LAPLACIAN RENORMALIZATION GROUP FOR HETEROGENEOUS NETWORKS: INFORMATION CORE AND ENTROPIC TRANSITIONS

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Laplacian paths in complex networks: Information core emerges from entropic transitions

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Laplacian renormalization group: an introduction to heterogeneous coarse-graining

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Laplacian renormalization group for heterogeneous networks

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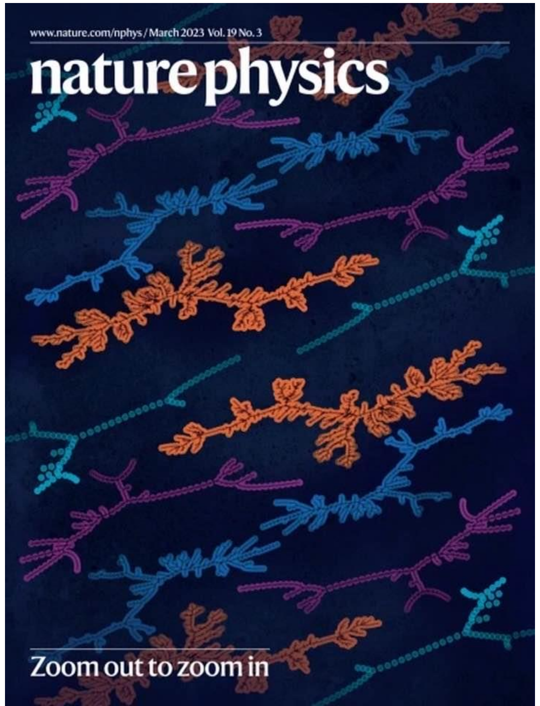
Pablo Villegas[1], Tommaso Gili[2], Guido Caldarelli[3,4,5,6,7] & Andrea Gabrielli[1,8]

The renormalization group is the cornerstone of the modern theory of universality and phase transitions and it is a powerful tool to scrutinize symmetries and organizational scales in dynamical systems. However, its



News & views

Renormalization group

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A zoom lens for networks

Konstantin Klemm

Check for updates

Renormalization is a technique based on a repeated coarse-graining procedure used to study scale invariance and criticality in statistical physics. Now, an expansion of the renormalization toolbox allows to explore scale invariance in real-world networks.

Imagine taking a series of photographs from the top of the Eiffel Tower: a rowboat on the Seine, the west facade of Notre Dame and, zooming out even more, a panoramic view of the whole city of Paris. Tourists look for novel and varying impressions at different spatial scales. Physicists, on the other hand, rejoice the most when things look similar despite zooming in and out. Fractal structures, such as the Koch curve, have a built-in self-similarity. The Ising model's critical point at the para- to ferro-magnetic phase transition is identified by invariance under coarse-graining. The renormalization group is a set of techniques to study the effects of such scale transformations in physical systems. Writing in *Nature Physics*, Pablo Villegas and colleagues[1] have now broadened the scope of renormalization to arbitrary networked systems beyond grid structures.

There are many examples of scale invariance in different areas of physics and mathematics. Take for instance fractal structures, which have a built-in self-similarity (Fig. 1a), or the Ising model's critical point at the para- to ferro-magnetic phase transition, which is identified by invariance under coarse-graining (Fig. 1b). A pedagogical renormalization approach to the Ising model, introduced by Leo Kadanoff[2], is to subdivide the system into equal-sized blocks and merge the spins of each subsystem into one block spin of the rescaled system. Once parameters such as coupling strength and temperature remain unchanged by the transformation, we have reached scale invariance.

Villegas and colleagues[1] broaden the scope of renormalization to arbitrary networked systems beyond grid structures. Various biological and technical networks, such as organisms' metabolic pathways and the Internet, turn out to be scale invariant under a suitable block formation scheme. Not all networked structures, however, share this property. Artificial networks such as random graphs and stochastic block models fail the test of scale invariance.

Physicists have analysed this kind of real network data and models for more than two decades. What has hindered a prompter reconciliation of networks with existing renormalization techniques? Crucially, Kadanoff's method assumes an underlying geometric space. Under the spatial partition into blocks, all bonds are short-range, connecting grid points in adjacent blocks only. Networks, however, are defined purely by the presence or absence of bonds. Nodes do not need spatial coordinates attached to them. Even when they have, bonds are not restricted to short-range. In the human brain, the spacing between neurons is on the scale of micrometres, whereas the axons – the fibres transmitting pulses between neurons – reach lengths of several centimetres.

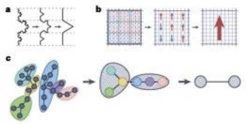


Fig. 1 | Iterated coarse-graining in geometric and networked systems. a, The Koch curve, a recursively constructed fractal, coarse-grained by inverting the local construction rule. **b**, The Ising model on a square grid is coarse-grained by Kadanoff's block method. The up/down spins in each 3×3 block are replaced by the majority spin orientation. **c**, A tree network (black, left panel) is partitioned into blocks shown as bubbles in different colours. The coarse-grained network (centre panel) is obtained by lumping together the nodes of each block in a supernode. The process is repeated by finding blocks (striped bubbles) and coarse-graining again. This leads to the two-node network (right panel).

A small share of these long-range connections is sufficient to endow networks with the small-world property[3] – colloquially dubbed 'six degrees of separation' for social networks. Any two persons are connected by a short chain of intermediate acquaintances – much shorter than expected if the network of acquaintances were a two-dimensional grid. In a small-world network, the diameter – the mean distance between nodes – scales logarithmically with the number of nodes. This is seen as the infinite dimension limit of the diameter scaling found for a grid of any dimensionality[4]. The small-world property, exhibited by most real-world networks, thus describes the absence of a finite dimension and hampers network embedding in low-dimensional Euclidian spaces.

A previous network renormalization approach[5] tackled this problem by embedding the network into a two-dimensional hyperbolic space, modelled as a Poincaré disk. The projection onto the boundary of the disk presented the desired blocks as clusters on this one-dimensional manifold. The method revealed clear-cut scale invariance in several real networks of biological, technical and social origin. In addition, it had a strong nexus with the existing theory of networks from hidden metric spaces. On the downside, the method was tailored to networks embeddable in hyperbolic geometry and was not applicable to other structures such as grids.

Doing away with assumptions about geometry altogether, Villegas et al[1]. considered a diffusion process across the network. They identified the blocks as sets of nodes with significant probability current under diffusion (Fig. 1c). The vector of probabilities evolves by a network version of the heat equation, governed by the Laplacian matrix – the discrete analogue of the Laplacian operator known from vector calculus. Just like the conventional Laplacian operator, the network Laplacian tightly couples temporal and spatial scales. In particular, the

TWO DIFFERENT AND CONNECTED ASPECTS

1) Structural/topological properties :

- Hierarchical organization
- Multiscale features
- Strong heterogeneity and correlations

Methods and tools:

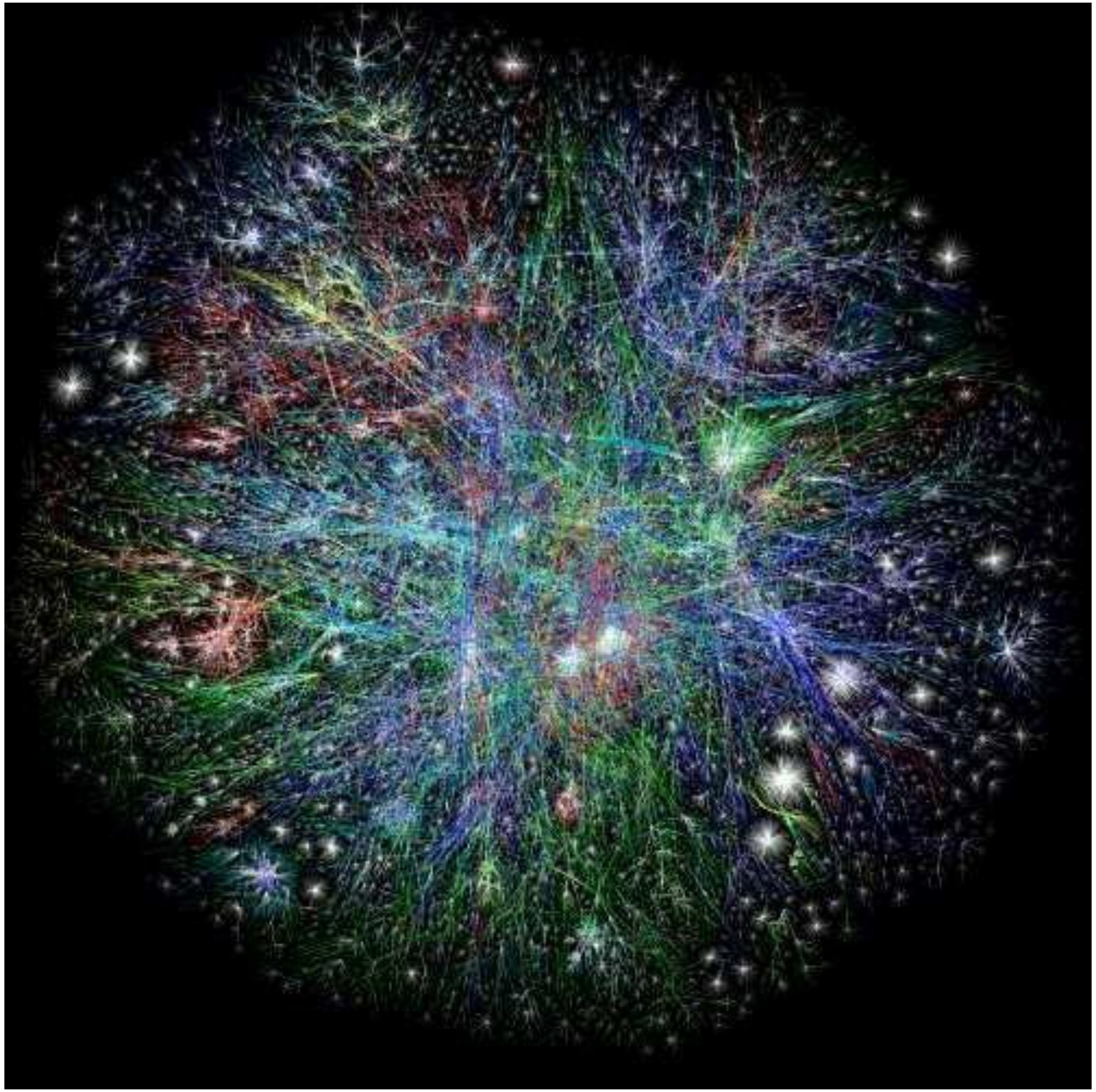
- Degree distribution P(k) (statistics of the number of neighbors)
- Nearest neighbors connectivity k_{nn}
- Clustering coefficient (fraction of complete triangles between all)
- Higher order clustering properties: communities

