



Université
de Paris

Frédéric van Wijland
Professor
Head of the Theory of Complex Systems group
Head of the ICFP Master 2 Theory track
Laboratoire Matière et Systèmes Complexes
Université de Paris
10 rue Alice Domon et Léonie Duquet
75013 Paris, France
Phone: +33 1 57 27 62 54
fvw@u-paris.fr
frederic.vanwijland.org

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Glassiness and chaotic dynamics in high space dimension

In collaboration with A. Altieri & J. Tailleur

About being glassy.— The emergence of glassiness in the dynamics of a system made of a large number of interacting particles rests on a combination of factors. On the one hand, the rugged energy landscape the particles evolve in, with its large number of degenerate minima, has been invoked as the main culprit for the slowing down of the dynamics below some typical temperature. On the other hand, there exist purely dynamical models of interacting degrees of freedom (spins, typically), whose phenomenology is similar to that of glasses, but which nevertheless possess a completely flat energy landscape, thereby casting doubt on the purely energetic interpretation of glassiness. These are called kinetically constrained models. However, there is no microscopics-based theory that supports the relevance of kinetically-constrained models to interacting particle systems. In a recent series of works, it has been shown that working in a space with infinitely many dimensions made some predictions and analyses considerably easier, albeit with the possibility that working in infinite dimensions brings in some spurious simplifications that may not hold in two or three dimensional systems. The project that is hereafter described lies within this framework:

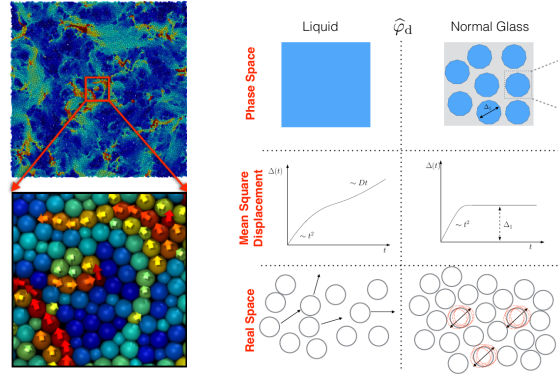


Figure 1: Left: a view of a dynamical heretogeneity in a two-dimensional glass former, taken from [8]. Right: Emergence of caging as density is increased, taken from [5].

this is an attempt to bring both approaches closer to each other using the technical simplifications that working in a space with a large number of dimensions allows for.

What do we know?— As a quick summary of the state of the art (details can be found in a recent book by Parisi, Urbani and Zamponi [11]), it is possible to show that the onset of dynamical glassiness coincides with the proliferation of metastable states in the energy landscape [10]. This remarkable coincidence (between static signatures of glassiness and dynamical ones) has been established mathematically for hard-spheres undergoing Langevin dynamics. However, in the course of this derivation, the microscopic and mesoscopic mechanisms by which glassiness sets in are somewhat blurred. In particular, such anisotropic structures as dynamical heretogeneities have been shown [8] to control the dynamics in the supercooled regime but, if they are still relevant in high space dimensions, they definitely have gone unnoticed.

What are the questions we would like to answer?—

1. A natural question is whether the infinite-dimensional limit simply bypasses dynamical heterogeneities (which could possible exist only in low space dimensions), or whether these do exist also in infinite-dimensions, in a guise yet to unravel.
2. The one-to-one mapping between static and dynamical properties works for Langevin dynamics (see [3] for an in-depth discussion in the field of spin dynamics). Can we devise alternative dynamical evolution rules, that nevertheless sample the same Boltzmann equilibrium

distribution, that allow for accelerated dynamics (and that would therefore circumvent the obstacles that slow the dynamics down in the regular Langevin dynamics). Can we use these fictitious dynamics to identify the relevant structures of phase space that actually cause glassiness.

3. The caging picture is appealing, and the vanishing of the diffusion constant is a way to capture this effect. But the anisotropic nature of dynamical heterogeneities is simply lacking. Perhaps more complex correlations involving *e.g.* the stress tensor, may provide alternative physical pictures.

What are the possible ways to take up these question?–

1. We speculate that the study of the tangent dynamics, because of its connections with the dynamics of local currents (see Chapter 2 in [12] for a pedagogical review) can perhaps be solved in infinitely-many dimensions. In addition, it will construct from the microscopics a vectorial observable known to characterize the transition from one local metastable structure to another. See also these references [15, 14, 9] for more details.
2. A theoretician has the ability to tune dynamical evolution rules while respecting the detailed balance condition so as to ensure the proper Boltzmann equilibrium distribution is sampled. It is possible to use that freedom to our advantage: by modifying the dynamics, and by trying to solve it in the infinite-dimensional limit, differences with standard dynamics will probably emerge, and these will point to the structures that actually matter for realistic physical evolution rules. These ideas are rather recent [7, 13, 16] so that their concrete consequences in the infinite-dimensional limit are yet to be explored.
3. The question of how to access transport properties is of course highly non-trivial (even for purely relaxational dynamics [6] early attempts show how difficult this is). However, with a newly developed scheme [4], we believe that sheared systems can be explored directly within their stationary state. In addition, we believe that exploring the dynamical correlations of observables more complex than the position (that gives access to the diffusion constant), such as the stress tensor, could be helpful in understanding the fate of dynamical heterogeneities. This is correlated to the recent series of works by Agoritsas, Maimbourg, Zamponi [1, 2].

