel

Script Generator

- New Calculator
  - Spin: Polarized
  - Exchange-correlation: SGGA.PBE
  - Electron temperature: 1200 Kelvin.
  - K-point sampling: (7,7,100)
- Initial State.
  - Initial State: User spin
  - Relative spin: 0 for Mg and O and 1 for Fe.
- MullikenPopulation
- Forces

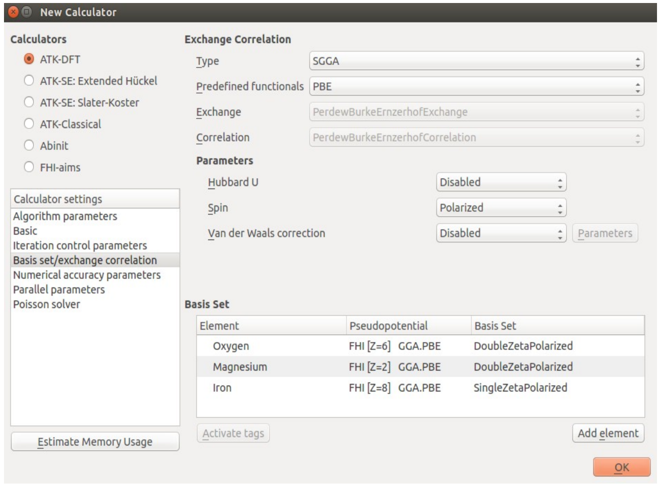


Script
- Device
- New Calculator
- Initial State
- MullikenPopulation
- Forces
- TransmissionSpectrum

Global IO

Default output file: ›p/MTJ/mgo_para.nc

Script detail: Minimal



Calculators
- ● ATK-DFT
- ○ ATK-SE: Extended Hückel
- ○ ATK-SE: Slater-Koster
- ○ ATK-Classical
- ○ Abinit
- ○ FHI-aims

Calculator settings
- Algorithm parameters
- Basic
- Iteration control parameters
- Basis set/exchange correlation
- Numerical accuracy parameters
- Parallel parameters
- Poisson solver

Exchange Correlation

Type: SGGA

Predefined functionals: PBE

Exchange: PerdewBurkeErnzerhofExchange

Correlation: PerdewBurkeErnzerhofCorrelation

Parameters

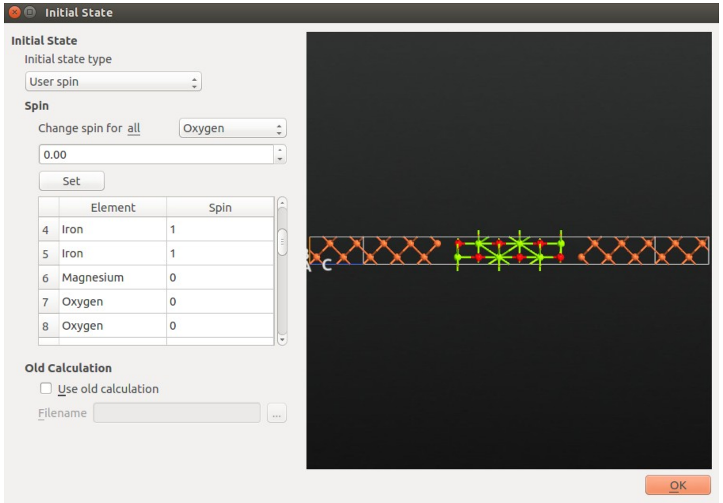
Hubbard U: Disabled

Spin: Polarized

Van der Waals correction: Disabled   Parameters

Basis Set

Element	Pseudopotential	Basis Set
Oxygen	FHI [Z=6] GGA.PBE	DoubleZetaPolarized
Magnesium	FHI [Z=2] GGA.PBE	DoubleZetaPolarized
Iron	FHI [Z=8] GGA.PBE	SingleZetaPolarized



Initial State

Initial state type: User spin

Spin

Change spin for all: Oxygen

0.00

	Element	Spin
4	Iron	1
5	Iron	1
6	Magnesium	0
7	Oxygen	0
8	Oxygen	0

Old Calculation

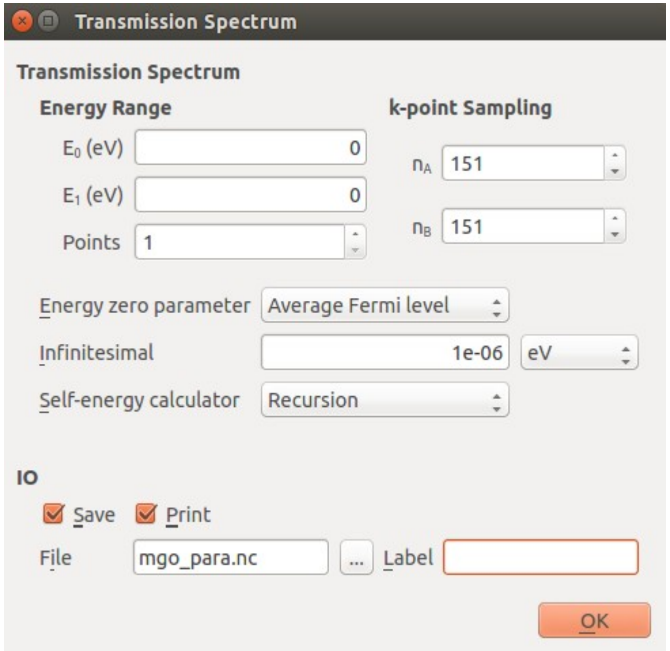
☐ Use old calculation

Filename

Setup the script for transmission calculation: spin parallel

Script Generator

- TransmissionSpectrum
  - E0=E1= 0 eV
  - Energy Points=1
  - K-points grid sampling: (151x151)



Transmission Spectrum

Transmission Spectrum

Energy Range

E_0 (eV) 0

E_1 (eV) 0

Points 1

k-point Sampling

n_A 151

n_B 151

Energy zero parameter: Average Fermi level

Infinitesimal: 1e-06 eV

Self-energy calculator: Recursion

IO

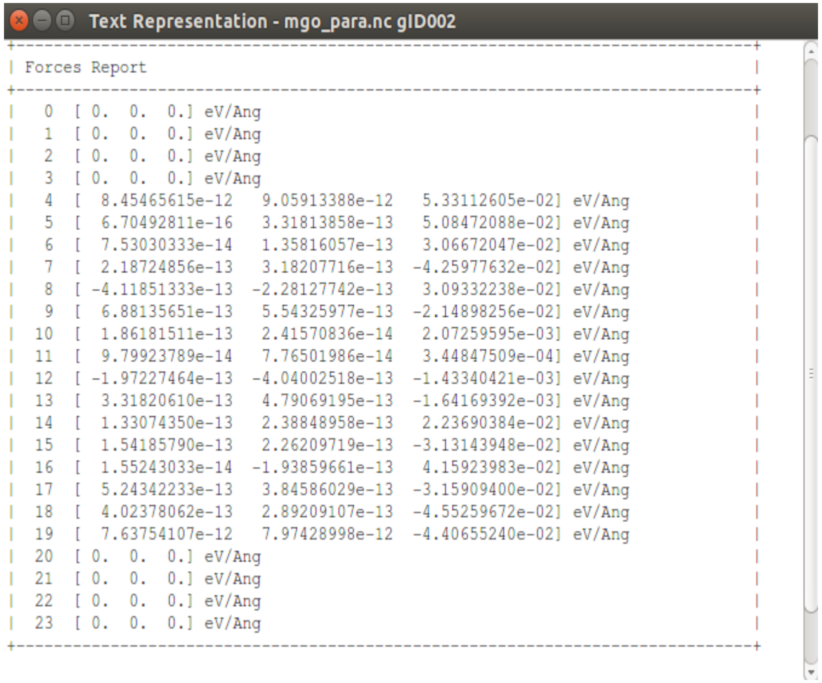
☑ Save ☑ Print

File: mgo_para.nc

Label:

Inspecting the forces

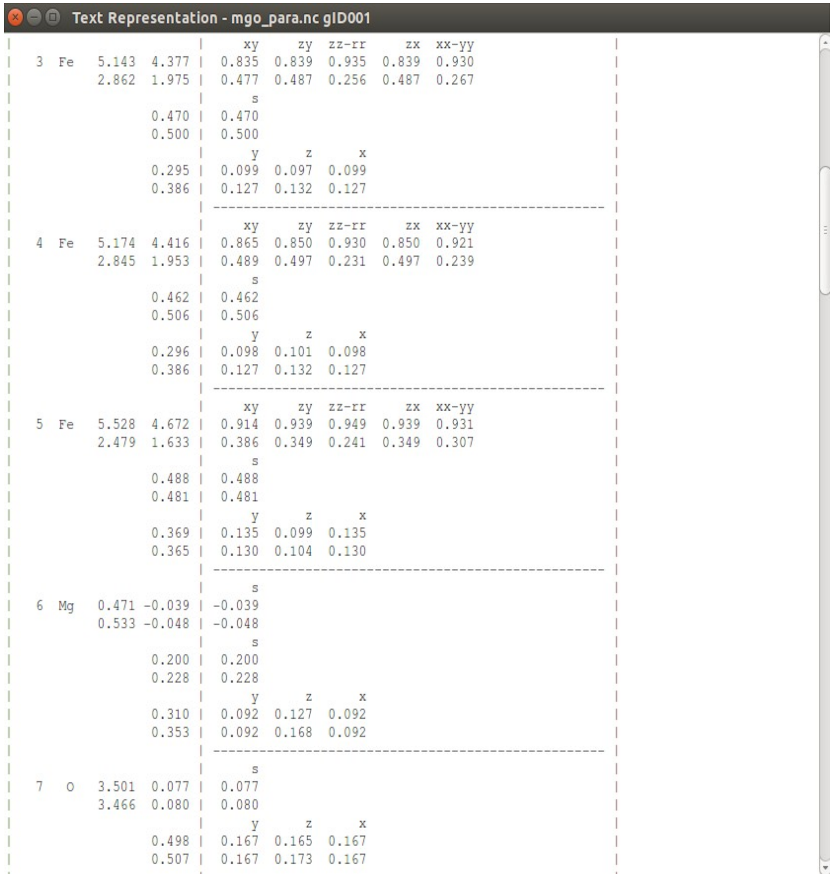
- From the *LabFloor*, select the **Forces** object.
- Next, click **Text Representation...** button.
- The forces on the equivalent electrode atoms inside the central cell are not calculated (zero).
- For the other atoms, the forces are small: relaxing the geometry is a good strategy for this system.



```
+-------------------------------------------------------------------------------+
| Forces Report                                                                 |
+-------------------------------------------------------------------------------+
|   0  [ 0.  0.  0.] eV/Ang                                                     |
|   1  [ 0.  0.  0.] eV/Ang                                                     |
|   2  [ 0.  0.  0.] eV/Ang                                                     |
|   3  [ 0.  0.  0.] eV/Ang                                                     |
|   4  [  8.45465615e-12   9.05913388e-12   5.33112605e-02] eV/Ang              |
|   5  [  6.70492811e-16   3.31813858e-13   5.08472088e-02] eV/Ang              |
|   6  [  7.53030333e-14   1.35816057e-13   3.06672047e-02] eV/Ang              |
|   7  [  2.18724856e-13   3.18207716e-13  -4.25977632e-02] eV/Ang              |
|   8  [ -4.11851333e-13  -2.28127742e-13   3.09332238e-02] eV/Ang              |
|   9  [  6.88135651e-13   5.54325977e-13  -2.14898256e-02] eV/Ang              |
|  10  [  1.86181511e-13   2.41570836e-14   2.07259595e-03] eV/Ang              |
|  11  [  9.79923789e-14   7.76501986e-14   3.44847509e-04] eV/Ang              |
|  12  [ -1.97227464e-13  -4.04002518e-13  -1.43340421e-03] eV/Ang              |
|  13  [  3.31820610e-13   4.79069195e-13  -1.64169392e-03] eV/Ang              |
|  14  [  1.33074350e-13   2.38848958e-13   2.23690384e-02] eV/Ang              |
|  15  [  1.54185790e-13   2.26209719e-13  -3.13143948e-02] eV/Ang              |
|  16  [  1.55243033e-14  -1.93859661e-13   4.15923983e-02] eV/Ang              |
|  17  [  5.24342233e-13   3.84586029e-13  -3.15909400e-02] eV/Ang              |
|  18  [  4.02378062e-13   2.89209107e-13  -4.55259672e-02] eV/Ang              |
|  19  [  7.63754107e-12   7.97428998e-12  -4.40655240e-02] eV/Ang              |
|  20  [ 0.  0.  0.] eV/Ang                                                     |
|  21  [ 0.  0.  0.] eV/Ang                                                     |
|  22  [ 0.  0.  0.] eV/Ang                                                     |
|  23  [ 0.  0.  0.] eV/Ang                                                     |
+-------------------------------------------------------------------------------+
```

