# TITAN: A code and its applications for time-dependent transport and angular momentum in nanostructures

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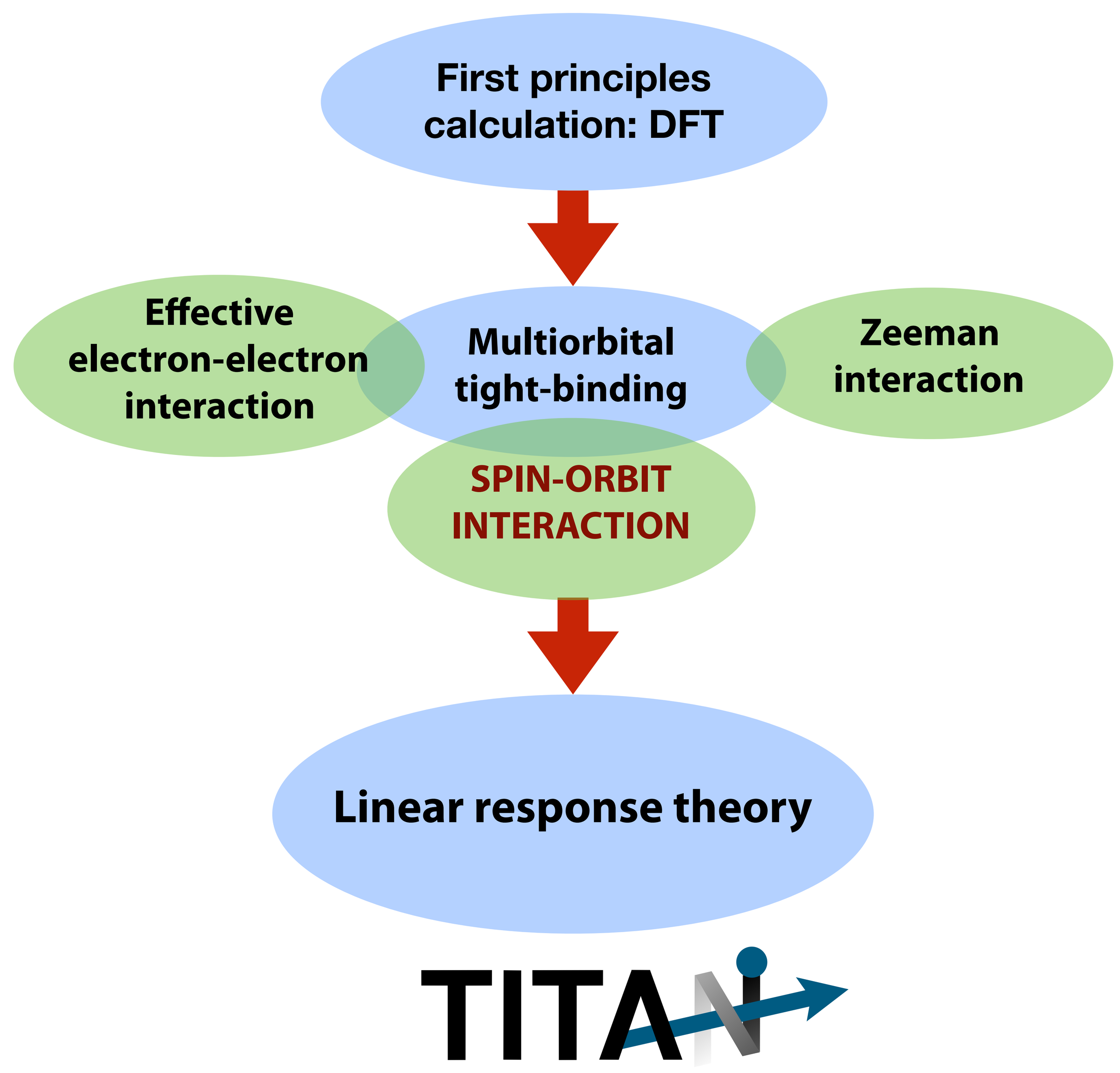
## Abstract

Spintronics has been a highly studied topic for decades, with already successful applications in technological devices and other promising routes for future implementations. In this work, we explore the magnetization dynamics using a multi-orbital tight-binding approach including the spin-orbit interaction by calculating the full magnetic susceptibility in a linear response formalism. This quantity is mapped into analytical expressions obtained from a phenomenological model to obtain all the relevant parameters - in particular, the damping constant (also known as Gilbert parameter). We use CLAIX, JURECA and JUQUEEN supercomputers to investigate typical magnetic bulk systems - Fe, Ni and Co - and compare the different methods available in the literature, establishing their range of validity.