- **2) Dynamical processes or physical models on networks:**
- **The network is the 'space' for dynamical processes**
- Random walks and diffusion
- Epidemic models (e.g. contact processes)
- Synchronization of intereacting oscillators
- Ising model on network
- Phase transitions and large scale

MANY SYSTEMS CAN BE SCHEMATIZED AS A SET OF N VERTICES JOINED BY EDGES REPRESENTING INTERACTIONS/DEPENDENCIES

(INTERNET, HUMAN BRAIN, SOCIAL-ECONOMIC-FINANCIAL-ECOLOGICAL AND BIOLOGICAL SYSTEMS)

(STANDARD) DYNAMICAL SYSTEMS ARE EMBEDDED IN THIS IRREGULAR AND NON-LOCAL SPACES: SCALES ARE INTERTWINED AND AFFECT SYSTEM BEHAVIOR AND POSSIBLE PHASE TRANSITIONS AND CRITICAL BEHAVIORS



RENORMALIZATION GROUP IN STATISTICAL PHYSICS: COLLECTIVE STATES AND CHARACTERISTIC SCALES

In **homogeneous metric spaces** (e.g. $\mathbb{R}^d$ or $\mathbb{Z}^d$) the multiscale features of **statistical and dynamical models** (e.g. Ising, CP) with **translationally invariant couplings** are optimally described by the Renormalization Group to study characteristic scales and scale invariant states

Renormalization Group:
Coarse-graining (collective block variables)
\+ spatio-temporal rescaling
\+ redefinition of coupling constants

Coarse graining: definition of block variables and/or integration of small wavelength modes

L. Kadanoff, *Scaling laws for ising models near Tc*, Physics **2**, 263 (1966)
K. G. Wilson and J. Kogut, *The Renormalization Group and the ε~expansion*, Phys. Rep. **12**, 75 (1974)

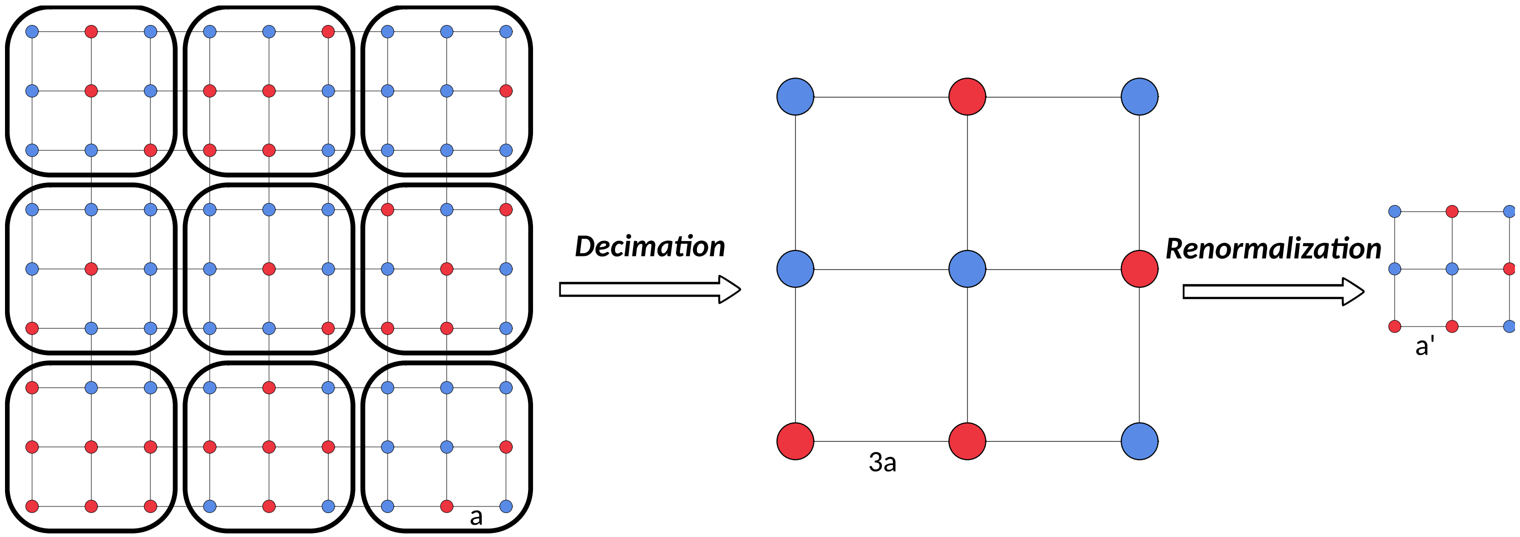
SPATIAL HOMOGENEITY SIMPLIFIES COARSE GRAINING

Implications of spatial homogeneity (and of couplings):

(i) Translational invariance of the system

(ii) Identical block variables at all points of the space (Kadanoff block variables)

(iii) Utility of the expansion in Fourier plane waves (Wilson RG)



WHAT ABOUT A RG FOR HETEROGENEOUS NETWORKS?

Spatial/topological heterogeneity is the main obstacle to the extension of an RG to graphs

Even with constant couplings, heterogeneous topology and connectivity are major problems

A meaningful coarse-graining of nodes and connections is the central issue

How to define statistical and dynamical equivalent block variables (macronodes) at different heterogeneous regions of the network?

PREVIOUS ATTEMPTS

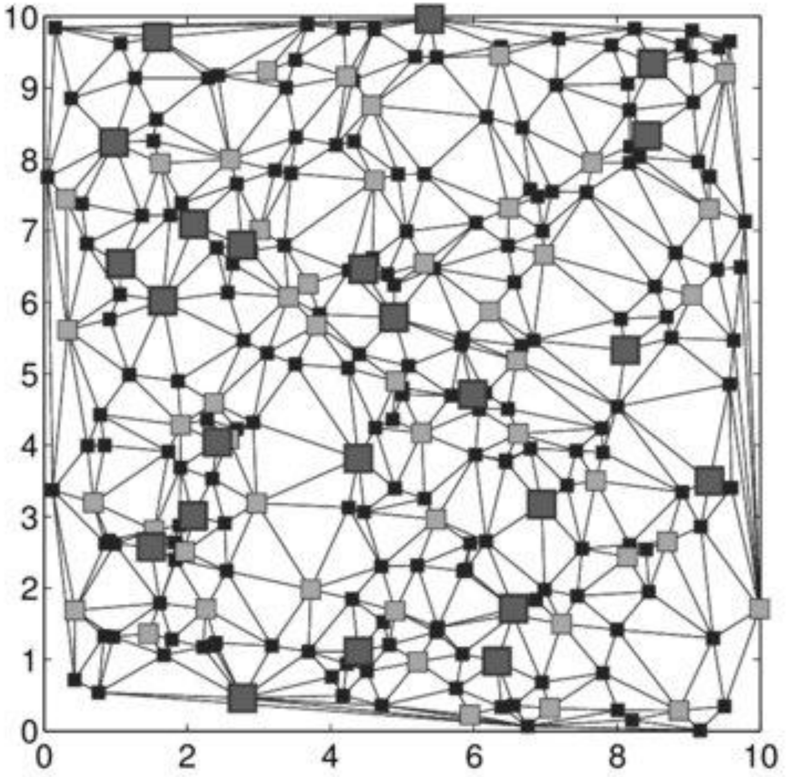
Ad hoc and heuristic definition of block variables for particular kind of networks (e.g for scale-free or core-periphery networks)

In planar graphs one can introduce a metric criterion of neighborhood to define block variables

Recently and *hyperbolic* RG approach has been introduced:

For each graph one can find a suitable hyperbolic space on which the graph is a sort of planar graph.

What is the physical meaning of the spatial dimension, curvature and distance?



