A multi-scale modelling roadmap is presented to simulate precipitation and precipitation hardening in metallic alloys. The first step of the simulation strategy is the modelling of precipitate nucleation and growth [1-2]. This is achieved using classical nucleation theory coupled with phase field simulations. The driving forces are controlled by the different energy contributions (chemical free energy, interfacial energy, lattice parameters, elastic constants) that are obtained from either computational thermodynamics databases or from first-principles density functional theory. Afterwards, two different strategies were used to determine the strengthening provided by either small precipitates that can be sheared by dislocations or large precipitates which are overcome by the formation of Orowan loops. In the first case, the rate at which the dislocations shear the precipitates is given by an Arrhenius equation with a pre-exponential factor and an activation energy, that can be obtained by means of molecular dynamics simulations [3]. In the second situation, the mechanisms of dislocation/precipitate interaction were studied by means of discrete dislocation dynamics, which include the effect of precipitate size, shape and spatial distribution as well as the influence of the elastic mismatch and of the stress-free transformation strains [4].

The multi-scale modelling strategy was applied to analyse precipitation hardening in Al-Cu alloys strengthened with Guinier-Preston zones, ’ and ’ precipitates. The simulation results in terms of the precipitate aspect ratio and spatial distribution as well as of critical resolved shear stress were compared with experimental results. It is demonstrated that quantitative estimations of the strengthening provided by precipitates in metallic alloys can be achieved using multi-scale modelling strategies based in first principles calculations.