## Methods




F. S. M. Guimarães et al., Sci. Rep. 7, 3686 (2017)
F. S. M. Guimarães et al., Phys. Rev. B 92, 220410(R) (2015)

## Magnetic perturbations

Dynamical magnetic susceptibility is the response of the magnetization to a time-dependent magnetic field:

$$\mathbf{m}(t) = \int \mathrm{d}t' \chi(t-t')\mathbf{B}(t')$$

It describes the single-particle (spin-flip) and collective (spin wave) excitation modes of the system.

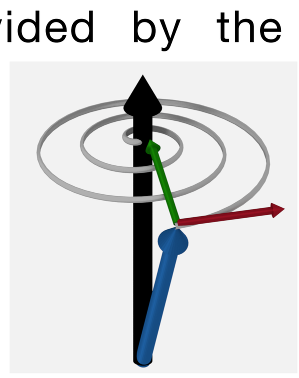
The quantum mechanical equation of motion:

$$\frac{\mathrm{d}\hat{\mathbf{S}}}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\left[\hat{\mathbf{S}}, \hat{H}_0 + \hat{H}_{\mathrm{SO}} + \hat{H}_{\mathrm{XC}}\right] = \mathbf{I}^{\mathrm{S}} + \mathbf{T}_{\mathrm{SO}} + \mathbf{T}_{\mathrm{XC}}$$

no spin pumping

is calculated in linear response and mapped into a phenomenological description provided by the Landau-Lifshitz-Gilbert equation:

$$\frac{\mathrm{d}\mathbf{M}}{\mathrm{d}t} = -\gamma\mathbf{M}\times\mathbf{B}^{\mathrm{eff}} + \frac{\alpha}{M}\mathbf{M}\times\frac{\mathrm{d}\mathbf{M}}{\mathrm{d}t}$$



## Damping parameter

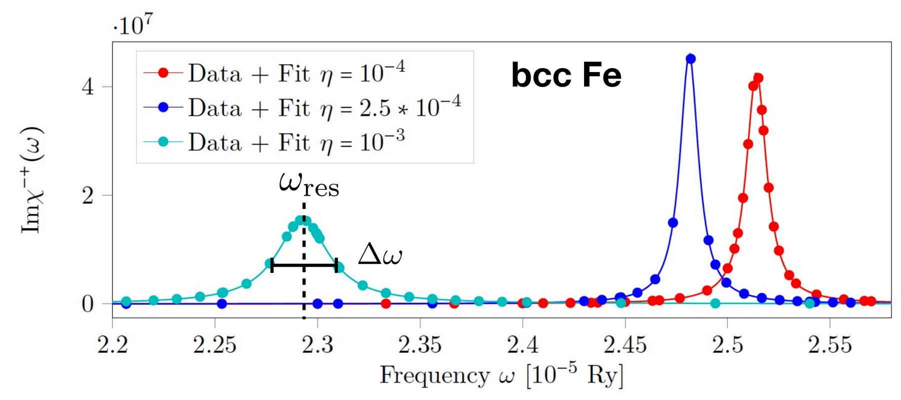
**There are many ways to obtain the damping parameter**

### Ferromagnetic resonance:

(similar to experiments)

$$\alpha = \frac{\Delta\omega}{\omega_{\mathrm{res}}}$$

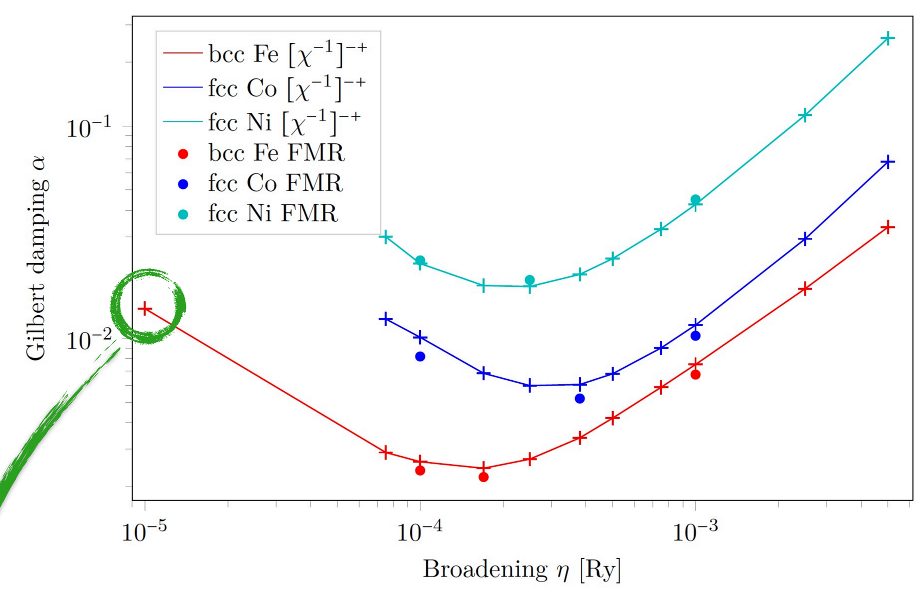
physica status solidi (b) **16**, K11 (1966)
J. Appl. Phys. **50**, 7726 (1979)




