Dynamical Mean-Field Theory in Statistical Physics: Glassy Dynamics, Ecosystems and Inter-Disciplinary Applications

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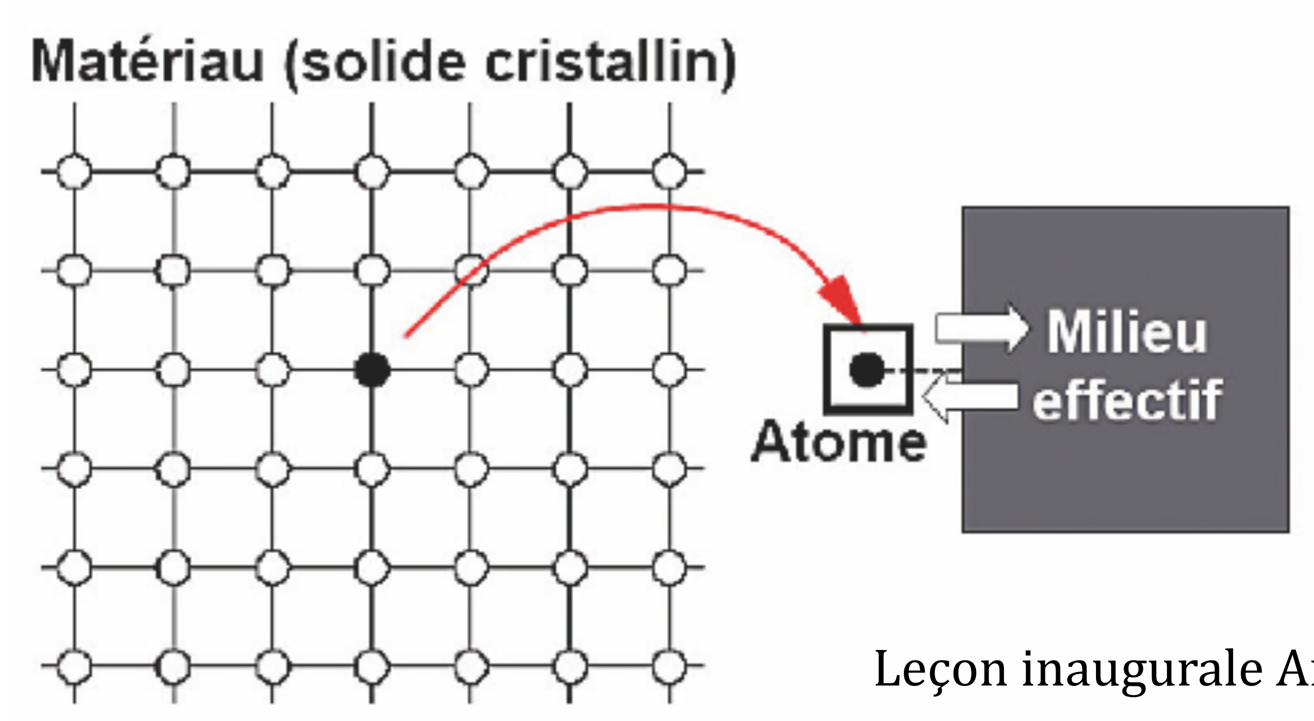
Dynamical Mean Field Theory in Strongly Correlated Electrons



Leçon inaugurale Antoine Georges

- ✦ DMFT for the Hubbard Model: theory of the Mott transition

Antoine Georges 2019 lectures

- ✦ Cluster extension of DMFT
    - theory of high-Tc superconductors
    - first principle methods for strongly correlated materials

Outline

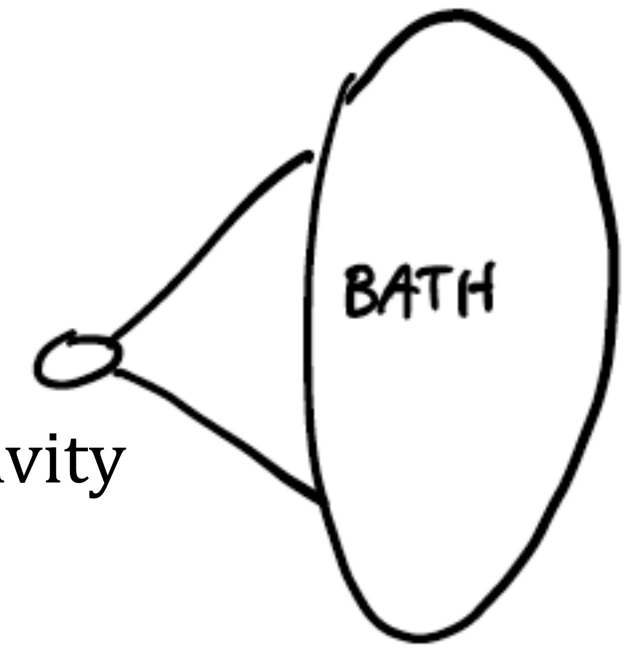
- The basis of DMFT in classical statistical physics:
    - thermal bath
    - self-consistency