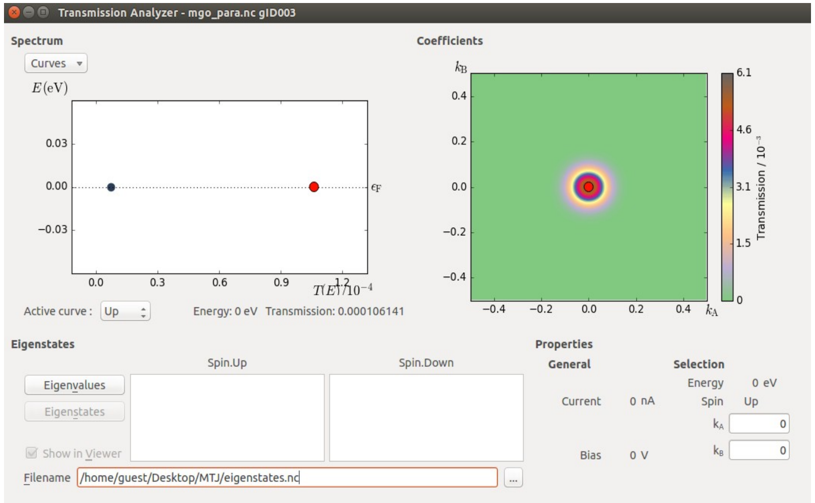
Inspecting the Mulliken Population

- From the *LabFloor*, select the **MullikenPopulation** object.
- Click **Text Representation…** button.
- Check that each atom is correctly spin polarized: Inspect the leftmost column, this shows the total Mulliken population per spin channel for each atom.
- All the Fe atoms polarized with their majority spin pointing up.
- The Mg atoms close to the interface couple antiparallel with Fe.
- The O atoms are unpolarized.



```
|                        |     xy     zy  zz-rr     zx  xx-yy               |
|   3  Fe   5.143  4.377 |  0.835  0.839  0.935  0.839  0.930               |
|           2.862  1.975 |  0.477  0.487  0.256  0.487  0.267               |
|                        |      s                                           |
|                  0.470 |  0.470                                           |
|                  0.500 |  0.500                                           |
|                        |      y      z      x                             |
|                  0.295 |  0.099  0.097  0.099                             |
|                  0.386 |  0.127  0.132  0.127                             |
|                        | ------------------------------------------------ |
|                        |     xy     zy  zz-rr     zx  xx-yy               |
|   4  Fe   5.174  4.416 |  0.865  0.850  0.930  0.850  0.921               |
|           2.845  1.953 |  0.489  0.497  0.231  0.497  0.239               |
|                        |      s                                           |
|                  0.462 |  0.462                                           |
|                  0.506 |  0.506                                           |
|                        |      y      z      x                             |
|                  0.296 |  0.098  0.101  0.098                             |
|                  0.386 |  0.127  0.132  0.127                             |
|                        | ------------------------------------------------ |
|                        |     xy     zy  zz-rr     zx  xx-yy               |
|   5  Fe   5.528  4.672 |  0.914  0.939  0.949  0.939  0.931               |
|           2.479  1.633 |  0.386  0.349  0.241  0.349  0.307               |
|                        |      s                                           |
|                  0.488 |  0.488                                           |
|                  0.481 |  0.481                                           |
|                        |      y      z      x                             |
|                  0.369 |  0.135  0.099  0.135                             |
|                  0.365 |  0.130  0.104  0.130                             |
|                        | ------------------------------------------------ |
|                        |      s                                           |
|   6  Mg   0.471 -0.039 | -0.039                                           |
|           0.533 -0.048 | -0.048                                           |
|                        |      s                                           |
|                  0.200 |  0.200                                           |
|                  0.228 |  0.228                                           |
|                        |      y      z      x                             |
|                  0.310 |  0.092  0.127  0.092                             |
|                  0.353 |  0.092  0.168  0.092                             |
|                        | ------------------------------------------------ |
|                        |      s                                           |
|   7   O   3.501  0.077 |  0.077                                           |
|           3.466  0.080 |  0.080                                           |
|                        |      y      z      x                             |
|                  0.498 |  0.167  0.165  0.167                             |
|                  0.507 |  0.167  0.173  0.167                             |
```

Analyzing the k-parallel transmission


Transmission Analyzer - mgo_para.nc gID003

Active curve : Up

Energy: 0 eV Transmission: 0.000106141

Current 0 nA

Bias 0 V

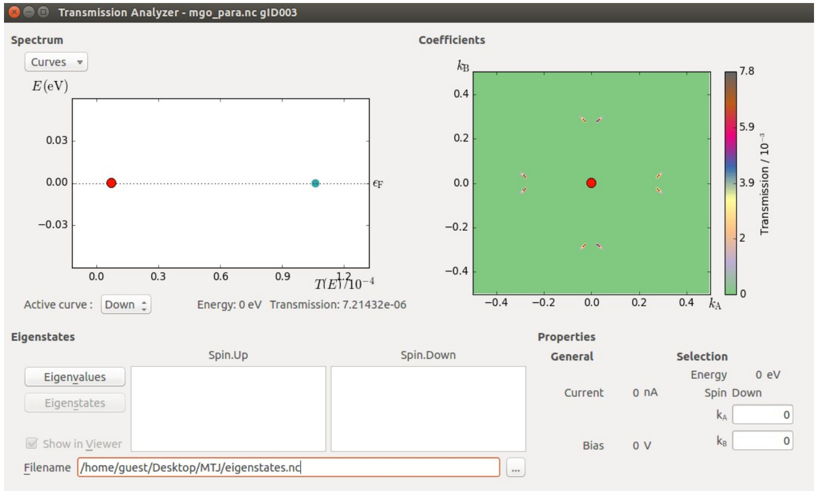
Energy 0 eV

Spin Up

k_A 0

k_B 0

Filename /home/guest/Desktop/MTJ/eigenstates.nc


Transmission Analyzer - mgo_para.nc gID003

Active curve : Down

Energy: 0 eV Transmission: 7.21432e-06

Current 0 nA

Bias 0 V

Energy 0 eV

Spin Down

k_A 0

k_B 0

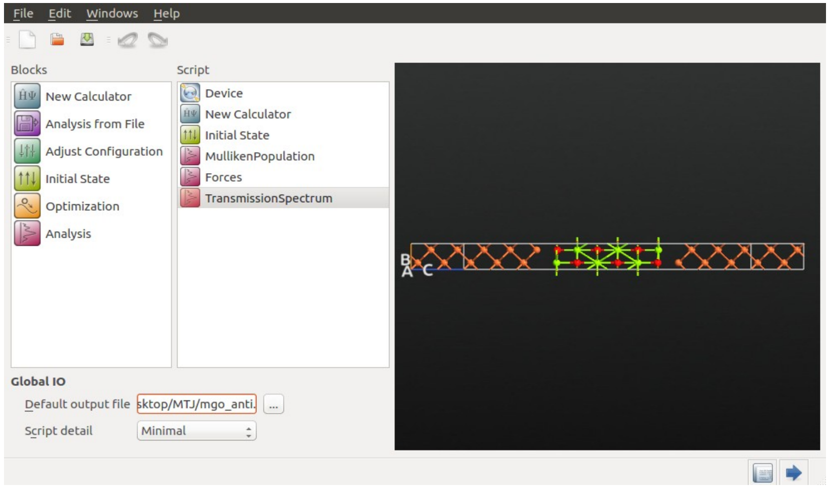
Filename /home/guest/Desktop/MTJ/eigenstates.nc

- ❖ It is clear from the plots that the down spin (minority) transmission is strongly supressed in magnitude and exhibits peaks at certain points in the Brillouin zone.

Setup the script for Transmission calculation: spin anti-parallel

Script Generator

- ❖ New Calculator
  - – Spin: Polarized
  - – Exchange-correlation: SGGA.PBE
  - – Electron temperature: 1200 Kelvin.
  - – K-point sampling: (7,7,100)
- ❖ Initial State.
  - – Initial State: User spin
  - – Relative spin: 0 for Mg and O and 1/-1 for Fe.
- ❖ MullikenPopulation
- ❖ Forces
- ❖ TransmissionSpectrum
  - – E0=E1= 0 eV
  - – Energy Points=1
  - – K-points grid sampling: (151x151)

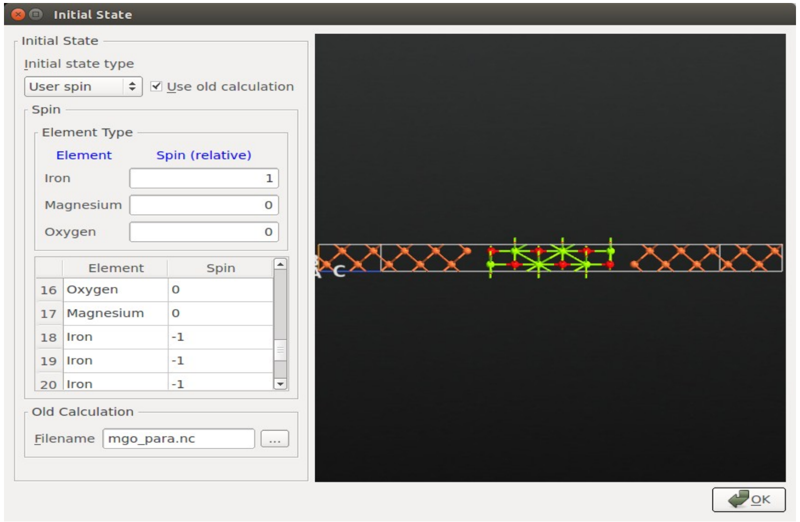


Script
- Device
- New Calculator
- Initial State
- MullikenPopulation
- Forces
- TransmissionSpectrum

Global IO

Default output file: sktop/MTJ/mgo_anti.