### Spin correlation slope:

$$\alpha = \frac{M}{\gamma}\lim_{\omega\to 0}\frac{[\chi^{-1}]^{-+}}{\omega}$$

Phys. Rev. B **79**, 064403 (2009)



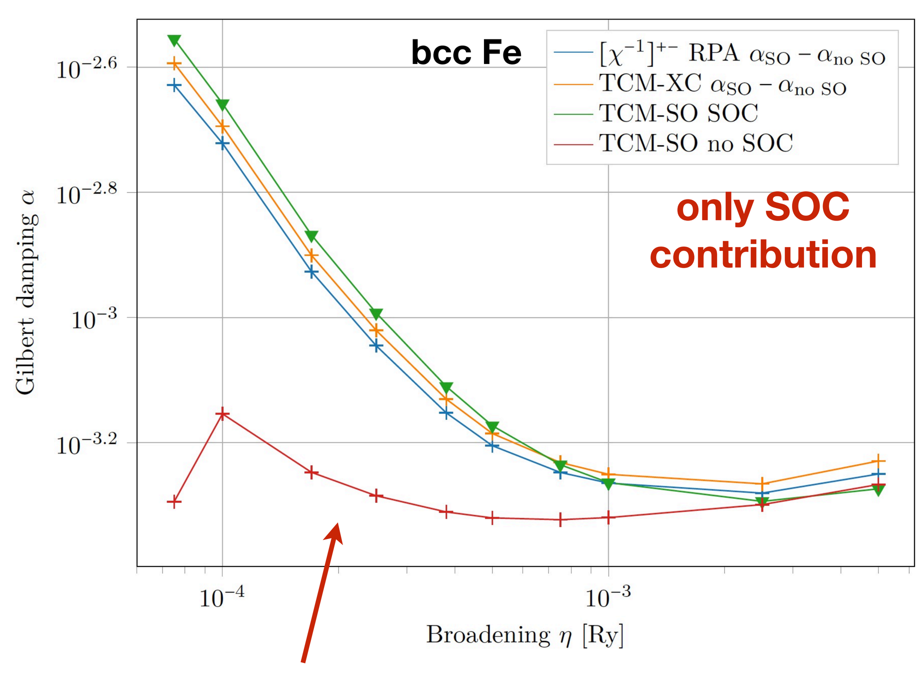

### Torque correlation methods:

$$\alpha = -\frac{1}{\pi\gamma M}\mathrm{Tr}\{\mathrm{Im}G(\epsilon_F)\hat{T}^{-}_{\mathrm{XC}}\mathrm{Im}G(\epsilon_F)\hat{T}^{+}_{\mathrm{XC}}\}$$ (TCM-XC)

Czech J. Phys. **26**, 1366–1383 (1976)
Phys. Rev. B **75**, 174434 (2007)

$$\alpha = -\frac{\gamma}{4\pi M}\mathrm{Tr}\{\mathrm{Im}G(\epsilon_F)\hat{T}^{-}_{\mathrm{SO}}\mathrm{Im}G(\epsilon_F)\hat{T}^{+}_{\mathrm{SO}}\}$$ (TCM-SO)

Phys. Rev. Lett. **101**, 037207 (2008)
Phys. Rev. Lett. **107**, 066603 (2011)