- Applications of Dynamical Mean Field Theory:
    - Aging dynamics in spin-glasses
    - Theory of the glass transition
    - Chaotic dynamics in ecosystems

The two key ingredients of DMFT

1. Identify the correct degree of freedom and treat the rest of the system as a bath

2. The bath is statistically identical to the singled-out degree of freedom: self-consistency



cavity

An intermezzo on thermal baths

Coupling to a thermal bath

$$H = H_{Syst} + H_{Env} + H_{Int}$$

$$H_{Syst} = \frac{p^2}{2m} + V(x)$$

$$H_{Env} = \sum_k \frac{P_k^2}{2} + \frac{\omega_k^2 Q_k^2}{2}$$

$$H_I = -\sum_k \gamma_k Q_k x$$

Thermal bath

$$\frac{d^2 Q_k}{dt^2} = -\omega_k^2 Q_k + \gamma_k X(t) \; ; \; m\frac{d^2 x}{dt^2} = -V'(x) + \sum_k \gamma_k Q_k$$

$$m\frac{d^2 x}{dt^2} + \underbrace{\int_0^t K(t-s)\,\dot{x}(s)\,ds}_{\text{Dissipation: friction}} = -V'(x) - V'_{eff}(x) + \underbrace{\xi(t)}_{\text{Noise: Gaussian force}}$$

$$K(t) = \sum_k \frac{\gamma_k^2}{\omega_k^2}\cos(\omega_k t)$$

$$\langle \xi(t)\,\xi(t')\rangle = k_B T\, K(t-t')$$

$$V_{eff}(x) = -\frac{1}{2}\sum_k \frac{\gamma_k^2}{\omega_k^2}\, x^2$$

From Newton to Langevin with *generalized friction* and *thermal noise*

The two key ingredients of DMFT

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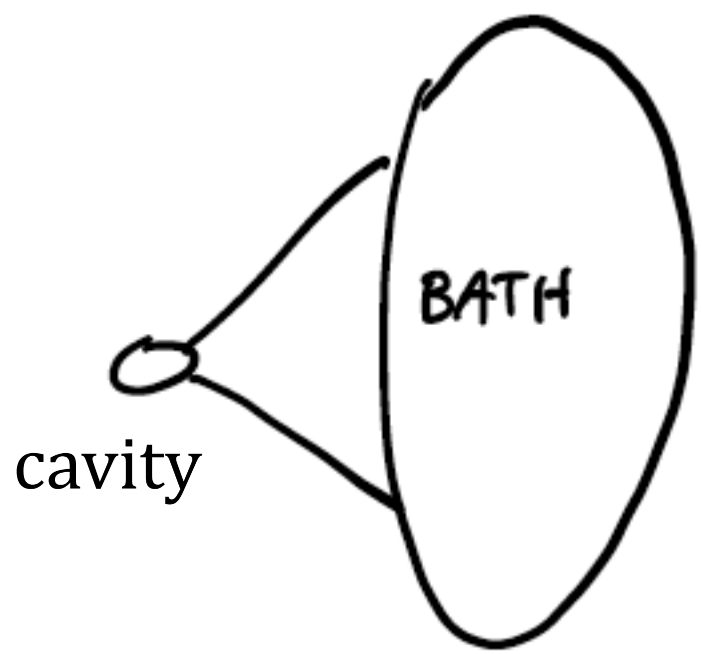


An example: mean-field spin glasses

$$\dot{S}_i = -\frac{\partial V}{\partial S_i} + \sum_{k(\neq i)} J_{ik} S_k + \xi_i(t)$$

$N \gg 1$

$$\overline{J_{ik}^2} = \frac{1}{N} \; ; \; V(S) = (S^2-1)^2 \; ; \; \langle \xi_i(t)\, \xi_k(t') \rangle = 2T \delta_{ik} \delta(t-t')$$

$$\dot{S}_k = -\frac{\partial V}{\partial S_k} + \sum_{\ell(\neq k,i)} J_{k\ell} S_\ell + J_{ki} S_i + \xi_k(t)$$

Solve the dynamics of the "bath" as a function of the cavity

An example: mean-field spin glasses

$$\dot{s}_k = -\frac{\partial V}{\partial s_j} + \sum_{\ell(\neq k,i)} J_{k\ell}\, s_\ell + J_{ki}\, S_i + \xi_k(t)$$

$N \gg 1$

$$\dot{S}_i = -\frac{\partial V}{\partial S_i} + \underbrace{\sum_{k(\neq i)} J_{ik}\, S_k^{0}}_{\text{Noise: Gaussian force}} + \underbrace{\sum_{k\neq i} J_{ik}\, \delta S_k^{0}}_{\text{Dissipation: Onsager reaction term}} + \xi_i(t)$$

$$\boxed{\dot{S}_i(t) - \int_0^t ds\, R(t,s)\, S_i(s) = -\frac{\partial V}{\partial S_i} + \xi_i(t) + \eta_i(t)}$$