Script detail: Minimal



Initial State

Initial state type: User spin ☑ Use old calculation

Spin

Element Type

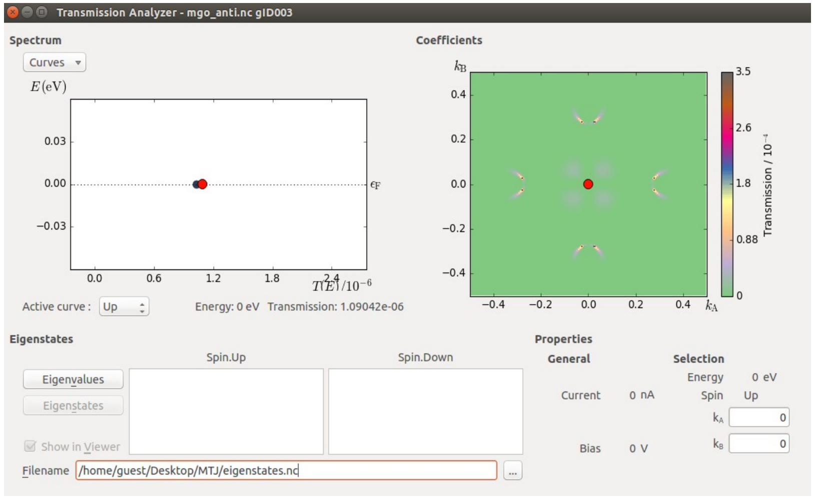
Element	Spin (relative)
Iron	1
Magnesium	0
Oxygen	0

	Element	Spin
16	Oxygen	0
17	Magnesium	0
18	Iron	-1
19	Iron	-1
20	Iron	-1

Old Calculation

Filename: mgo_para.nc

Analysis of k anti-parallel transmission



Transmission Analyzer - mgo_anti.nc gID003

Active curve : Up

Energy: 0 eV Transmission: 1.09042e-06

☑ Show in Viewer

Filename /home/guest/Desktop/MTJ/eigenstates.nc

Current 0 nA

Bias 0 V

Energy 0 eV

Spin Up

k_A 0

k_B 0

- In this case the transmission for the up and down will be identical due to the mirror symmetry of the system. Note: due to the time inversion symmetry, propagation from left to right is always identical to propagation from right to left.
- The up components of the transmission spectrum corresponds to up electrons from the left transmission propagating into the right electrode.
- The down component of the transmission spectrum corresponds to the down electrons in the right propagating into the left electrode.

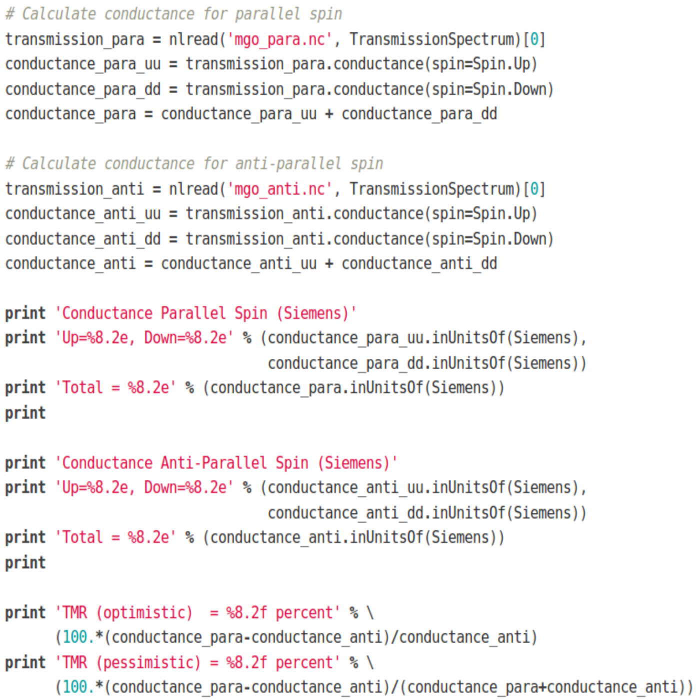
Tunneling magnetoresistance

❖ The tunneling magneto resistance (TMR) is defined as:

$$\mathrm{TMR} = \frac{G_P - G_{AP}}{G_{AP}},$$

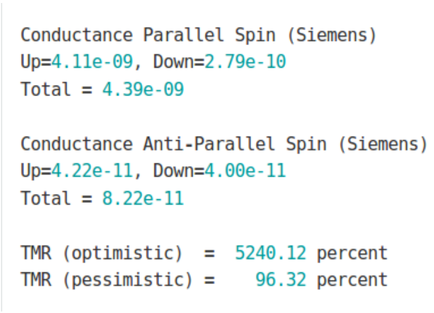
G_P is the conductance through the junction with parallel spin alignment
G_{AP} is the conductance for the anti-parallel spin alignment

❖ Script provided (**tmr.py**) to calculate the conductance from the transmission spectra of the junction with parallel and anti-parallel spin aligment:



```
# Calculate conductance for parallel spin
transmission_para = nlread('mgo_para.nc', TransmissionSpectrum)[0]
conductance_para_uu = transmission_para.conductance(spin=Spin.Up)
conductance_para_dd = transmission_para.conductance(spin=Spin.Down)
conductance_para = conductance_para_uu + conductance_para_dd

# Calculate conductance for anti-parallel spin
transmission_anti = nlread('mgo_anti.nc', TransmissionSpectrum)[0]
conductance_anti_uu = transmission_anti.conductance(spin=Spin.Up)
conductance_anti_dd = transmission_anti.conductance(spin=Spin.Down)
conductance_anti = conductance_anti_uu + conductance_anti_dd

print 'Conductance Parallel Spin (Siemens)'
print 'Up=%8.2e, Down=%8.2e' % (conductance_para_uu.inUnitsOf(Siemens),
                                conductance_para_dd.inUnitsOf(Siemens))
print 'Total = %8.2e' % (conductance_para.inUnitsOf(Siemens))
print

print 'Conductance Anti-Parallel Spin (Siemens)'
print 'Up=%8.2e, Down=%8.2e' % (conductance_anti_uu.inUnitsOf(Siemens),
                                conductance_anti_dd.inUnitsOf(Siemens))
print 'Total = %8.2e' % (conductance_anti.inUnitsOf(Siemens))
print

print 'TMR (optimistic)  = %8.2f percent' % \
      (100.*(conductance_para-conductance_anti)/conductance_anti)
print 'TMR (pessimistic) = %8.2f percent' % \
      (100.*(conductance_para-conductance_anti)/(conductance_para+conductance_anti))
```

❖ Execute the script and find the TMR:



```
Conductance Parallel Spin (Siemens)
Up=4.11e-09, Down=2.79e-10
Total = 4.39e-09

Conductance Anti-Parallel Spin (Siemens)
Up=4.22e-11, Down=4.00e-11
Total = 8.22e-11

TMR (optimistic)  =  5240.12 percent
TMR (pessimistic) =    96.32 percent
```

Adaptive k-grid

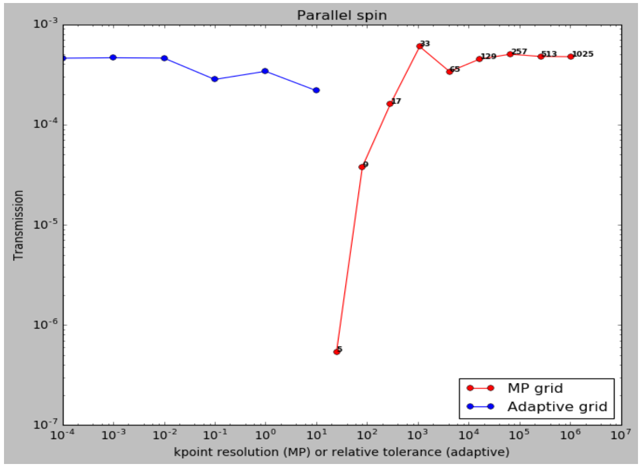
Adaptive k-grid

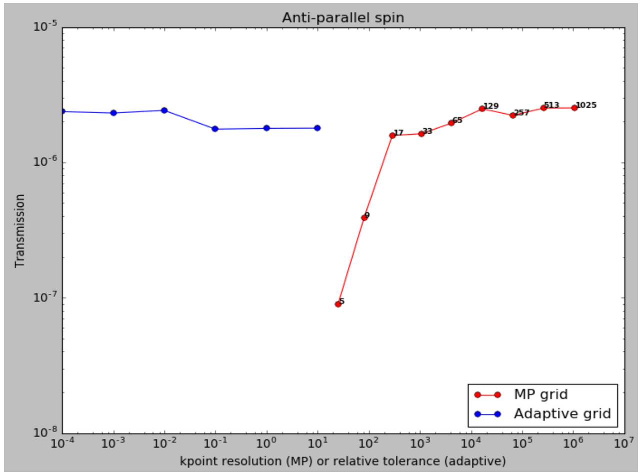
- Object for defining the k-point sampling used for the calculation of transmission and spin-transfer torque.
- **Application**: automatically zoom in on the significant features of the electron transmission spectrum. Useful when the k-dependent transmission is dominated by localized peaks and the total computed transmission may depend critically on resolving those peaks.
- **Adaptive algorithm**: divides the Brillouin zone into triangles and integrates over each triangle. Each triangle becomes increasingly small in an iterative manner until convergence is reaced, but stops if the number of refinement levels reaches the **max_number_of_levels** (20 by default).
- The integral over each triangle is estimated as:
- In order to estimate whether or not the I_o integral is converged, two types of errors available:
  - Absolute: converged when the absolute value of the Brillouin zone integral in all triangles is lower than the chosen tolerance
  - Relative: converged when the relative value of the Brillouin zone integral in all triangles is lower than the chosen tolerance.
- Absolute or Relative error? If one have knowledge about the function values, the use of Absolute error may be advantageous, otherwise the use of Relative error will be more useful.