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SYMMETRIC LAPLACIAN AS A INTRINSIC SCALES DETECTOR

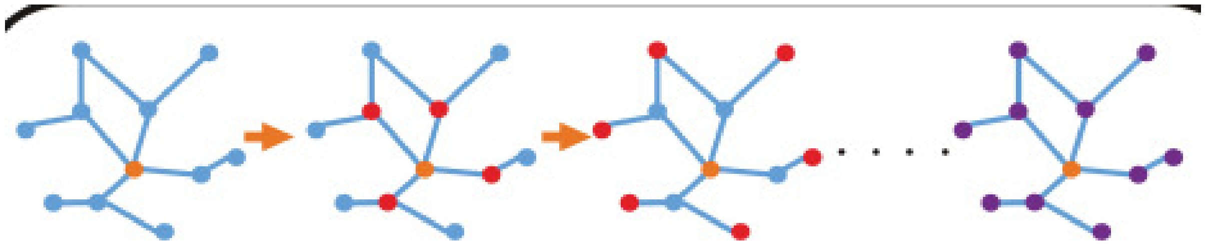
To detect the characteristic structures in a network, we use heat diffusion dynamics

$\hat{L} = \widehat{D} - \hat{A} =$ symmetric Laplacian matrix

$\hat{A} =$ symmetric adjacency matrix (undirected)

$\widehat{D} =$ diagonal degree matrix → $D_{ij} = (\sum_l A_{il})\delta_{ij} = k_i\delta_{ij}$

(i) For connected undirected graphs eigenvalues are all positive but one $\lambda_1 = 0$ with a corresponding uniform eigenvector $\vec{\lambda}_1$. (ii)The eigenvectors form an orthogonal basis



TIME EVOLUTION OPERATOR FOR DIFFUSION

Diffusion/heat equation on undirected graphs: $\dot{\vec{\phi}} = -\hat{L}\vec{\phi}$

$\vec{\phi}(t) = e^{-t\hat{L}}\,\vec{\phi}(0) = \hat{\rho}(t)\vec{\phi}(0)$ with $\phi_i(t)$ = information at site i

$\hat{L}$ is semi-definite positive and symmetric: spectral theorem

$$\boxed{|\phi(t)\rangle(t) = \sum_\lambda e^{-\lambda t}\,|\lambda\rangle\langle\lambda|\phi(0)\rangle}$$

$$\boxed{p(\lambda, t) = \frac{e^{-\lambda t}}{Z(t)} = \text{statistical weight of the } \lambda^{th} \text{ mode}}$$

$$\boxed{\rho_{ij}(t) = \left(e^{-t\hat{L}}\right)_{ij} = \text{fraction of information flowing from node } i \text{ to node } j \text{ in time } t}$$

In $\mathbb{R}^d$ or $\mathbb{Z}^d \Longrightarrow \hat{L} = -\nabla^2$ is a translational invariant counter of wavelengths l :

Eigenvalues are $k^2 \sim 1/l^2$ and eigenvectors e^{ikx} (i.e. tiling with identical boxes in real space)

Diffusion/heat equation: $\partial_t \varphi(x,t) = \nabla^2 \varphi(x,t)$

We can use it to define «block variables» in homogeneous spaces at different wave-vectors $k^2 \sim 1/t$

Diffusion from each point defines increasing block variables or wavelengths of modes $l \sim \sqrt{t}$

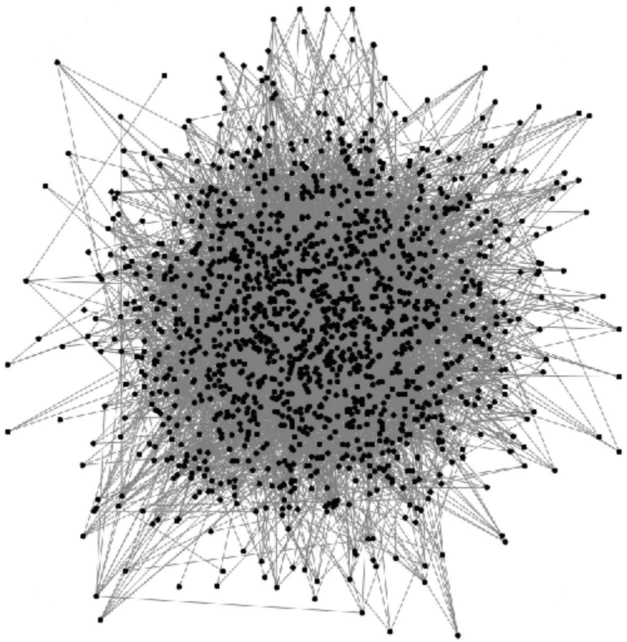
In the Wilson RG the coarse graining is done by integrating out larger and larger wave-lengths l

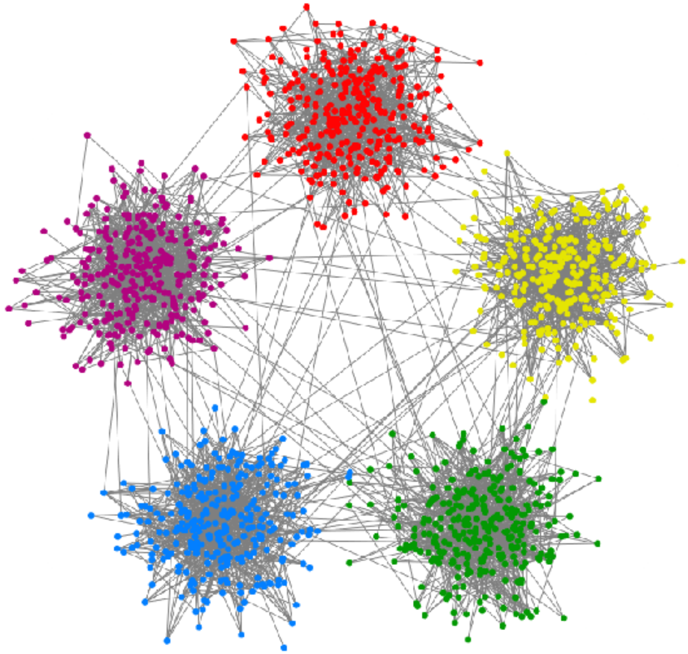
We adopt exactly the same approach for networks replacing $-\nabla^2$ with its graph counterpart $\hat{L}$

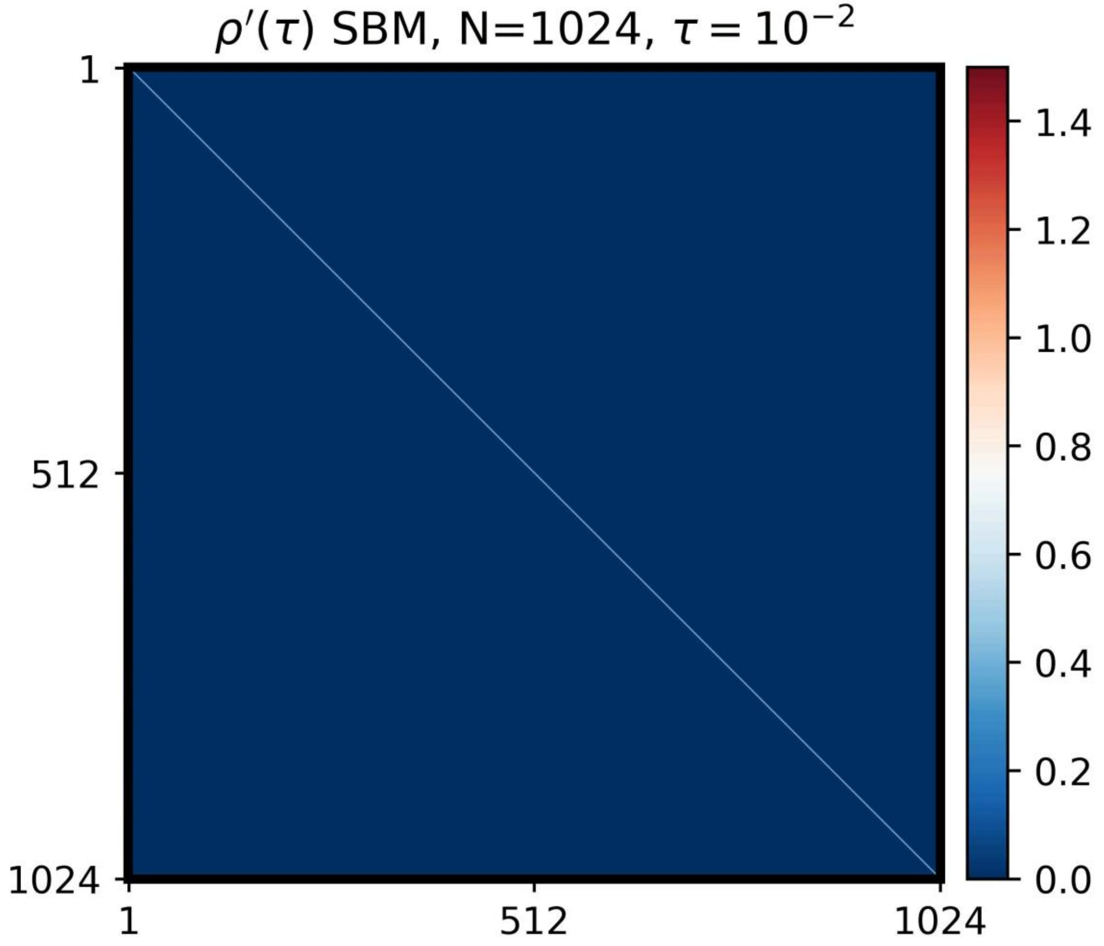
The time evolution operator $\hat{\rho}\ \ (t) = e^{-t\hat{L}}$ defines *equivalent* macronodes at each «wavelength» t