Self-consistency

$$R(t,s) = \frac{1}{N}\sum_k \left.\frac{\delta S_k(t)}{\delta h_k(s)}\right|_{h_k=0}$$

$$\langle \eta_i(t)\,\eta_i(s)\rangle = \frac{1}{N}\sum_k S_k(t)\, S_k(s) = C(t,s)$$

DMFT in statistical physics

1. Identify the correct degree of freedom and treat the rest of the system as a bath

The effect on the cavity on the rest of the system treated at first order in perturbation theory

Generalized friction kernel and thermal noise

2. The bath is statistically identical to the singled out degree of freedom: self-consistency

Generalized friction kernel
thermal noise

Cavity dynamics

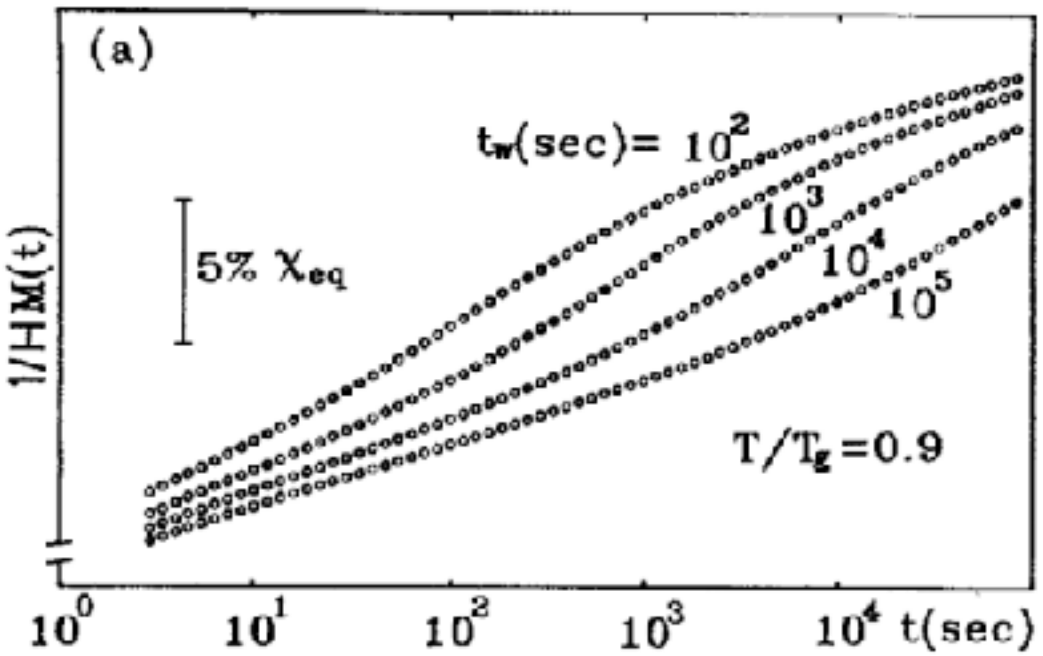
Sompolinsky, Zippelius PRB 1982
Mézard, Parisi, Virasoro, Spin Glass and Beyond