What are the prerequisites?–

1. a strong background education in statistical mechanics, in and out of equilibrium, including stochastic calculus and field-theoretic approaches;
2. a strong interest for theoretical questions many people have stumbled on;
3. a certain taste for mathematical elegance.

References

- [1] Elisabeth Agoritsas, Thibaud Maimbourg, and Francesco Zamponi. Out-of-equilibrium dynamical equations of infinite-dimensional particle systems i. the isotropic case. *Journal of Physics A: Mathematical and Theoretical*, 52(14):144002, 2019.
- [2] Elisabeth Agoritsas, Thibaud Maimbourg, and Francesco Zamponi. Out-of-equilibrium dynamical equations of infinite-dimensional particle systems. ii. the anisotropic case under shear strain. *Journal of Physics A: Mathematical and Theoretical*, 52(33):334001, 2019.
- [3] Ada Altieri, Giulio Biroli, and Chiara Cammarota. Dynamical mean-field theory and aging dynamics. *Journal of Physics A: Mathematical and Theoretical*, 53(37):375006, aug 2020. URL: <https://doi.org/10.1088%2F1751-8121%2Faba3dd>, doi:10.1088/1751-8121/aba3dd.
- [4] Thibaut Arnoulx de Pirey, Gustavo Lozano, and Frédéric van Wijland. Active hard spheres in infinitely many dimensions. *Phys. Rev. Lett.*, 123:260602, Dec 2019. URL: <https://link.aps.org/doi/10.1103/PhysRevLett.123.260602>, doi:10.1103/PhysRevLett.123.260602.
- [5] Patrick Charbonneau, Jorge Kurchan, Giorgio Parisi, Pierfrancesco Urbani, and Francesco Zamponi. Glass and jamming transitions: From exact results to finite-dimensional descriptions. *Annual Review of Condensed Matter Physics*, 8:265–288, 2017.
- [6] Yves Elskens and Harry L Frisch. Kinetic theory of hard spheres in infinite dimensions. *Physical Review A*, 37(11):4351, 1988.
- [7] Hugo Jacquin, Bongsoo Kim, Kyozi Kawasaki, and Frédéric Van Wijland. Brownian dynamics: from glassy to trivial. *Physical Review E*, 91(2):022130, 2015.

- [8] Aaron S Keys, Lester O Hedges, Juan P Garrahan, Sharon C Glotzer, and David Chandler. Excitations are localized and relaxation is hierarchical in glass-forming liquids. *Physical Review X*, 1(2):021013, 2011.
- [9] Tanguy Laffargue, Julien Tailleur, and Frédéric Van Wijland. Lyapunov exponents of stochastic systems—from micro to macro. *Journal of Statistical Mechanics: Theory and Experiment*, 2016(3):034001, 2016.
- [10] Thibaud Maimbourg, Jorge Kurchan, and Francesco Zamponi. Solution of the dynamics of liquids in the large-dimensional limit. *Phys. Rev. Lett.*, 116:015902, Jan 2016. URL: <https://link.aps.org/doi/10.1103/PhysRevLett.116.015902>, doi:10.1103/PhysRevLett.116.015902.
- [11] Giorgio Parisi, Pierfrancesco Urbani, and Francesco Zamponi. *Theory of simple glasses: exact solutions in infinite dimensions*. Cambridge University Press, 2020.
- [12] Massimiliano Picciani. *Rare events in many-body systems: reactive paths and reaction constants for structural transitions*. PhD thesis, 2012.
- [13] Grzegorz Szamel. Theory for the dynamics of glassy mixtures with particle size swaps. *Physical Review E*, 98(5):050601, 2018.
- [14] Julien Tailleur, Sorin Tănase-Nicola, and Jorge Kurchan. Kramers equation and supersymmetry. *Journal of statistical physics*, 122(4):557–595, 2006.
- [15] Sorin Tănase-Nicola and Jorge Kurchan. Topological methods for searching barriers and reaction paths. *Physical review letters*, 91(18):188302, 2003.
- [16] Matthieu Wyart and Michael E Cates. Does a growing static length scale control the glass transition? *Physical review letters*, 119(19):195501, 2017.