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Amyloid aggregation: numerical challenges to understanding the onset of oligomerisation

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Amyloid aggregation is associated with a number of degenerative diseases such as Alzheimers and Parkinsons diseases. During amyloid formation, various proteins, that are often disordered as monomers, assemble into toxic beta-sheet dominated oligomers. This off-equilibrium dynamical process is difficult to characterize experimentally and even the basic properties of these oligomers remain unknown although some universal structural features have been demonstrated indirectly. To go beyond experimental limitations, it is useful to turn to computational atomistic simulations. These can provide much needed insights about the microscopic nature of the oligomerization process as well as provide support for interpreting experimental results. Yet, challenges are numerous in the computational side too, associate both with limitations of the computational tools and the gaps in the basic physics of this process. Building on work done within my group and numerous collaborators, I will discuss these challenges and identify some way to address them.