Quantum: Georges, Kotliar, Krauth, Rozenberg, RMP 1996

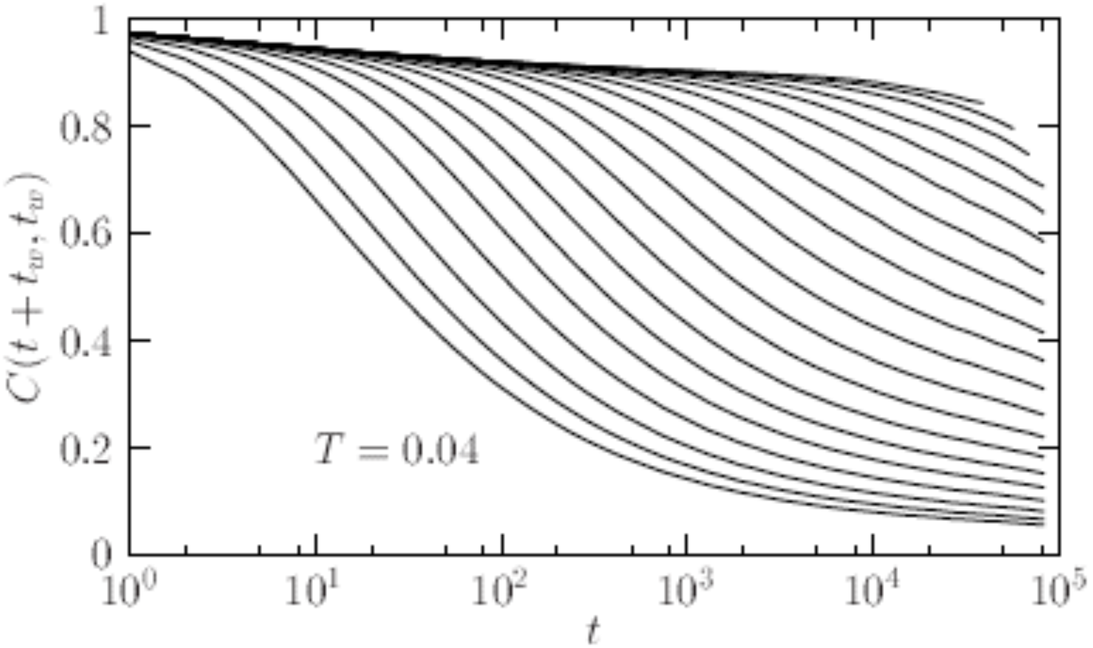
Applications

Aging in spin-glasses

At low temperature spin-glasses display a very slow off-equilibrium dynamics



Zero-Field cooled susceptibility from Zeidlindh et al PRB 87



Heisenberg spin-glass from Berthier Young PRB 04

Aging DMFT

$$\boxed{\dot{S}_i(t) - \int_0^t ds\, R(t,s) S_i(s) = -\frac{\partial V}{\partial S_i} + \xi_i(t) + \eta_i(t)}$$

Self-consistency

$$\underline{R(t,s)} = \frac{1}{N} \sum_k \frac{\delta S_k(t)}{\delta h_k(s)}\bigg|_{h_k=0}$$

$$\langle \eta_i(t) \eta_i(s) \rangle = \frac{1}{N} \sum_k S_k(t) S_k(s) = \underline{C(t,s)}$$

Equilibrium dynamics: R and C are related by FDT and time-translation invariant

Aging dynamics: R and C are slow, the thermal bath is aging together with the system

Aging DMFT

- Ergodicity breaking transition: the system remains always out of equilibrium below Tc

Cugliandolo, Kurchan, PRL 1993;…
Franz, Mezard 1994,…

- Infinite hierarchy of time-scales and time-sectors: effective temperatures out of equilibrium, and dynamical version of Parisi Full Replica Symmetry Breaking

Cugliandolo, Kurchan PRB 1994; JPSJ 2000,…

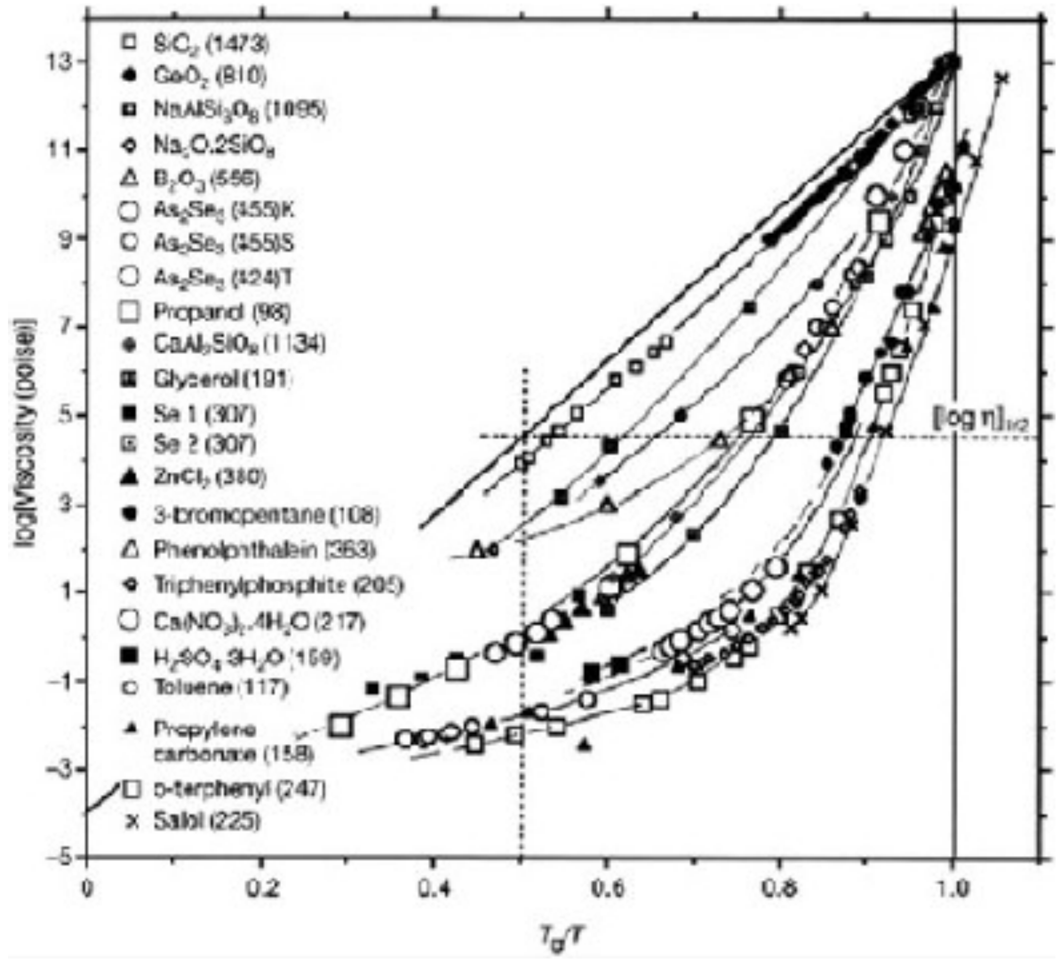
Altieri, Cammarota, Biroli J. Phys. A 2020