Time t is the scale parameter to define heterogeneos block variables

HOW TO USE $\rho(t)$ TO DETECT NETWORK STRUCTURES
STOCHASTIC BLOCK MODEL







https://arxiv.org/abs/2301.04514

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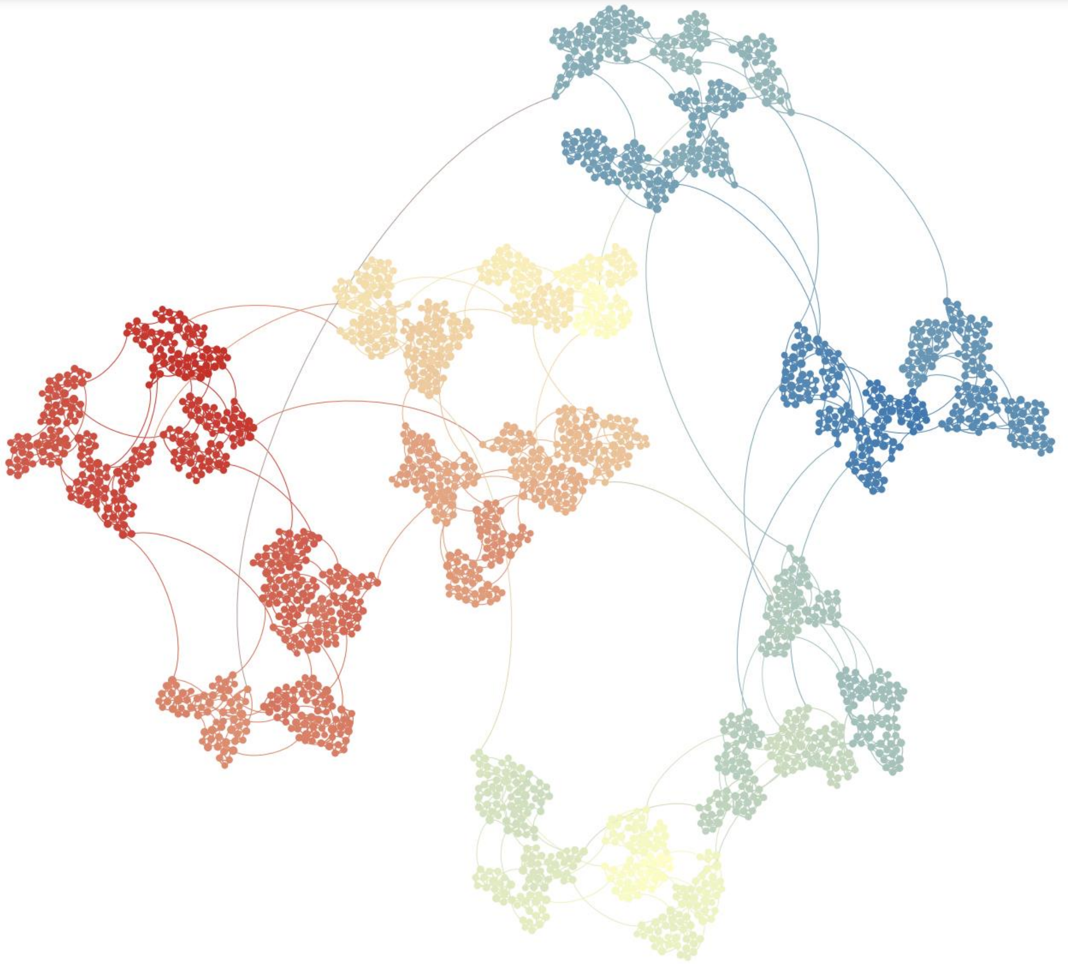
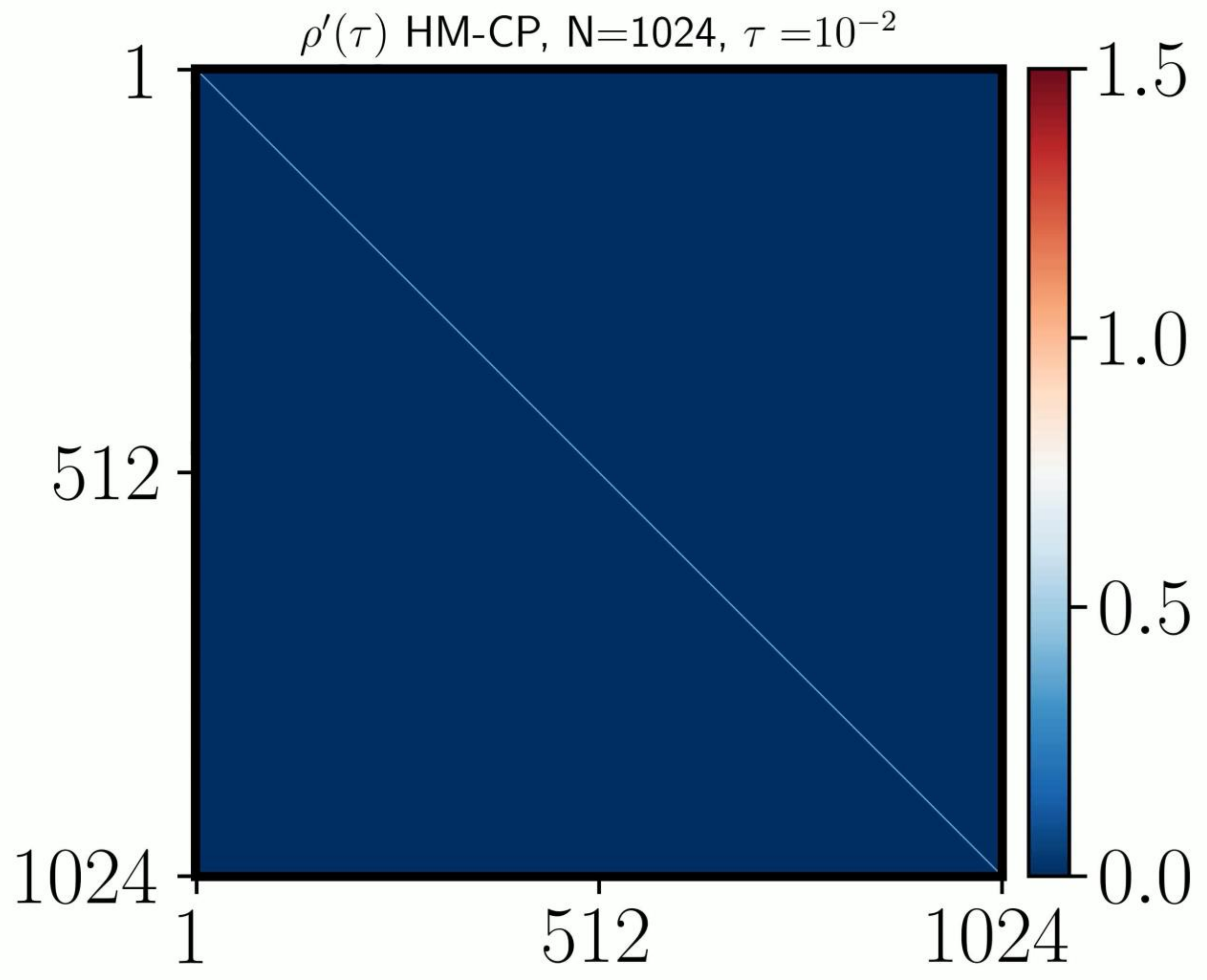
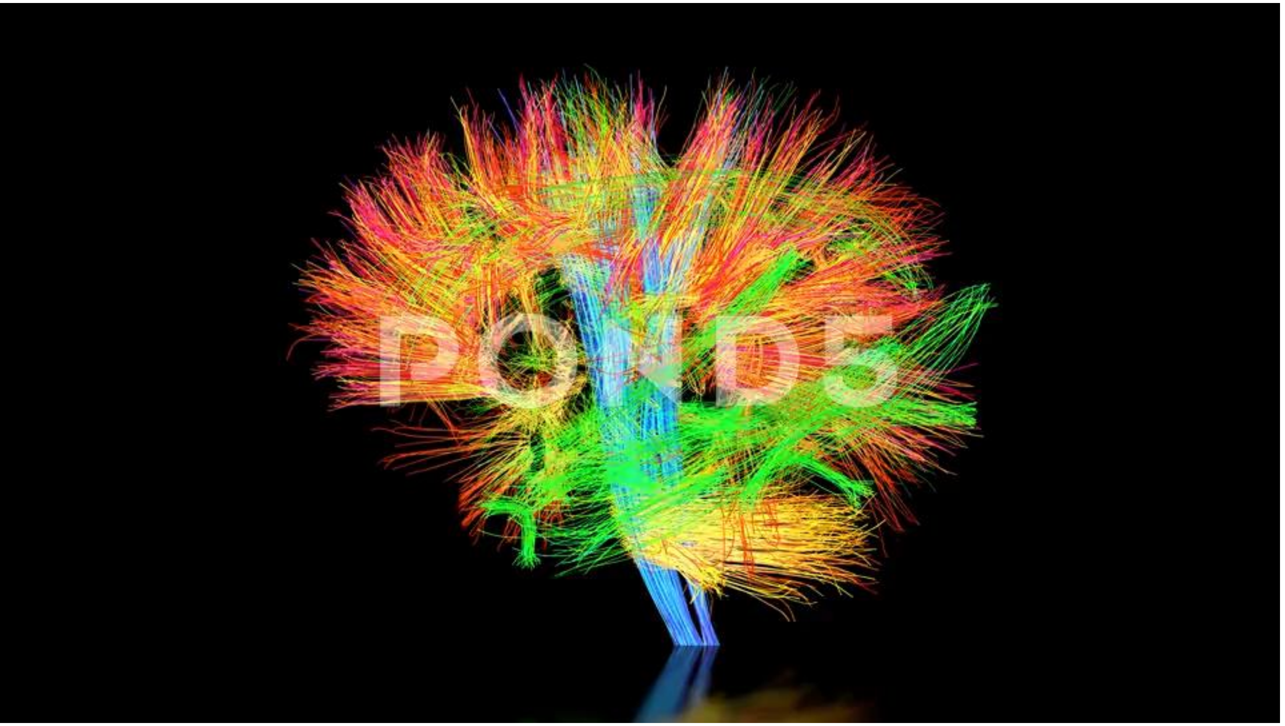
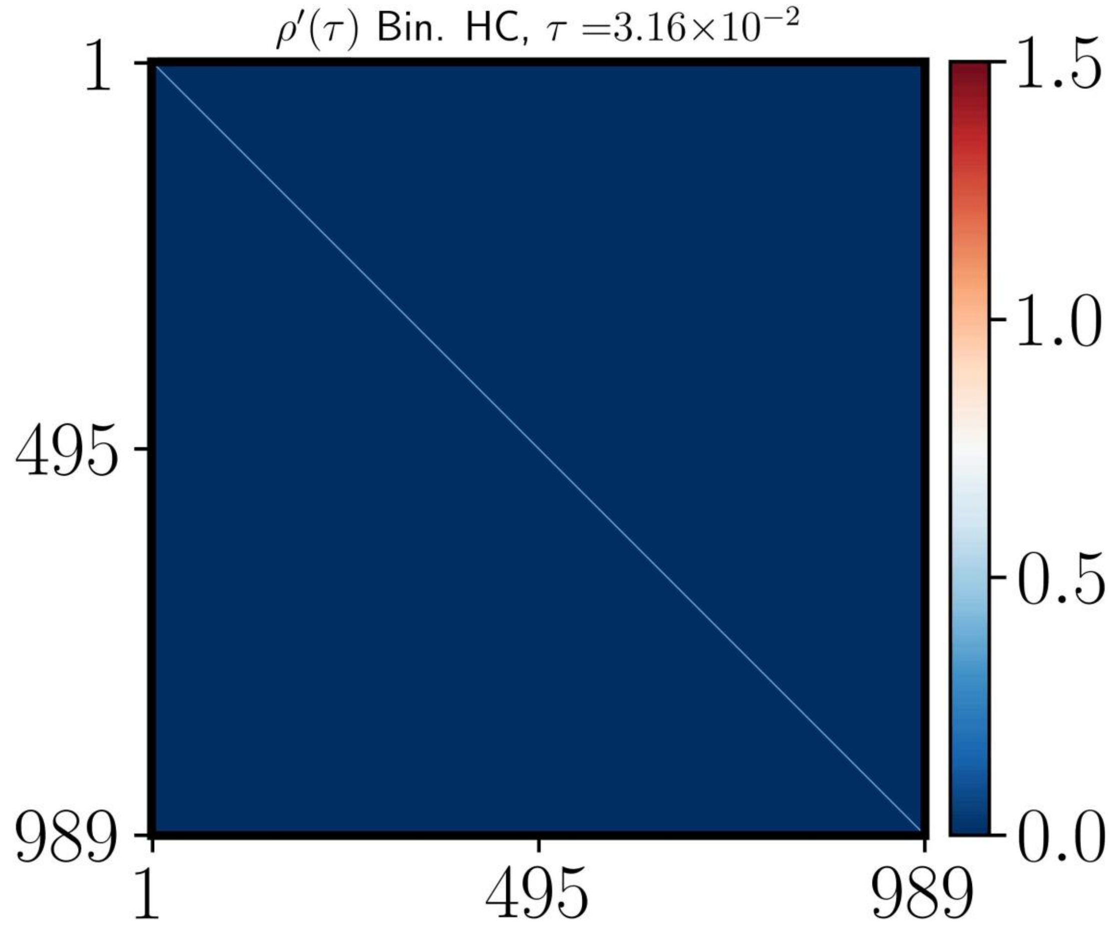
HIERARCHICAL MODULAR WITH CORE-PERIPHERY STRUCTURE