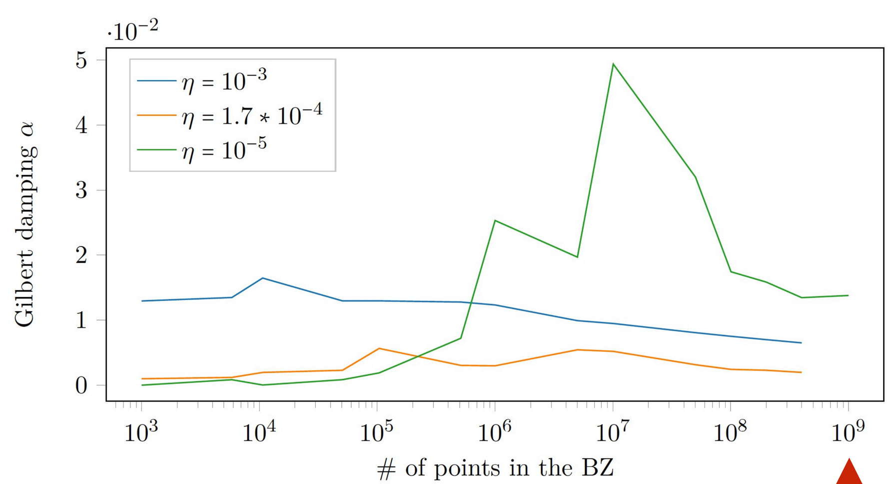



J. Phys.: Condens. Matter **28**, 086004 (2016)

**Different methods give distinct contributions**

## Convergence

**Low broadenings require a large amount of k-points**

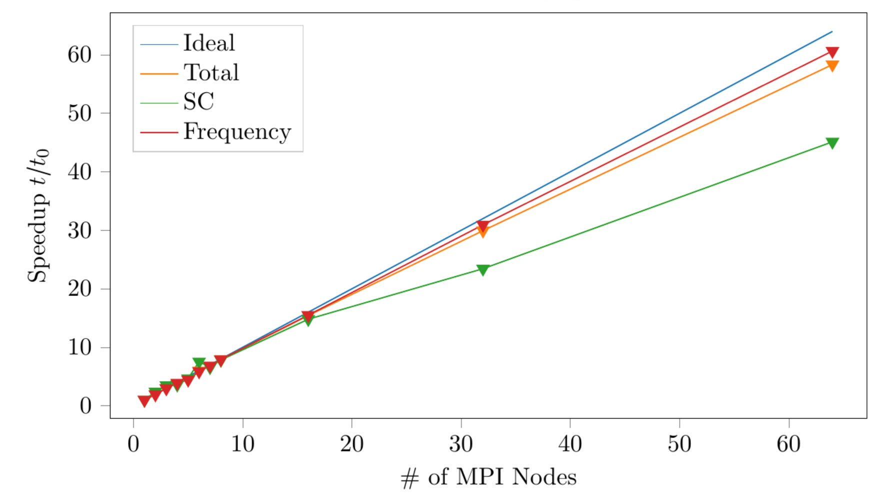



**1 billion k-points needed!**

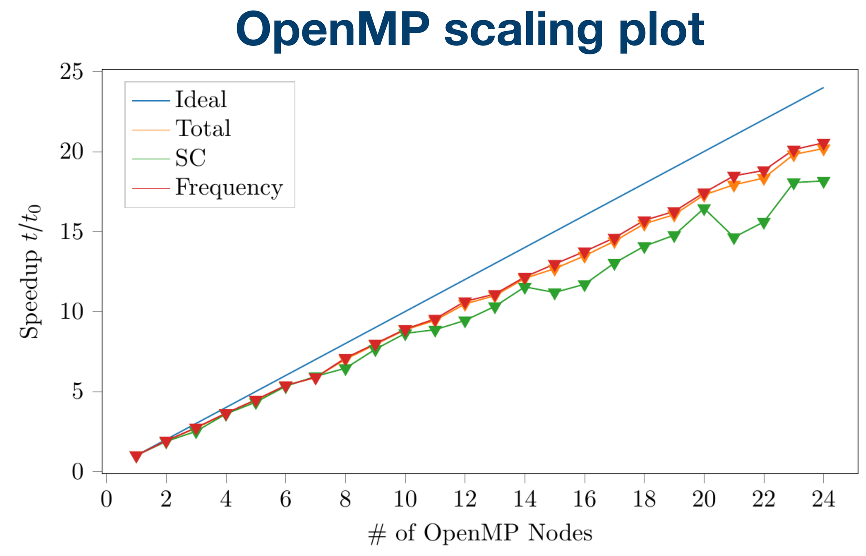
## Performance

**Hybrid parallelization**
**+**
**Local generation of workload**

### MPI scaling plot




### OpenMP scaling plot



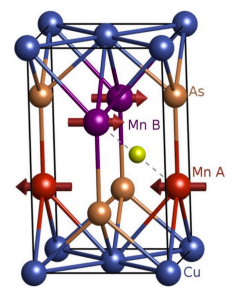

**Efficient use of large number of computing nodes**

## Conclusions

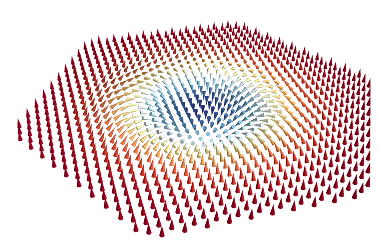
- TITAN is a powerful tool to calculate dynamical quantities, such as the damping parameter
- Systematic assessment of the Gilbert damping is necessary to unravel its nature
- Damping diverges in the clean system limit, if the spin-orbit interaction is present
- Spin-correlation methods yield total damping while torque-correlation (SO) only includes spin-orbit contribution

## Perspectives

We are interested in the dynamical properties of



Antiferromagnets



Topological spin textures

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