- Generalisation to quantum systems

Cugliandolo, Lozano PRB 1999
Biroli, Parcollet PRB 2002

DMFT of the glass transition

Molecular liquids display a dramatic slowing down associated to the glass transition



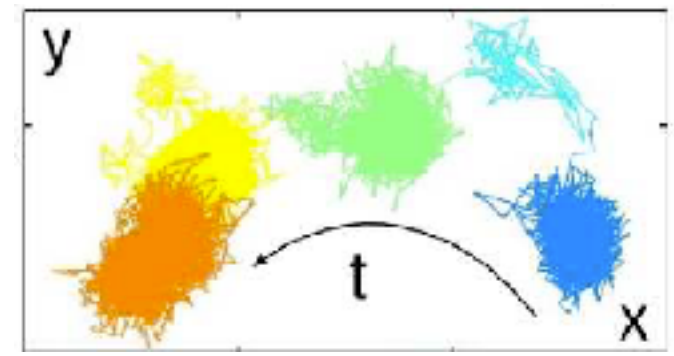
The relaxation time increases by 14 orders of magnitude

DMFT of the glass transition

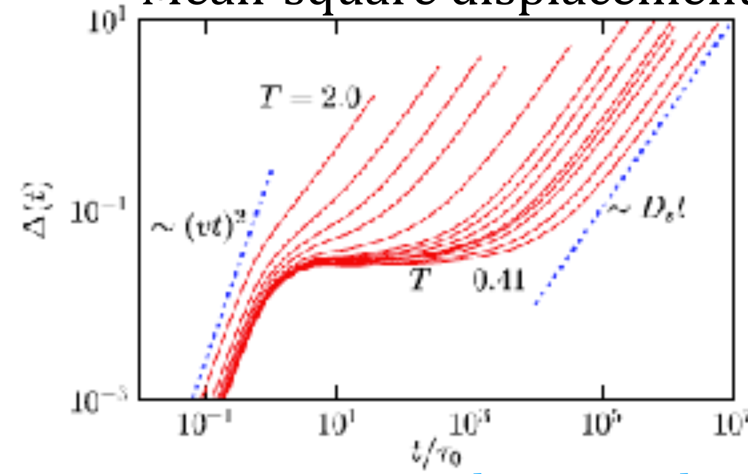
$$H = \sum_i \frac{P_i^2}{2m} + \sum_{\langle i\neq j\rangle} V(R_i - R_j)$$