THE HUMAN CONNECTOME





UNIVERSITÀ DEGLI STUDI ROMA TRE

1. At an arbitrary scale t^* let us divide the spectrum in *slow modes* $\lambda_i < 1/t^*$ with $i = 1, \dots, N-M$ and *fast modes* $\lambda_i \geq 1/t^*$ with $i = N-M+1, \dots, \mathrm{N}$

2. <u>k-space</u>: Let us consider a reduced Laplacian operator $\widehat{L'} = \sum_{i=1}^{N-M} \lambda_i \, |\lambda_i\rangle\langle\lambda_i|$ (eliminate fast modes)

3. $\hat{L}' = \widehat{D}'$- $\hat{A}'$ defines a new Hermitian $(N-M) \times (N-M)$ (weighted) adjacency matrix $\hat{A}'$

4. <u>Real space</u>: The macronodes are defined by ordering in decreasing order the matrix elements $\rho_{ij}(t^*)$ and progressively aggregating nodes up to obtain $(N-M)$ clusters → macronodes

5. Rescaling $t \to \frac{t}{t^*}$ and $\lambda \to \lambda t^*$

6. Binarize for visualization: e.g. the new edge exists if $|\rho'_{ij}(t^*)| \geq \min\left[\left|\rho'_{ii}(t^*),\right|\left|\rho'_{jj}(t^*)\right|\right]$

P. Villegas, T. Gili, G. Caldarelli, A. Gabrielli, Nature Physics **19**, 445–450 (2023)

EXAMPLE in k-space

$$p[\vec{\phi}] = e^{-H[\vec{\phi}]}/Z$$

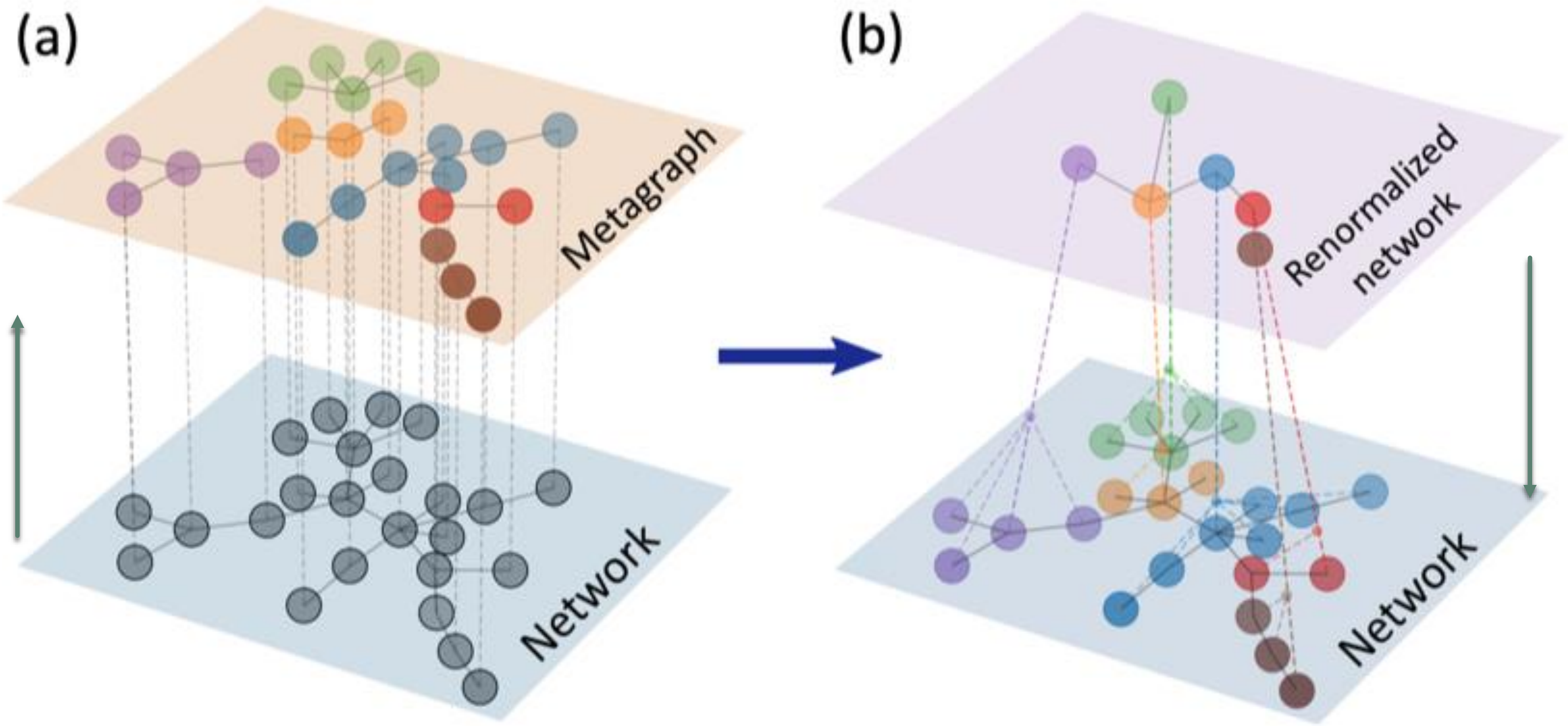
$$H[\vec{\phi}] = \vec{\phi} \cdot \hat{L}\vec{\phi} + m^2\vec{\phi} \cdot \vec{\phi} + F[\vec{\phi}] = \sum_{i,j}^{1,N} \phi_i \left(L_{ij} + m^2\delta_{ij}\right)\phi_j \; + F[\vec{\phi}] = \sum_{\lambda=0}^{\lambda_{max}} (\lambda + m^2)\, |\phi_\lambda|^2 + F[\vec{\phi}]$$