Adaptive grid vs. MonkhorstPack grid: total transmission convergence at 0 eV

Transmission computed for Parallel and antiparallel configurations

- Basis set: *DoubleZetaPolarized* for Mg and O. *SingleZetaPolarized* for Fe.
- Exchange and correlation: SGGA.PBE
- K-point sampling: 6,6,100
- Electron temperature: 1200 Kelvin
- Adaptive k-grid
  - Relative Tolerance: 10, 1, 0.1, 0.01, 0.001, 0.0001 and 0.00001.
- Monkhorst-Pack grid
  - K-pont sampling: (5x5), (9x9), (17x17), (33x33), (65x65), (129x129), (257x257), (513x513), (1025x1025)

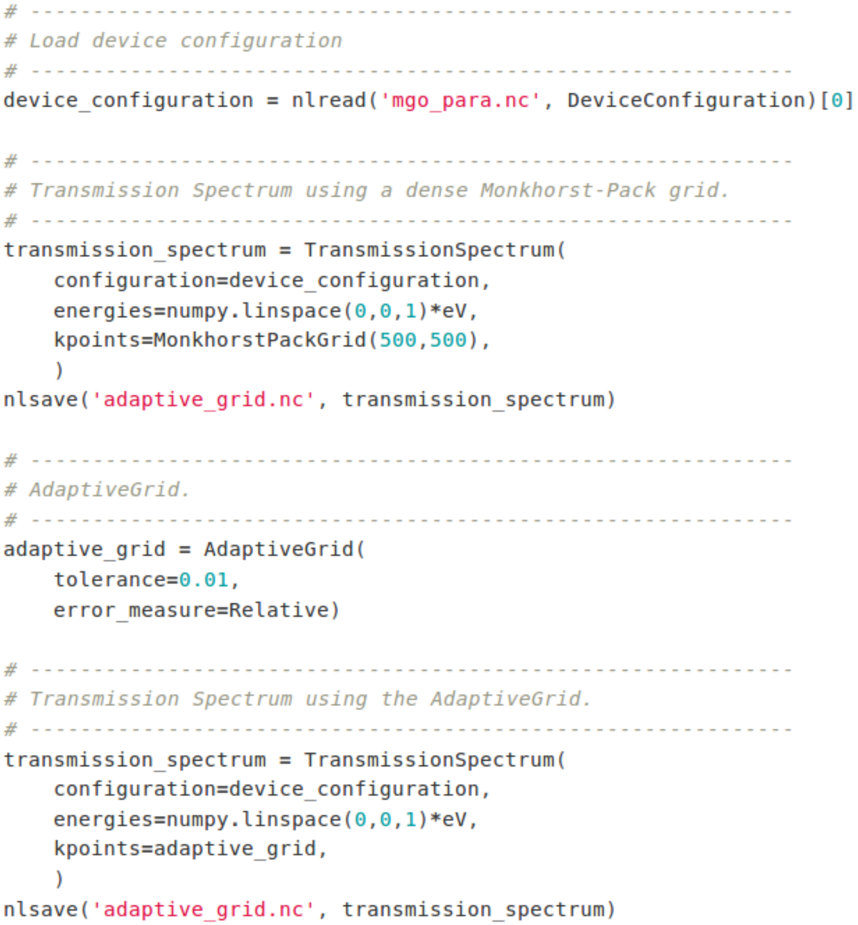




Well converged calculations of the total transmission through the MTJ obtained with no less than 10^3 Monkhorst-Pack k-points and with a relative tolerance of 10^{-2} using the adaptive k-point grid.

Parallel transmission

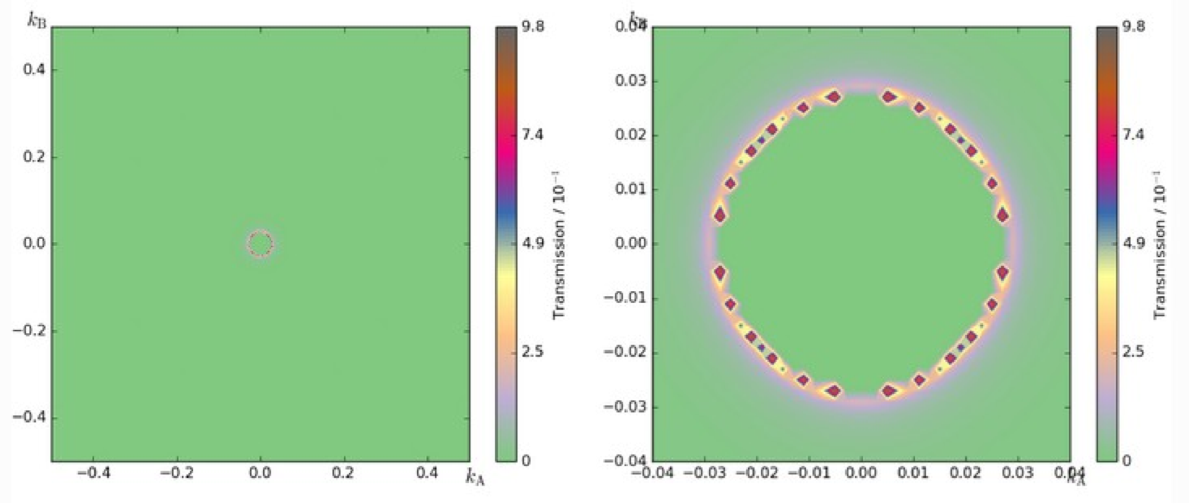
- ❖ Provide the adaptive_grid.py script.
- ❖ This script calculates the transmission for the Fe|MgO|Fe device with parallel spin orientation using both a dense MP grid and the AdaptiveGrid method.
- ❖ Monkhorst-Pack grid: 500x500 k-points
- ❖ Adaptive grid: relative tolerance of 10^{-2}.
- ❖ Download and run the script.



```
# -------------------------------------------------------------
# Load device configuration
# -------------------------------------------------------------
device_configuration = nlread('mgo_para.nc', DeviceConfiguration)[0]

# -------------------------------------------------------------
# Transmission Spectrum using a dense Monkhorst-Pack grid.
# -------------------------------------------------------------
transmission_spectrum = TransmissionSpectrum(
    configuration=device_configuration,
    energies=numpy.linspace(0,0,1)*eV,
    kpoints=MonkhorstPackGrid(500,500),
    )
nlsave('adaptive_grid.nc', transmission_spectrum)

# -------------------------------------------------------------
# AdaptiveGrid.
# -------------------------------------------------------------
adaptive_grid = AdaptiveGrid(
    tolerance=0.01,
    error_measure=Relative)

# -------------------------------------------------------------
# Transmission Spectrum using the AdaptiveGrid.
# -------------------------------------------------------------
transmission_spectrum = TransmissionSpectrum(
    configuration=device_configuration,
    energies=numpy.linspace(0,0,1)*eV,
    kpoints=adaptive_grid,
    )
nlsave('adaptive_grid.nc', transmission_spectrum)
```

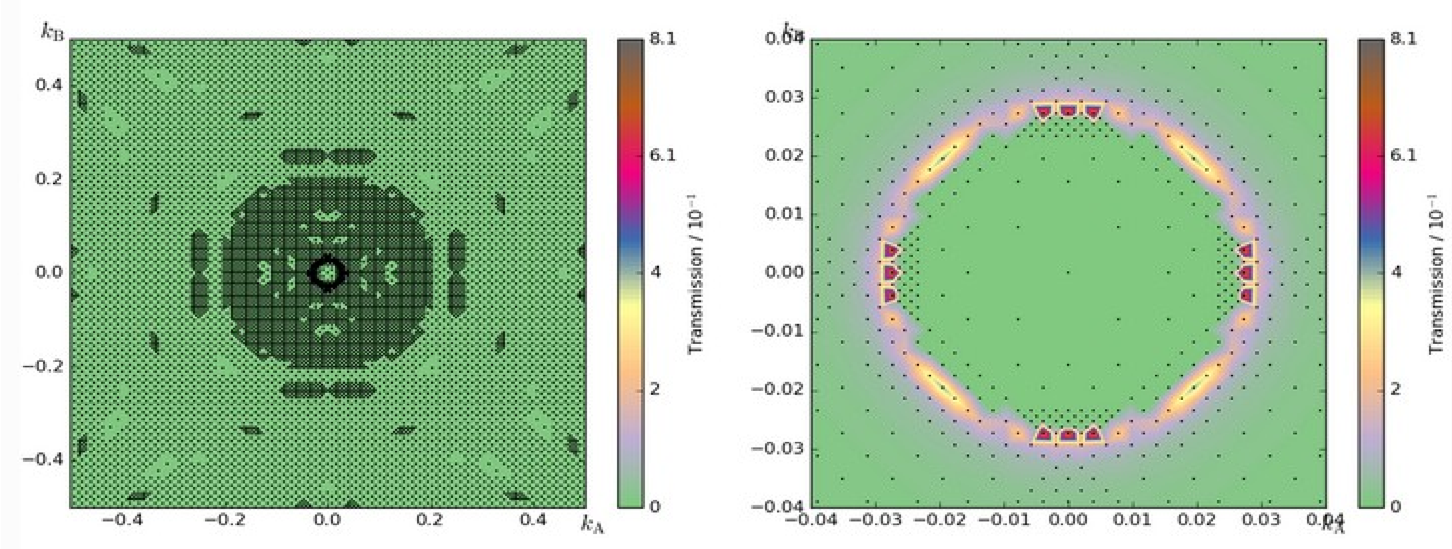
Spin-up transmission – Monkhorst-Pack grid

- Transmission spectrum obtained using a MP grid of (500x500) k-point sampling.



- The transmission spectrum obtained with the dense MP grid is different from the one obtained before using (151x151) k-point sampling.
  - Now circular feature in the middle of the spectrum with zero transmission immediately around the gamma point.
  - The improved k-point sampling has only increased the total k-point averaged spin-up transmission by a factor of 4.