$$m\ddot{R}_i = -\sum_{j(\neq i)} \nabla V(R_i - R_j)$$

N interacting particles
in the continuum



Mean-square displacement



Berthier, Biroli RMP 2011

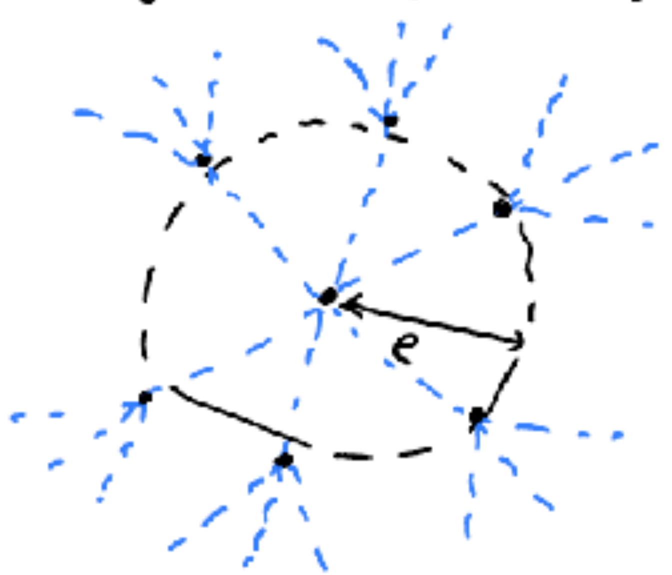
Large dimensional limit

$d \to \infty$

$$u_i(t) = R_i(t) - R_i(0)$$

$$V(R) = \bar{v}\left(d\left(\frac{R}{\ell} - 1\right)\right)$$

$$u_i^2 \sim \frac{1}{d}$$



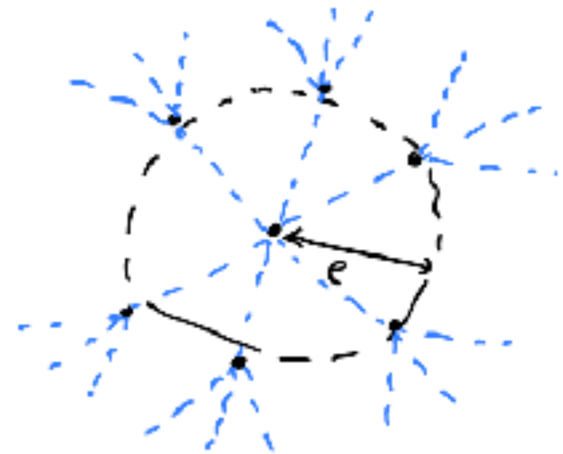
Cavity degree of freedom

$$u_{i,a}(t)$$

DMFT of the glass transition

The rest of the system acts like a thermal bath

$$m\ddot{u}_{i,\alpha}(t) = F_{i\alpha}(t) - \frac{1}{k_BT}\int_0^t K(t-s)\,\dot{u}_{i\alpha}(s)\,ds$$



$$\langle F_{i\alpha}(t)\,F_{i\alpha}(t')\rangle = K(t-t')$$

Self-consistency

$$m\ddot{u}_{i,\beta_{ij}} = -\nabla_{\beta_{ij}} V(R_i(t)-R_j(t)) + F_{i\beta_{ij}}(t) - \frac{1}{k_BT}\int_0^t K(t-s)\,\dot{u}_{i,\beta}(s)\,ds$$

$$m\ddot{u}_{j,\beta_{ij}} = -\nabla_{\beta_{ij}} V(R_j(t)-R_i(t)) + F_{j,\beta_{ij}}(t) - \frac{1}{k_BT}\int_0^t K(t-s)\,\dot{u}_{j,\beta_{ij}}(s)\,ds$$

$$K(t-t') = \sum_{j} \langle \nabla_{\beta_{ij}} V(R_i(t)-R_j(t)) \cdot \nabla_{\beta_{ij}} V(R_i(t')-R_j(t')) \rangle$$

Agoritsas, Maimbourg, Zamponi J Phys A 2019
Chen, Biroli, Reichman, Szamel 2021

DMFT of the glass transition

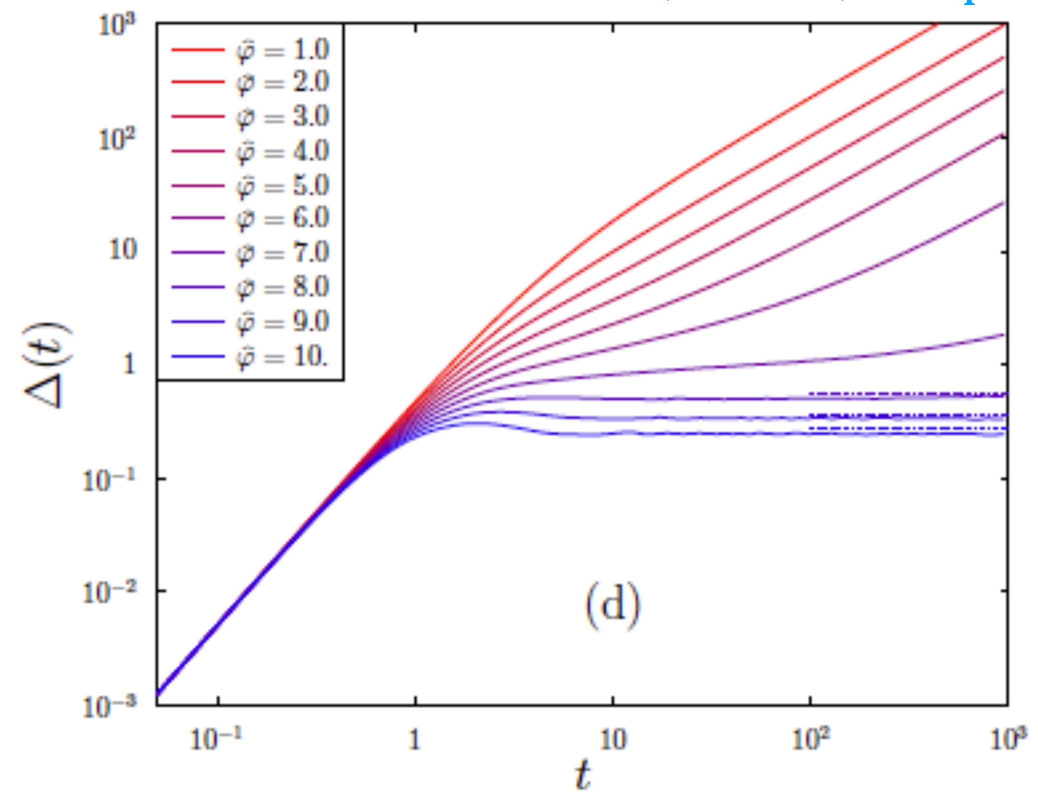
- Exact solution of infinite-d many particle dynamics

Maimbourg, Kurchan, Zamponi PRL 2016

- Glass transition at Td with the same properties of Mode-Coupling theory

Maimbourg, Kurchan, Zamponi PRL 2016

Manacorda, Schehr, Zamponi JCP 2020



- Detailed description of glassy dynamics but fails to obtain super-Arrhenius behavior (non-perturbative in 1/d)

Perspective: cluster extension to obtain a full description of glassy dynamics

Chen, Biroli, Reichman, Szamel 2021

DMFT for many-species ecosystems

"Traditional" ecosystems

"Modern" ecosystems

MANY INTERACTING SPECIES

- Communities formed by individuals belonging to different species.
- Interactions between individuals intra and inter species.
- Competition for resources--Cooperation.
- Abundances of species vary dynamically due to the births and deaths.