Integrate modes with λ between $\lambda^* = 1/t^*$ and λ_{max}

$$H'[\vec{\phi}'] = \sum_{\lambda=0}^{\lambda^*} (\lambda + m'^2)\, |\phi'_\lambda|^2 + F'[\vec{\phi}]'$$

General statistical dynamical model

$$\frac{\partial \rho(\mathrm{r},\mathrm{t})}{\partial t} = \mathrm{a}\rho(\mathrm{r},\mathrm{t}) - \mathrm{b}\rho^2(\mathrm{r},\mathrm{t}) + \mathrm{D}\nabla^2\rho(\mathrm{r},\mathrm{t}) + \mathrm{F}[\rho(\mathrm{r},\mathrm{t})]\,\eta(\mathrm{r},\mathrm{t})$$



P. Villegas, T. Gili, G. Caldarelli, A. Gabrielli, Nature Physics **19**, 445–450 (2023)

Eigenvalues of $e^{-t\hat{L}}$ define a probability measure on the diffusion modes (eigenvectors) at time t

$p(\lambda, t) = \frac{e^{-\lambda t}}{Z(t)}$ with $Z(t) = \sum_{\lambda'} e^{-\lambda' t}$ is the time-dependent normalized weight of the eigenvector $\vec{\lambda}$ of $\hat{L}$

$p(\lambda, 0) = \frac{1}{N}$ (all nodes isolated) and $p(\lambda, t \to \infty) = \delta_{\lambda,0}$ (all nodes with uniform information)

$S[p(\lambda,t)] = -\sum_{\lambda} p(\lambda,t) \log[p(\lambda,t)]$ is the Shannon entropy of this distribution

$$S[p(\lambda,t)] = S[\hat{\rho}(t)] = -\operatorname{tr}[\hat{\rho}(t) \log \hat{\rho}(t)]$$

Von Neumann entropy of the «density matrix» $\hat{\rho}(t)$ over the eigenstates of $\hat{L}$

Where $\hat{\rho}(t) = \frac{e^{-t\hat{L}}}{Z(t)}$ with $Z(t) = \operatorname{tr}(e^{-t\hat{L}}) = \sum_{\lambda} e^{-\lambda t}$

M. De Domenico and J. Biamonte, Phys. Rev. X **6**, 041062

ENTROPIC SUSCEPTIBILITY AND STRUCTURAL PHASE TRANSITIONS

Quantum Statistical Mechanics

$\hat{H}$ Hermitian and lower bounded

$\hat{\rho}(\beta) = \frac{e^{-\beta\hat{H}}}{Z(\beta)} =$ density matrix

$S[\hat{\rho}(\beta)] =$ Von Neumann entropy

$C(\beta) = -\frac{\partial S}{\partial \log \beta} =$ Heat capacity

Divergence/peak in $C(\beta)$ → critical point/phase transition

Laplacian diffusion on networks

$\hat{L}$ Hermitian and lower bounded

$\hat{\rho}(t) = \frac{e^{-t\hat{L}}}{Z(t)} =$ diffusion evolution operator

$S[\hat{\rho}(t)]$ = Laplacian diffusion entropy

$C(t) = -\frac{\partial S}{\partial \log t} =$ Laplacian susceptibility

Divergence/peak in $C(t)$ → structural phase transition

Characteristic diffusion scale

P. Villegas, A. Gabrielli, F. Santucci, G. Caldarelli, T. Gili, Phys. Rev. Res. **4**, 033196 (2022)

PROPERTIES OF THE ENTROPIC SUSCEPTIBILITY $C(t)$
A CONSTANT $C(t)$ MEANS LAPLACIAN SCALE INVARIANCE

$$C(t) = -\frac{\partial S}{\partial \log t} = -t^2 \frac{d\langle\lambda\rangle_t}{dt} \quad \text{where } \langle\lambda\rangle_t = \frac{\sum_\lambda \lambda e^{-\lambda t}}{Z(t)} \sim \frac{1}{t}$$

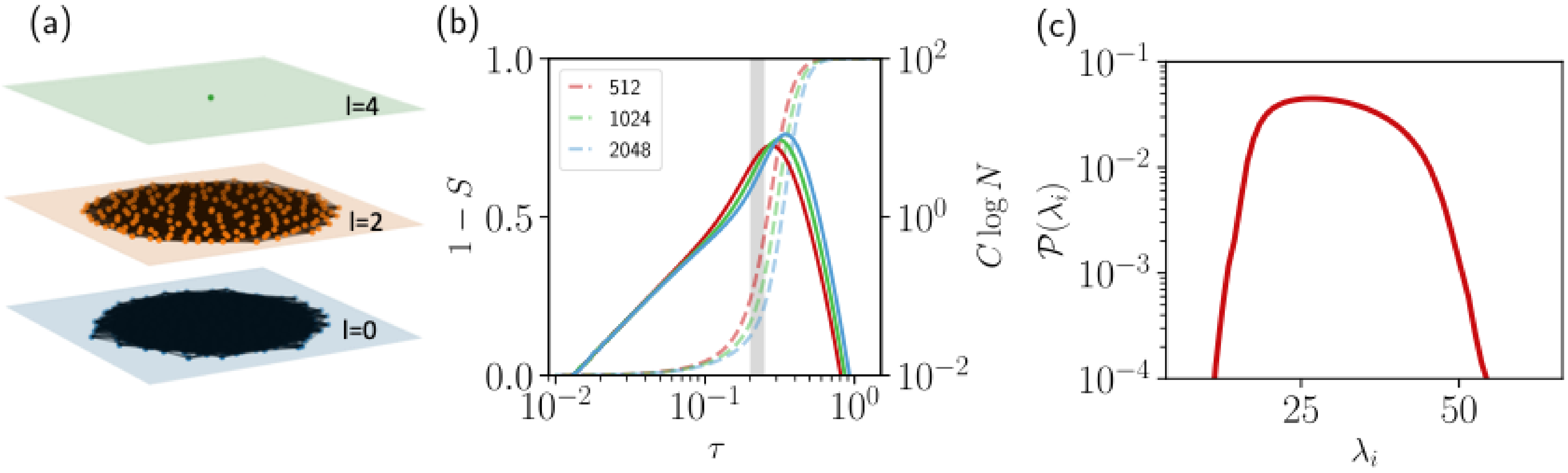
$C(t) = C_0 > 0 \Longrightarrow \langle\lambda\rangle_t \sim \frac{1}{t}$ which implies, in the limit of continuous spectrum $n(\lambda)$,

$n(\lambda) \sim \lambda^\gamma$ for small λ with $\gamma = C_0 - 1, \bar{d} = 2C_0 =$ spectral dimension

This is typical of lattices and random trees, which have no characteristic scale

P.Villegas, T. Gili, G. Caldarelli, A. Gabrielli, Nature Physics **19**, 445–450 (2023)

