

## Folding and Unfolding of Proteins

Ana Carpio, Universidad Complutense de Madrid

Single-molecule atomic force spectroscopy probes elastic properties of proteins such as titin and ubiquitin [3, 4]. We analyze bioprotein folding dynamics under both force and length-clamp conditions by modeling polyprotein modules as particles in a bistable potential, connected by harmonic springs [1, 2]. The study of multistable equilibria in these models explains recorded sawtooth force-extension curves. We show that bifurcations and transitions through quasi-stationary domain configurations [5, 6, 7] modified by thermal noise [8] are involved in observed stepwise and abrupt refolding and unfolding phenomena under force-clamp conditions. These predictions agree with experimental observations [2].

### References

- [1] L.L. Bonilla, A. Carpio, A. Prados, Theory of force-extension curves for modular proteins and DNA hairpins, *Physical Review E* 91, 052712, 2015
- [2] L.L. Bonilla, A. Carpio, A. Prados, Protein unfolding and refolding as transitions through virtual states, *EPL (Europhysics Letters)* 108, 28002, 2014
- [3] A. Prados, A. Carpio, L.L. Bonilla, Sawtooth patterns in force-extension curves of biomolecules: an equilibrium-statistical-mechanics theory, A. Prados, A. Carpio, L.L. Bonilla, *Physical Review E* 88, 012704, 2013
- [4] A. Prados, A. Carpio, L.L. Bonilla, Spin-oscillator model for the unzipping of biomolecules by mechanical force, *Physical Review E* 86, 021919, 2012
- [5] A. Carpio, I. Peral, Propagation failure along myelinated nerves, *Journal of Nonlinear Science* 21, 499-520, 2011
- [6] A. Carpio, Wave trains, self-oscillations and synchronization in discrete media, *Physica D-Nonlinear Phenomena* 207, 117-136, 2005

- [7] A. Carpio, Asymptotic construction of pulses in the discrete Hodgkin-Huxley model for myelinated nerves, *Physical Review E* 72, 011905, 2005
- [8] A. Carpio, L.L. Bonilla, A. Luzon, Effects of disorder on the wave front depinning transition in spatially discrete systems, *Physical Review E* 65, 035207, 2002