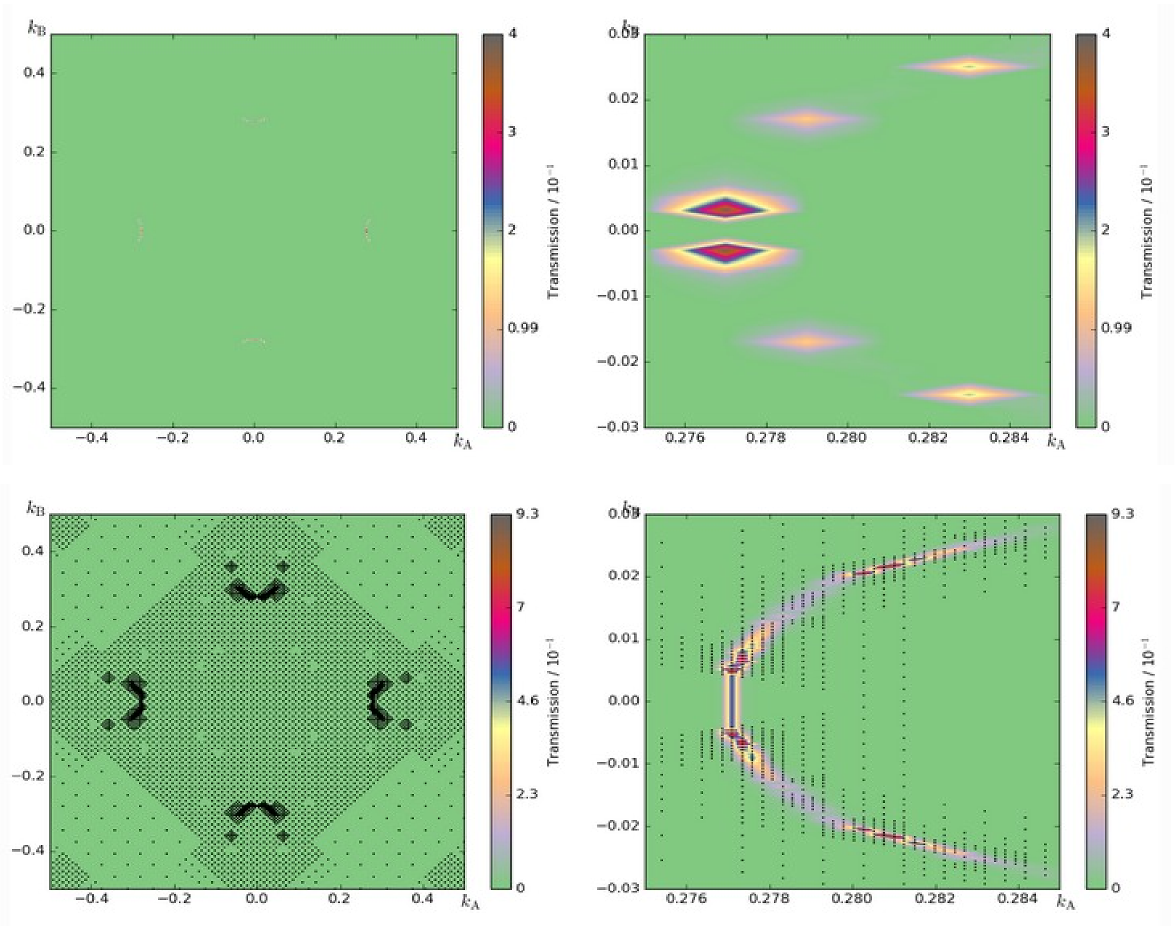
Spin-up transmission – Adaptive grid



- ❖ Spin-up transmission spectrum evaluated using the Adaptive grid with a 10^{-2} relative tolerance.
- ❖ Black dots indicate the sampled k-points.
- ❖ The adaptive grid has zoomed in on the circular feature of the k-dependent transmission, causing a larger k-point density around the circular feature.

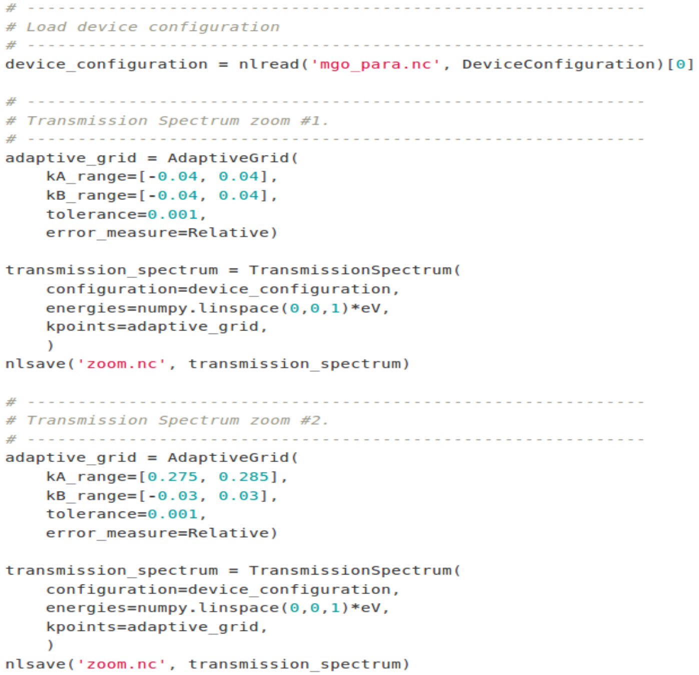
Spin-down transmission

- Above, transmission obtained using Monkhorst-Pack grid. The total k-point averaged spin-down transmission is 3.7 10^{-5}.
- Below, transmission obtained using Adaptive grid. The total k-point averaged spin-down transmission is 3.5 10^{-5}.
- The adaptive grid has zoomed in on the transmission peaks.
- The total k-point averaged spin-down transmission has changed 5%.

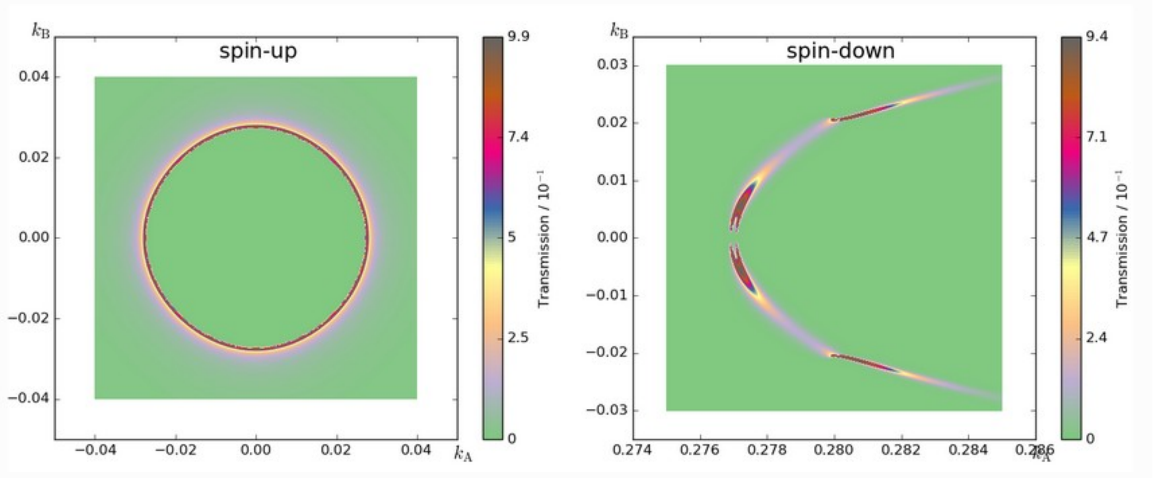


Restricting the grid range

- Provide the zoom.py script.
- This script shows how the adaptive grid class can be used to resolve only a specific features of the spin-up and spin-down k-dependent transmission.
- A relative tolerance of 10^{-3} is used to fully resolve the transmission features.
- The below figures show the spin-up and spin-down transmissions.



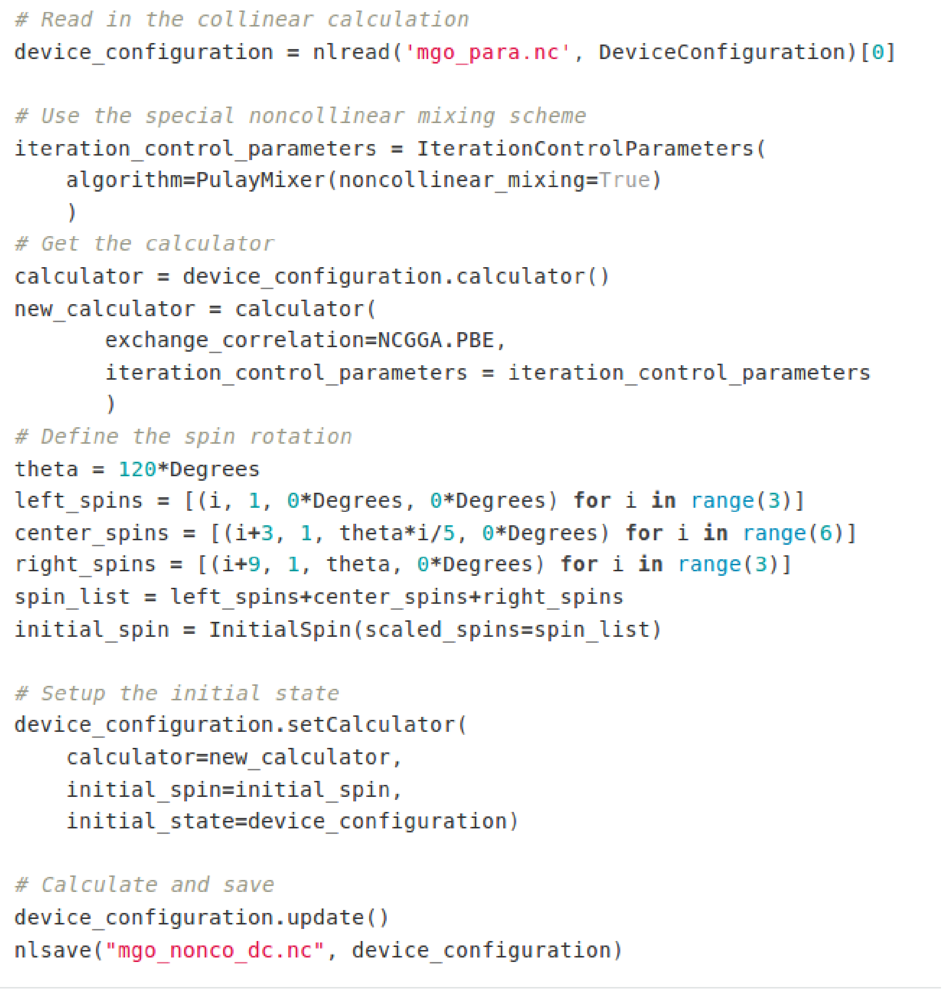
```
# -------------------------------------------------------------
# Load device configuration
# -------------------------------------------------------------
device_configuration = nlread('mgo_para.nc', DeviceConfiguration)[0]

# -------------------------------------------------------------
# Transmission Spectrum zoom #1.
# -------------------------------------------------------------
adaptive_grid = AdaptiveGrid(
    kA_range=[-0.04, 0.04],
    kB_range=[-0.04, 0.04],
    tolerance=0.001,
    error_measure=Relative)

transmission_spectrum = TransmissionSpectrum(
    configuration=device_configuration,
    energies=numpy.linspace(0,0,1)*eV,
    kpoints=adaptive_grid,
    )
nlsave('zoom.nc', transmission_spectrum)

# -------------------------------------------------------------
# Transmission Spectrum zoom #2.
# -------------------------------------------------------------
adaptive_grid = AdaptiveGrid(
    kA_range=[0.275, 0.285],
    kB_range=[-0.03, 0.03],
    tolerance=0.001,
    error_measure=Relative)

transmission_spectrum = TransmissionSpectrum(
    configuration=device_configuration,
    energies=numpy.linspace(0,0,1)*eV,
    kpoints=adaptive_grid,
    )
nlsave('zoom.nc', transmission_spectrum)
```



Computing the non-collinear device configuration

Editor

- ❖ Requires non-collinear definition of the electron spin.
- ❖ Device configuration: read the collinear configuration mgo_para.nc
- ❖ New Calculator : replace SGGA.PBE by NCGGA.PBE exchange and correlation.
- ❖ Define the spin rotation: theta= 120 degrees
- ❖ Setup the initial state: new calculator and spin
- ❖ Update and save the device configuration.