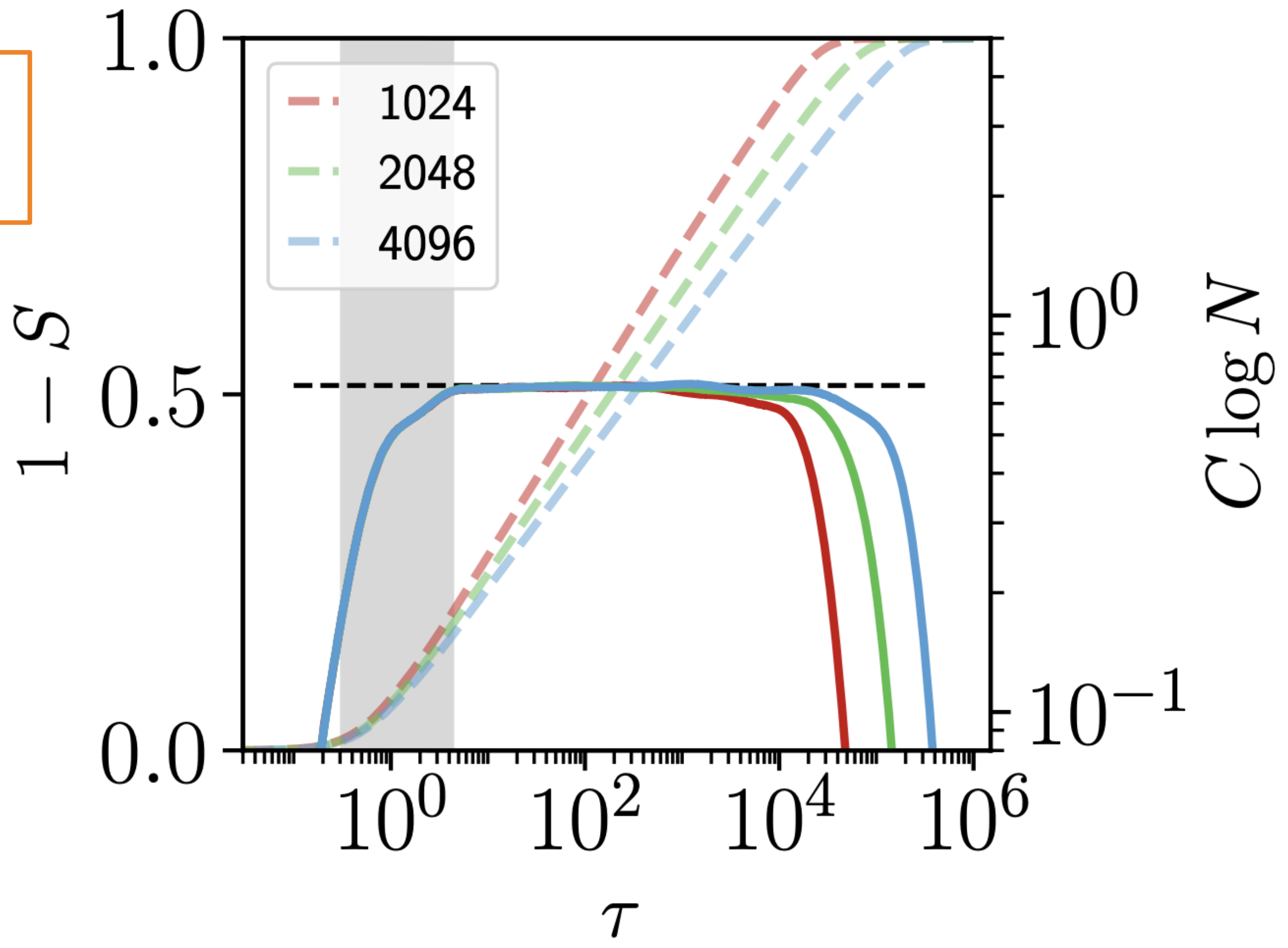
LAPLACIAN RG FOR THE ER RANDOM GRAPH



LAPLACIAN SCALE INVARIANT CASES: RANDOM TREE

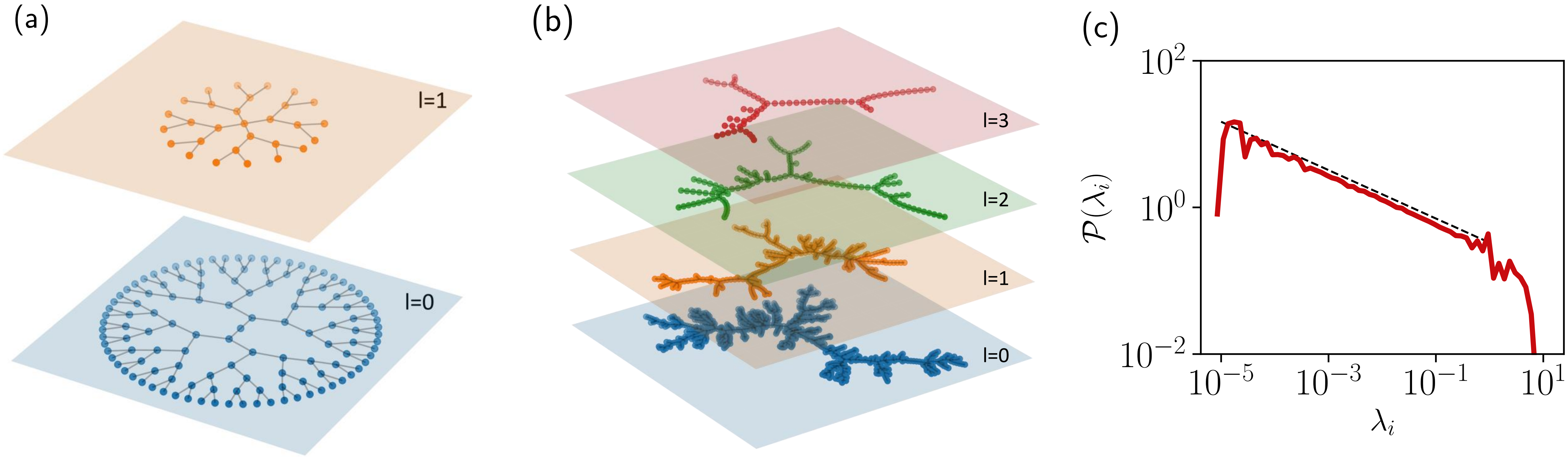
Random tree with finite mean branching ratio and finite variance

- Similarly to the regular lattice no single peak, but a large flat one.
- This is due to the scale invariance of the Laplacian spectrum (see below)
- This is connected to the geometrical scale invariance of the structure



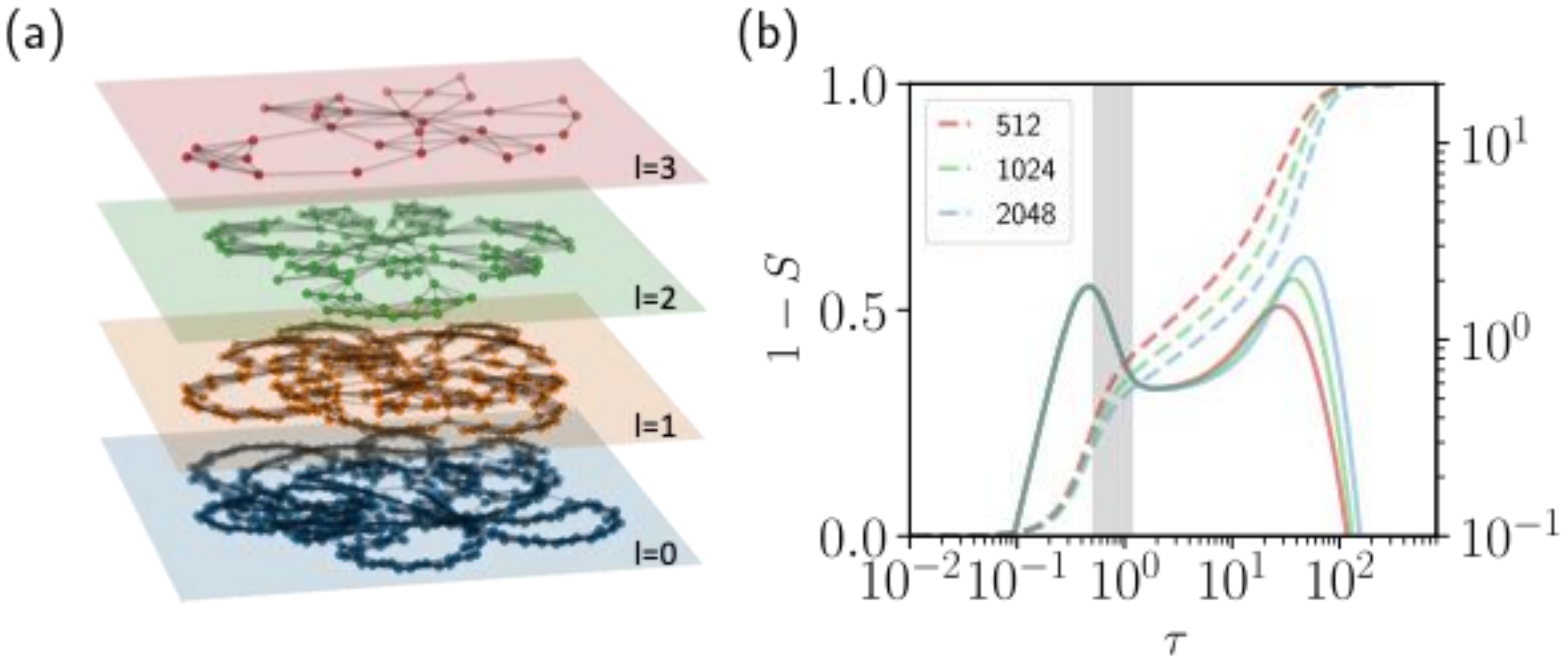
A. Poggialini, P. Villegas, M.A. Munoz, A. Gabrielli, https://arxiv.org/abs/2406.19104

RANDOM TREE

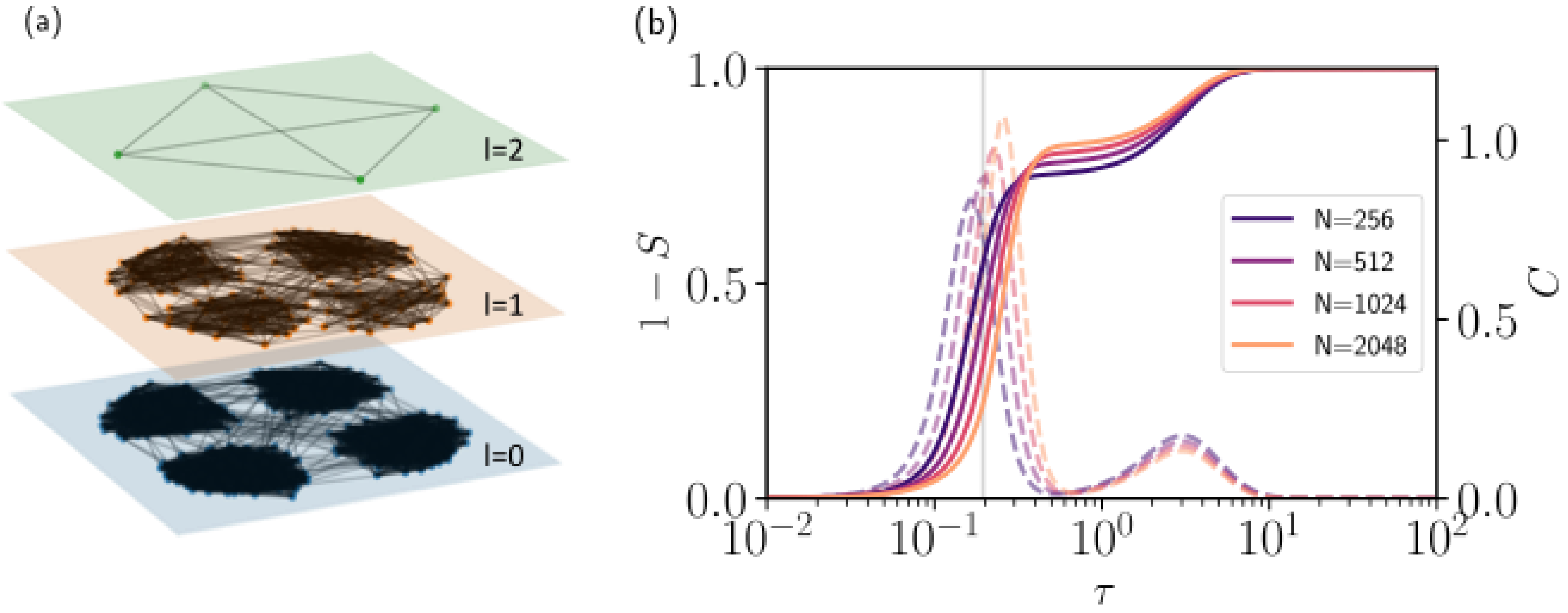


(a)
l=1
l=0
(b)
l=3
l=2
l=1
l=0
(c)
10^2
10^0
10^{-2}
$\mathcal{P}(\lambda_i)$
10^{-5}
10^{-3}
10^{-1}
10^1
λ_i