Many interesting open questions

- Can endogenous fluctuations survive in a large interacting ecosystem?

Endogenous versus exogenous fluctuations

"Are ecological systems chaotic—and if not, why not?" Berryman, Millstein 1989

DMFT of large ecosystems

$$\frac{dN_i}{dt} = N_i \left[r_i (K_i - N_i) - \sum_{j(\neq i)} \alpha_{ij} N_j \right] + \lambda_i$$

$$i = 1, \dots, N \qquad (N \gg 1) \; ; \; N_i \geq 0$$

Mean-Field Version

$$\overline{\alpha_{ij}^2}^c = \frac{\sigma^2}{N} \; ; \; \overline{\alpha_{ij}\alpha_{ji}}^c = \gamma \frac{\sigma^2}{N} \; ; \; \overline{\alpha_{ij}} = \frac{\mu}{S}$$

Bunin, PRE 2017
Barbier et al PNAS 2018

$$\frac{dN_i}{dt} = N_i \left[r_i (K_i - N_i) \underbrace{- \mu m(t) + \gamma \sigma^2 \int_0^t R(t,s) N_i(s) ds + \eta_i(t)}_{\text{“bath”}} \right] + \lambda_i$$

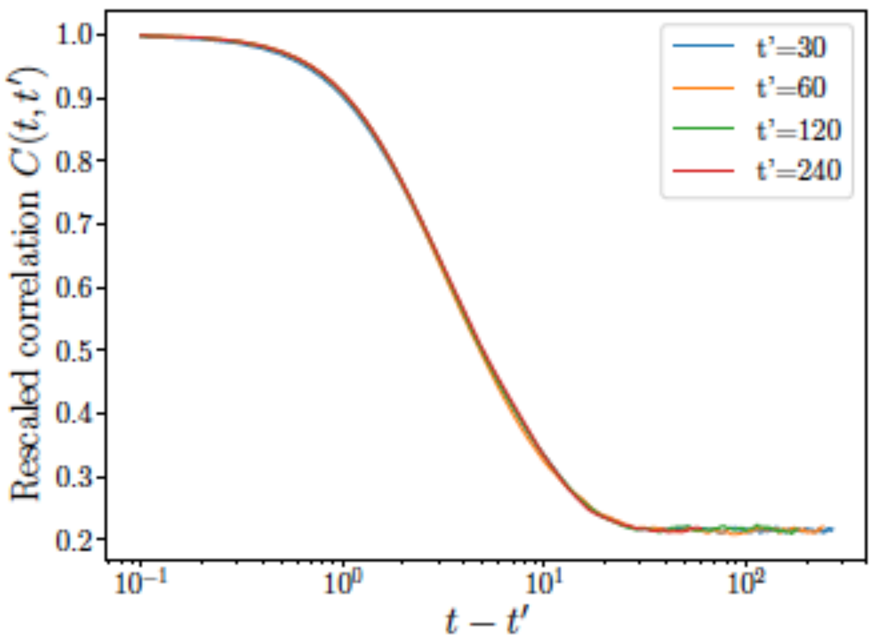
Self-consistency

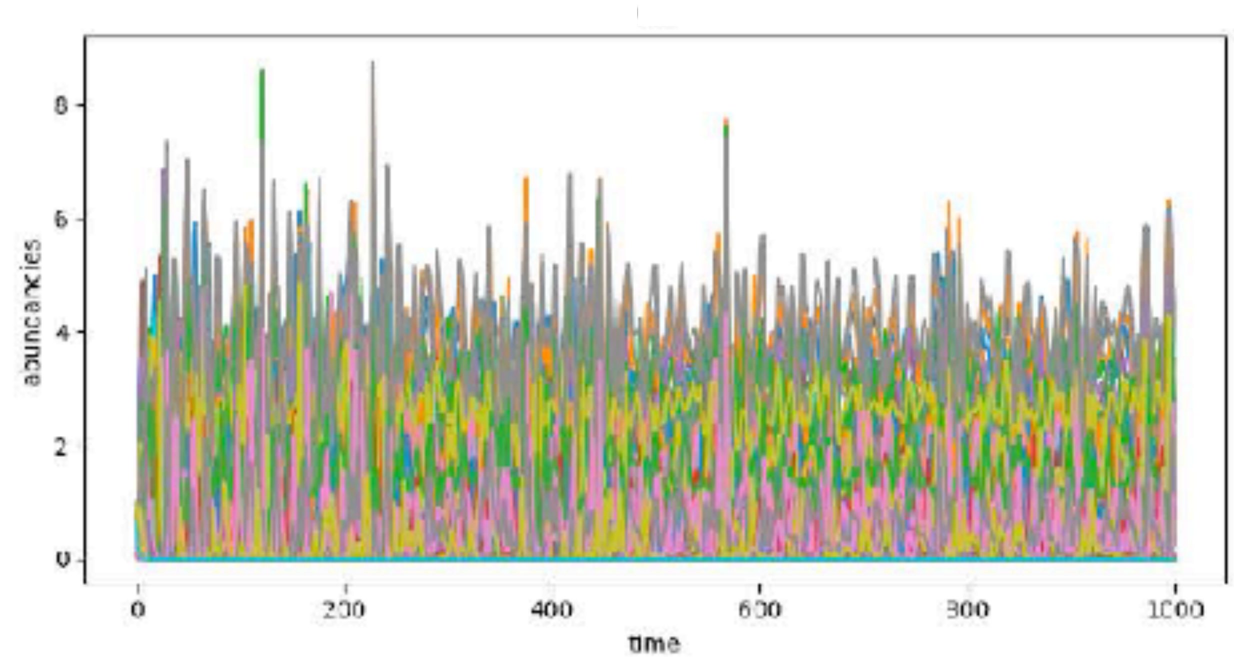