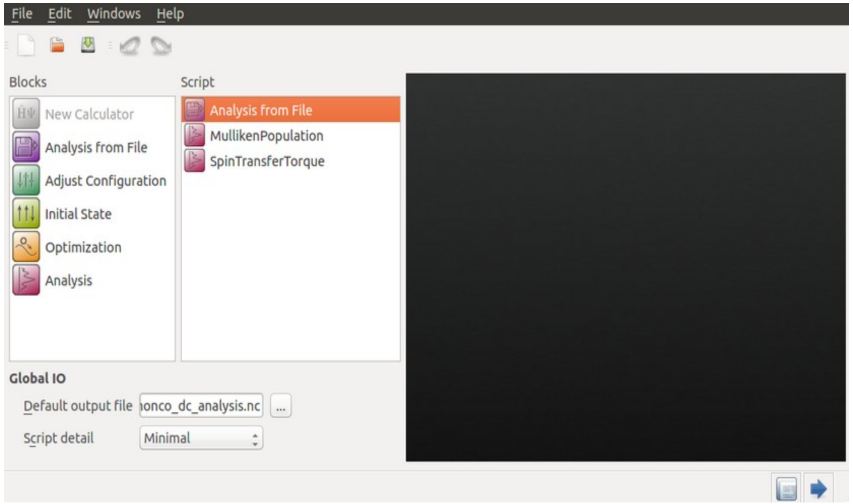


```
# Read in the collinear calculation
device_configuration = nlread('mgo_para.nc', DeviceConfiguration)[0]

# Use the special noncollinear mixing scheme
iteration_control_parameters = IterationControlParameters(
    algorithm=PulayMixer(noncollinear_mixing=True)
    )
# Get the calculator
calculator = device_configuration.calculator()
new_calculator = calculator(
       exchange_correlation=NCGGA.PBE,
       iteration_control_parameters = iteration_control_parameters
       )
# Define the spin rotation
theta = 120*Degrees
left_spins = [(i, 1, 0*Degrees, 0*Degrees) for i in range(3)]
center_spins = [(i+3, 1, theta*i/5, 0*Degrees) for i in range(6)]
right_spins = [(i+9, 1, theta, 0*Degrees) for i in range(3)]
spin_list = left_spins+center_spins+right_spins
initial_spin = InitialSpin(scaled_spins=spin_list)

# Setup the initial state
device_configuration.setCalculator(
    calculator=new_calculator,
    initial_spin=initial_spin,
    initial_state=device_configuration)

# Calculate and save
device_configuration.update()
nlsave("mgo_nonco_dc.nc", device_configuration)
```

Mulliken population and Spin Transfer Torque

Scripter

- ❖ Analysis from file
  - – Select the mgo_nonco_dc.nc file
- ❖ MullikenPopulation
- ❖ SpinTransferTorque.
  - – Energy: 0eV
  - – Contributions: Left to calculate **left → right** linear response current.
  - – Send the script to the Editor and replace the Monkhorst-Pack grid by the Adaptive grid.

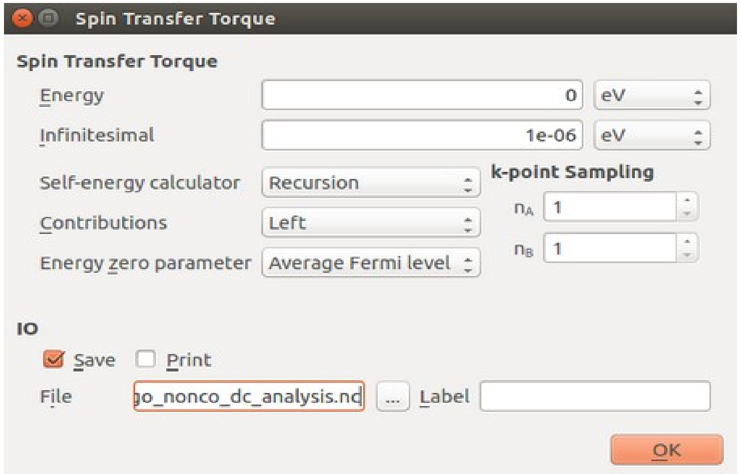


Script: Analysis from File, MullikenPopulation, SpinTransferTorque

Global IO

Default output file: ıonco_dc_analysis.nc

Script detail: Minimal



Spin Transfer Torque

Energy	0	eV
Infinitesimal	1e-06	eV
Self-energy calculator	Recursion	
Contributions	Left	
Energy zero parameter	Average Fermi level	

k-point Sampling

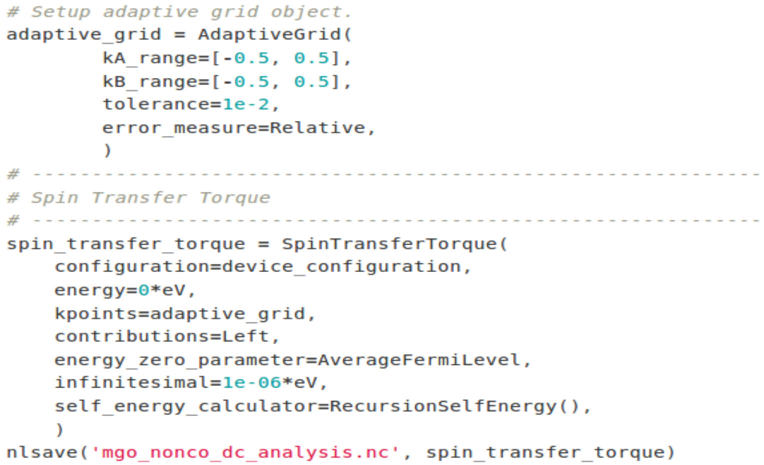
n_A: 1

n_B: 1

IO

☑ Save □ Print

File: jo_nonco_dc_analysis.nc Label:

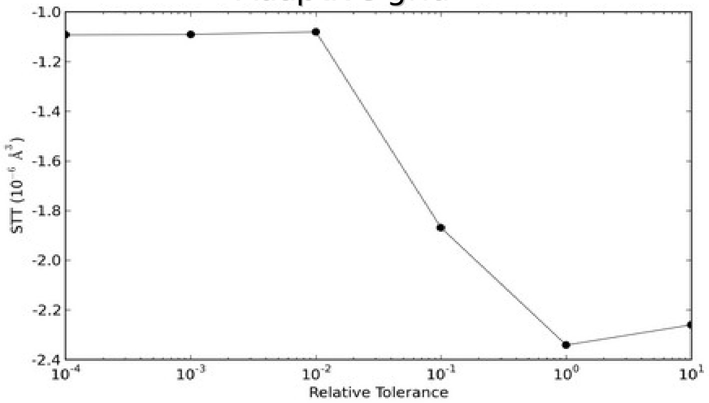


```
# Setup adaptive grid object.
adaptive_grid = AdaptiveGrid(
        kA_range=[-0.5, 0.5],
        kB_range=[-0.5, 0.5],
        tolerance=1e-2,
        error_measure=Relative,
        )
# -------------------------------------------------------------
# Spin Transfer Torque
# -------------------------------------------------------------
spin_transfer_torque = SpinTransferTorque(
    configuration=device_configuration,
    energy=0*eV,
    kpoints=adaptive_grid,
    contributions=Left,
    energy_zero_parameter=AverageFermiLevel,
    infinitesimal=1e-06*eV,
    self_energy_calculator=RecursionSelfEnergy(),
    )
nlsave('mgo_nonco_dc_analysis.nc', spin_transfer_torque)
```

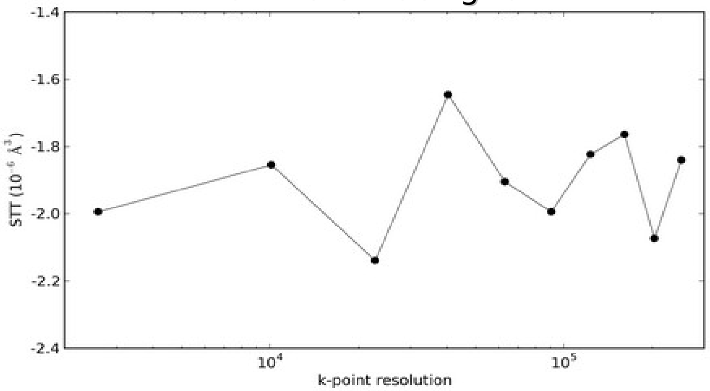
Convergence of the total spin-transfer torque

- We are using a **relative tolerance of 10^{-2}** for the adaptive grid.
- The spin-transfer torque must be computed using the relative tolerance at which the total transferred torque at the right side is converged.
- We have calculated the total spin-transfer torque in the right side for different relative tolerances.
- Use of 10-2 relative tolerance seems to be sufficient.
- Using a Monkhorst-Pack grid the total spin-transfer torque does not reach the convergence.

