I present two developments that aim to improve the description of strongly correlated systems. First, I detail the implementation of the ”charge-only-DFT”$+U$ method proposed in Refs. [1]. It intents to improve the description of exchange in usual DFT+$U$. I show the benchmark of the implementation on magnetic effects on iron and I show the application of this method for properties of actinides [2]. Secondly, I present the implementation of $k$-resolved spectral function in DFT+DMFT. It requires the analytic continuation of the self energy from the imaginary frequency axis to the real frequency axis. I show the example of OmegaMaxent [3] which uses the Maximum Entropy method to do this continuation. I benchmark the implementation of spectral function in SrVO$_3$, and I show the application to $\alpha$-cerium (cf Fig 1).

Figure 1: $k$ resolved LDA+DMFT spectral function of $\alpha$-cerium (U=6 eV)

References