$$\langle \eta_i(t) \eta_i(s) \rangle = \frac{1}{N} \sum_j N_j(t) N_j(t') \qquad m(t) = \frac{1}{N} \sum_j N_j(t)$$

$$R(t, s) = \frac{1}{N} \sum_j \left. \frac{\delta N_j(t)}{\delta h_j(s)} \right|_{h_j = 0}$$

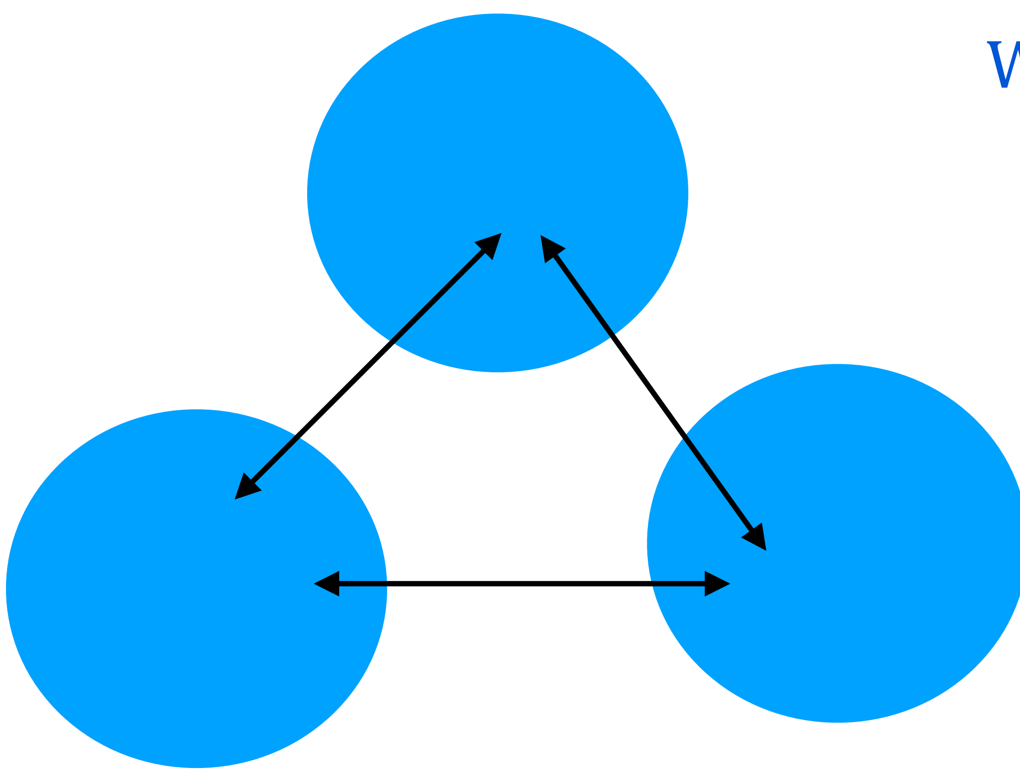
Chaos & Endogeneous fluctuations

Transition from one equilibrium phase to Stable high-dimensional chaos with immigration





Roy, Bunin, Biroli, Cammarota, JPA 2019



Without migration chaos is metastable for many communities and with diffusion

Roy, Barbier, Biroli, Bunin PLOS 2020

D. S. Fisher, A. Agarwala, M. Pearce PNAS 2019

Conclusion

DMFT in classical statistical physics: a powerful method to analyze and unveil complex dynamical phenomena

Many different applications

- Aging dynamics in spin-glasses
- Very slow relaxation and glass transition
- Complex phenomena in large interacting ecosystems
- Chaos in recurrent neural networks
- Optimization algorithms in computer science