Adaptive grid



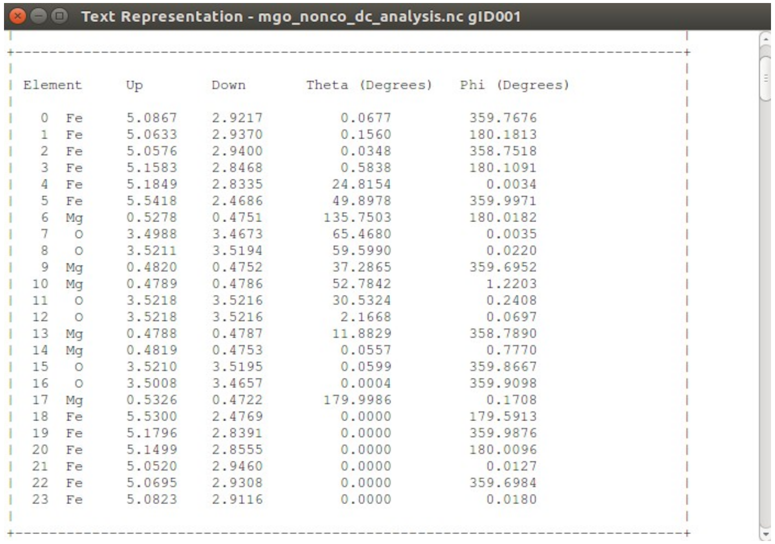
Monkhorst-Pack grid



Analysis of the results

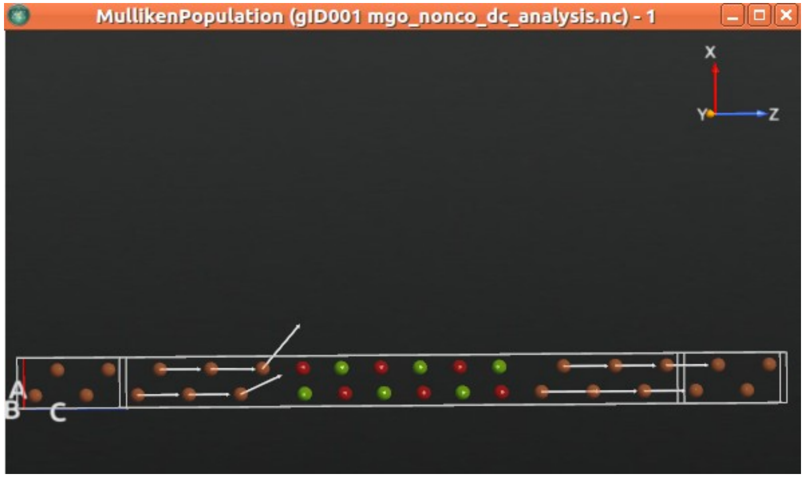
Mulliken Population

- Inspect the Mulliken charge and the components of the spin polarization vector using the text representation.
- The sum of up and down populations corresponds to the Mulliken charge (number of electrons) .
- The difference of these populations combined with the two angles (Theta and Phi) forms the spin polarization vector. This vector can be visualized using the Viewer.



Text Representation - mgo_nonco_dc_analysis.nc gID001

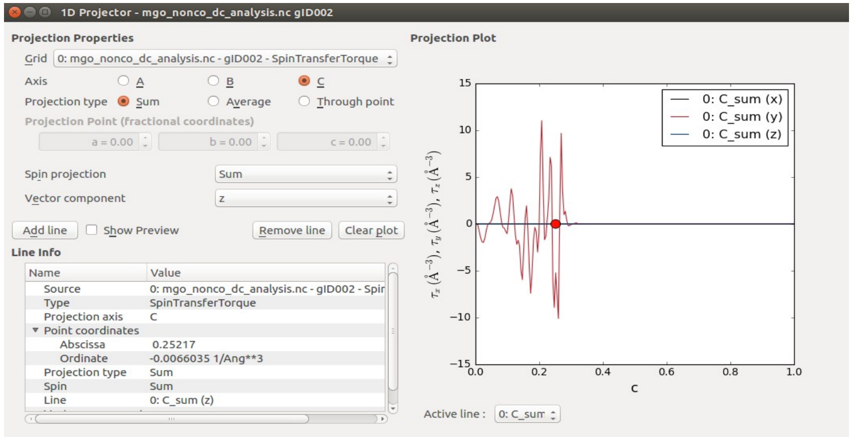
```
|
+------------------------------------------------------------------------------+
|
| Element      Up         Down         Theta (Degrees)   Phi (Degrees)
|
|   0  Fe     5.0867     2.9217         0.0677           359.7676
|   1  Fe     5.0633     2.9370         0.1560           180.1813
|   2  Fe     5.0576     2.9400         0.0348           358.7518
|   3  Fe     5.1583     2.8468         0.5838           180.1091
|   4  Fe     5.1849     2.8335        24.8154             0.0034
|   5  Fe     5.5418     2.4686        49.8978           359.9971
|   6  Mg     0.5278     0.4751       135.7503           180.0182
|   7   O     3.4988     3.4673        65.4680             0.0035
|   8   O     3.5211     3.5194        59.5990             0.0220
|   9  Mg     0.4820     0.4752        37.2865           359.6952
|  10  Mg     0.4789     0.4786        52.7842             1.2203
|  11   O     3.5218     3.5216        30.5324             0.2408
|  12   O     3.5218     3.5216         2.1668             0.0697
|  13  Mg     0.4788     0.4787        11.8829           358.7890
|  14  Mg     0.4819     0.4753         0.0557             0.7770
|  15   O     3.5210     3.5195         0.0599           359.8667
|  16   O     3.5008     3.4657         0.0004           359.9098
|  17  Mg     0.5326     0.4722       179.9986             0.1708
|  18  Fe     5.5300     2.4769         0.0000           179.5913
|  19  Fe     5.1796     2.8391         0.0000           359.9876
|  20  Fe     5.1499     2.8555         0.0000           180.0096
|  21  Fe     5.0520     2.9460         0.0000             0.0127
|  22  Fe     5.0695     2.9308         0.0000           359.6984
|  23  Fe     5.0823     2.9116         0.0000             0.0180
|
+------------------------------------------------------------------------------+
```



Analysis of the results

Spin-transfer torque

- The spatial components of the spin-transfer torque can be plotted using the **1D Projector**.
- Visualize the spatial components of the Spin-transfer torque using the Viewer. The below figure shows the isosurface of the "y" component.



1D Projector - mgo_nonco_dc_analysis.nc gID002

Projection Properties

Grid: 0: mgo_nonco_dc_analysis.nc - gID002 - SpinTransferTorque

Axis: ○ A ○ B ● C

Projection type: ● Sum ○ Average ○ Through point

Projection Point (fractional coordinates): a = 0.00 b = 0.00 c = 0.00

Spin projection: Sum

Vector component: z

Add line □ Show Preview Remove line Clear plot

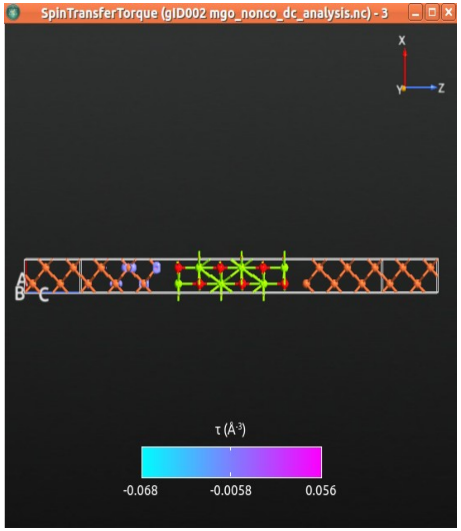
Line Info

Name	Value
Source	0: mgo_nonco_dc_analysis.nc - gID002 - Spir
Type	SpinTransferTorque
Projection axis	C
▾ Point coordinates	
Abscissa	0.25217
Ordinate	-0.0066035 1/Ang**3
Projection type	Sum
Spin	Sum
Line	0: C_sum (z)

Projection Plot

15
10
5
0
−5
−10
−15
$\tau_x\,(\mathrm{\AA}^{-3}),\ \tau_y\,(\mathrm{\AA}^{-3}),\ \tau_z\,(\mathrm{\AA}^{-3})$
0.0
0.2
0.4
0.6
0.8
1.0
C
0: C_sum (x)
0: C_sum (y)
0: C_sum (z)

Active line : 0: C_sum



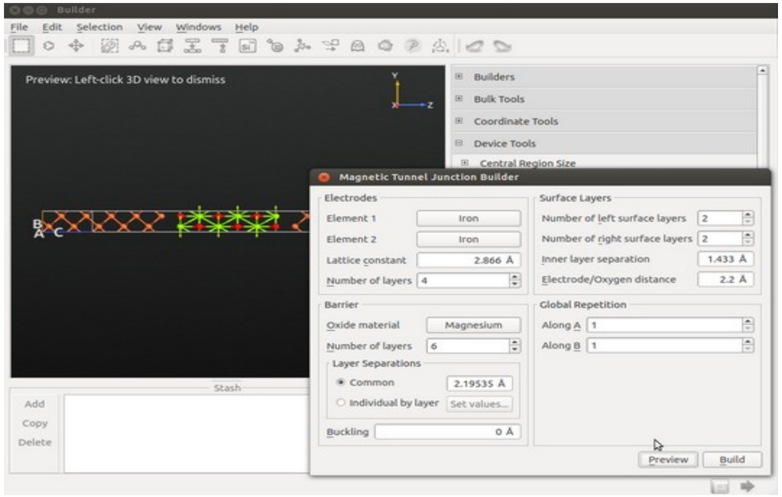
SpinTransferTorque (gID002 mgo_nonco_dc_analysis.nc) - 3

Optimizing the junction geometry

Builder

1.- Use Add → From Plugin → Magnetic Tunnel Junction (FeMgO-style). Change the number the barriers to 6 and number to surface layers to 2 on both left and right side and leave the other parameters as they are by default.

2.- Convert the device geometry to bulk send the structure to the Script Generator to optimize it by keeping **Rigid** the last two layers of Fe.



Magnetic Tunnel Junction Builder

Electrodes
Element 1: Iron
Element 2: Iron
Lattice constant: 2.866 Å
Number of layers: 4

Surface Layers
Number of left surface layers: 2
Number of right surface layers: 2
Inner layer separation: 1.433 Å
Electrode/Oxygen distance: 2.2 Å

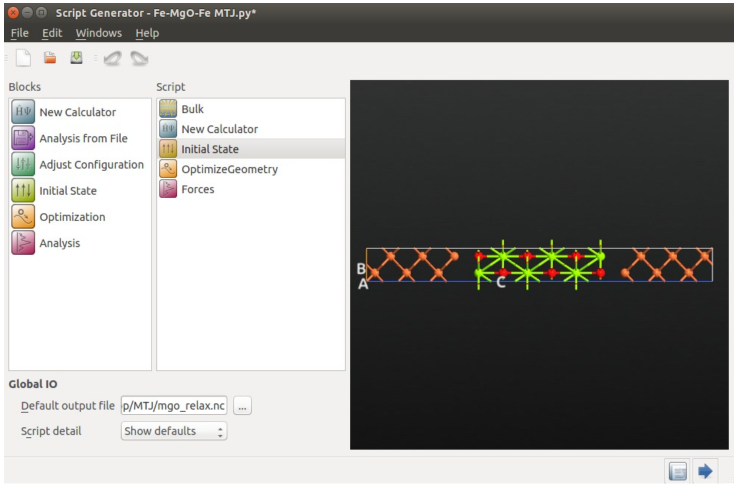
Barrier
Oxide material: Magnesium
Number of layers: 6
Layer Separations
● Common: 2.19535 Å
○ Individual by layer: Set values...
Buckling: 0 Å

Global Repetition
Along A: 1
Along B: 1

Optimizing the junction geometry

Script Generator

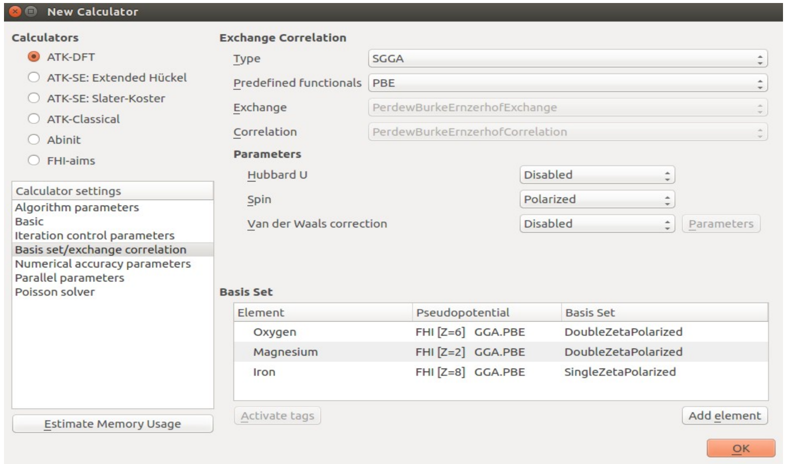
- New Calculator
  - Spin: Polarized
  - Exchange-correlation: SGGA.PBE
  - Electron temperature: 1200 Kelvin.
  - K-point sampling: (7,7,100)
- Initial State.
  - Initial State: User spin
  - Relative spin: 0 for Mg and O and 1 for Fe.



Global IO

Default output file: p/MTJ/mgo_relax.nc

Script detail: Show defaults



Calculators:
● ATK-DFT
○ ATK-SE: Extended Hückel
○ ATK-SE: Slater-Koster
○ ATK-Classical
○ Abinit
○ FHI-aims

Exchange Correlation

Type: SGGA

Predefined functionals: PBE

Exchange: PerdewBurkeErnzerhofExchange

Correlation: PerdewBurkeErnzerhofCorrelation

Parameters

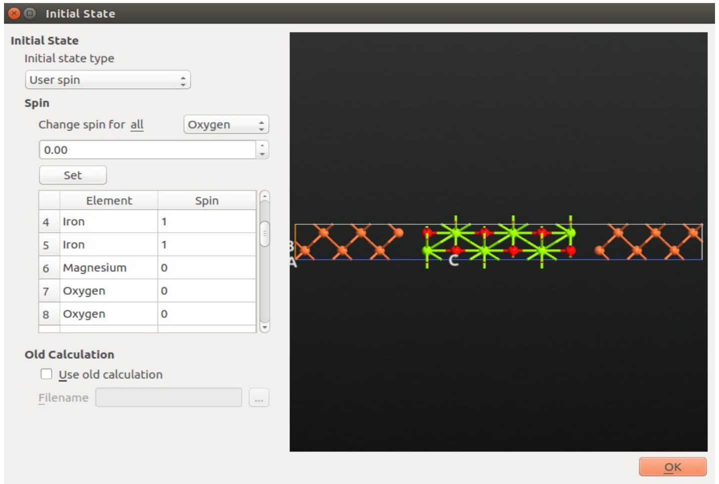
Hubbard U: Disabled

Spin: Polarized

Van der Waals correction: Disabled

Basis Set

Element	Pseudopotential	Basis Set
Oxygen	FHI [Z=6] GGA.PBE	DoubleZetaPolarized
Magnesium	FHI [Z=2] GGA.PBE	DoubleZetaPolarized
Iron	FHI [Z=8] GGA.PBE	SingleZetaPolarized



Initial State

Initial state type: User spin

Spin

Change spin for all: Oxygen

0.00

	Element	Spin
4	Iron	1
5	Iron	1
6	Magnesium	0
7	Oxygen	0
8	Oxygen	0

Old Calculation

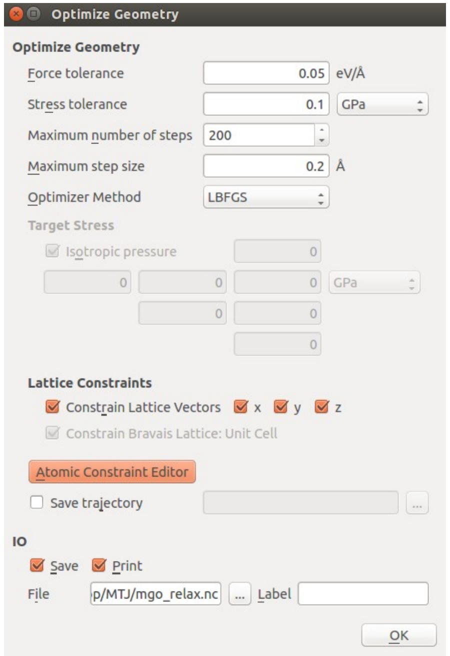
□ Use old calculation

Filename

Optimizing the junction geometry

Script Generator

- OptimizeGeometry
  - Keep the first and last four atoms rigid.
- Forces



Optimize Geometry

Optimize Geometry

Force tolerance: 0.05 eV/Å

Stress tolerance: 0.1 GPa

Maximum number of steps: 200

Maximum step size: 0.2 Å

Optimizer Method: LBFGS

Target Stress

☑ Isotropic pressure: 0

0 0 0 GPa

0 0

0

Lattice Constraints

☑ Constrain Lattice Vectors ☑ x ☑ y ☑ z

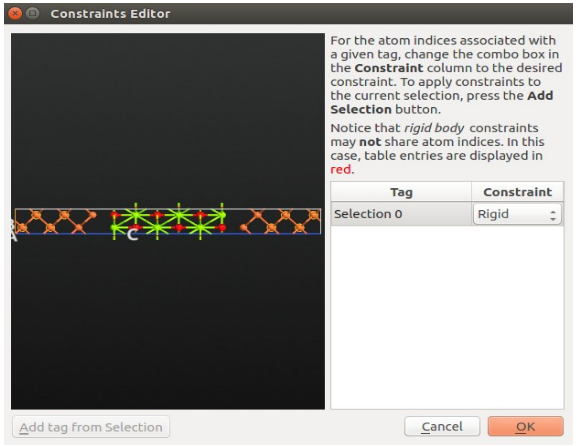
☑ Constrain Bravais Lattice: Unit Cell

□ Save trajectory

IO

☑ Save ☑ Print

File: p/MTJ/mgo_relax.nc ... Label:



Constraints Editor

For the atom indices associated with a given tag, change the combo box in the **Constraint** column to the desired constraint. To apply constraints to the current selection, press the **Add Selection** button.

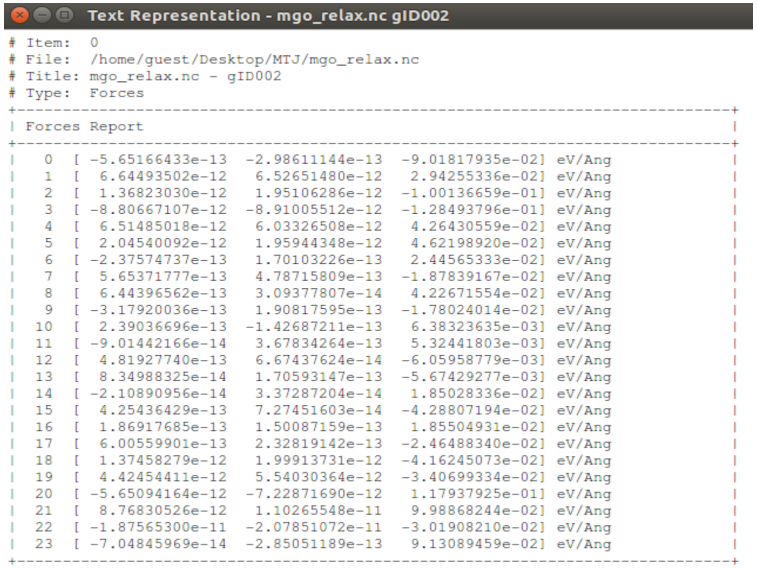
Notice that *rigid body* constraints may **not** share atom indices. In this case, table entries are displayed in red.

Tag	Constraint
Selection 0	Rigid

Analysis of the results

Forces

- Zero in x-y direction.
- Less that the optimization criteria (0.05 eV/Ang) for atoms which have been relaxed.
- For the electrode extension the forces are slightly larger and the force vectors point out of the cell (cell under compressive strain).
- Adding more surface to increase the cell length in z direction would lower the strain but would have very little effect on the results in the present case.



```
# Item:  0
# File:  /home/guest/Desktop/MTJ/mgo_relax.nc
# Title: mgo_relax.nc - gID002
# Type:  Forces
+------------------------------------------------------------------------------+
| Forces Report                                                                |
+------------------------------------------------------------------------------+
|   0  [ -5.65166433e-13  -2.98611144e-13  -9.01817935e-02] eV/Ang             |
|   1  [  6.64493502e-12   6.52651480e-12   2.94255336e-02] eV/Ang             |
|   2  [  1.36823030e-12   1.95106286e-12  -1.00136659e-01] eV/Ang             |
|   3  [ -8.80667107e-12  -8.91005512e-12  -1.28493796e-01] eV/Ang             |
|   4  [  6.51485018e-12   6.03326508e-12   4.26430559e-02] eV/Ang             |
|   5  [  2.04540092e-12   1.95944348e-12   4.62198920e-02] eV/Ang             |
|   6  [ -2.37574737e-13   1.70103226e-13   2.44565333e-02] eV/Ang             |
|   7  [  5.65371777e-13   4.78715809e-13  -1.87839167e-02] eV/Ang             |
|   8  [  6.44396562e-13   3.09377807e-14   4.22671554e-02] eV/Ang             |
|   9  [ -3.17920036e-13   1.90817595e-13  -1.78024014e-02] eV/Ang             |
|  10  [  2.39036696e-13  -1.42687211e-13   6.38323635e-03] eV/Ang             |
|  11  [ -9.01442166e-14   3.67834264e-13   5.32441803e-03] eV/Ang             |
|  12  [  4.81927740e-13   6.67437624e-14  -6.05958779e-03] eV/Ang             |
|  13  [  8.34988325e-14   1.70593147e-13  -5.67429277e-03] eV/Ang             |
|  14  [ -2.10890956e-14   3.37287204e-14   1.85028336e-02] eV/Ang             |
|  15  [  4.25436429e-13   7.27451603e-14  -4.28807194e-02] eV/Ang             |
|  16  [  1.86917685e-13   1.50087159e-13   1.85504931e-02] eV/Ang             |
|  17  [  6.00559901e-13   2.32819142e-13  -2.46488340e-02] eV/Ang             |
|  18  [  1.37458279e-12   1.99913731e-12  -4.16245073e-02] eV/Ang             |
|  19  [  4.42454411e-12   5.54030364e-12  -3.40699334e-02] eV/Ang             |
|  20  [ -5.65094164e-12  -7.22871690e-12   1.17937925e-01] eV/Ang             |
|  21  [  8.76830526e-12   1.10265548e-11   9.98868244e-02] eV/Ang             |
|  22  [ -1.87565300e-11  -2.07851072e-11  -3.01908210e-02] eV/Ang             |
|  23  [ -7.04845969e-14  -2.85051189e-13   9.13089459e-02] eV/Ang             |
+------------------------------------------------------------------------------+
```