WATTS-STROGATZ SMALL WORLD NETWORK



STOCHASTIC BLOCK MODEL



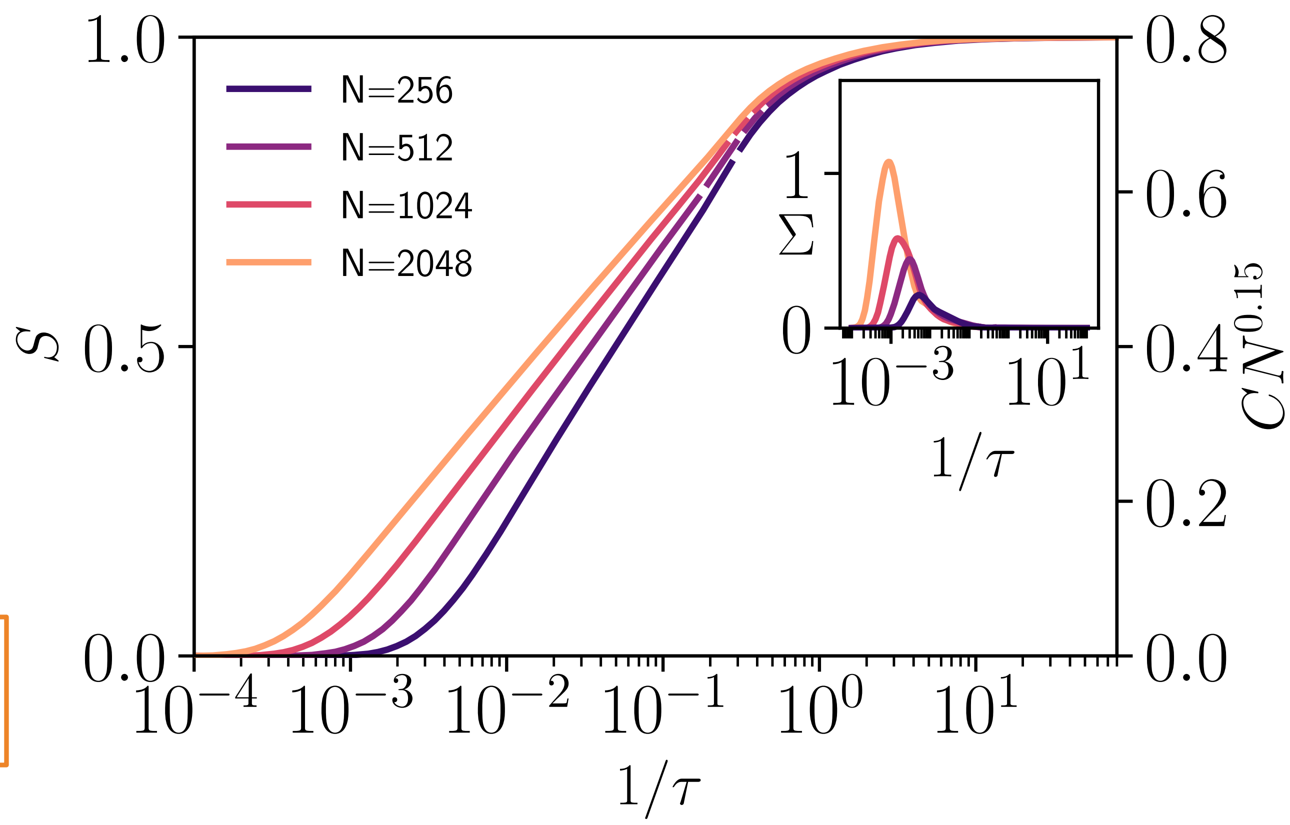
SCALE FREE CASE: BARABASI- ALBERT MODEL WITH $m = 1$ (PREFERENTIAL ATTACHMENT)

A new node is added at each time step bringing $m = 1$ edges which is attached to a node of the network with a probability proportinal to the degree of the receiving node

With $m = 1$

$P(k) \sim k^{-3}$ (scale-freeness)

A flat large peak → a scale invariant region as in lattice or tree



INFORMATION CORE AND SYNCHRONIZATION

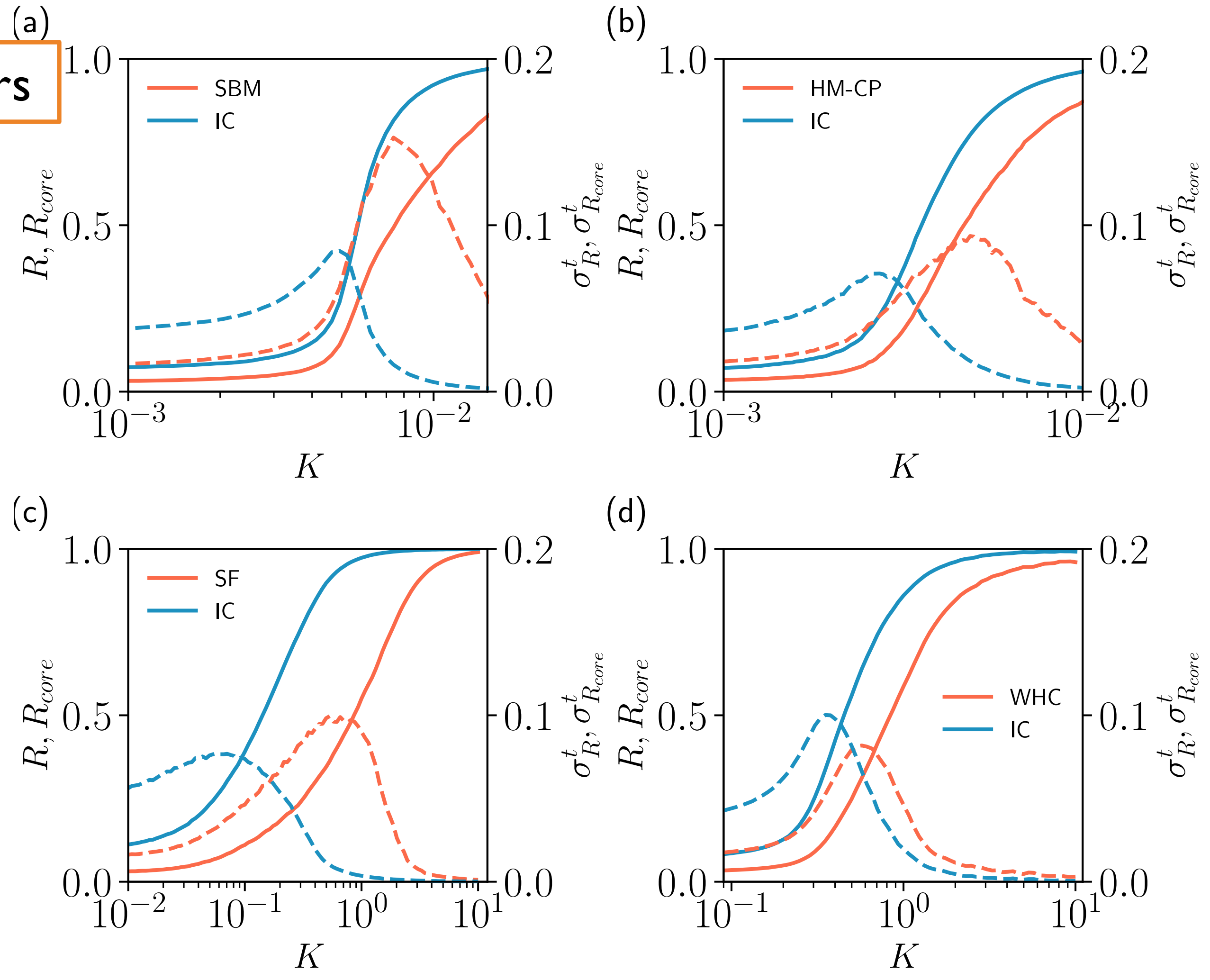
Kuramoto model of interacting non-linear oscillators

$$\dot{\theta}_i = \omega_i + K \sum_{j=1}^{N} A_{ij} \sin(\theta_j(t) - \theta_i(t)) + \sigma\eta_i(t),$$

At small angles it becomes

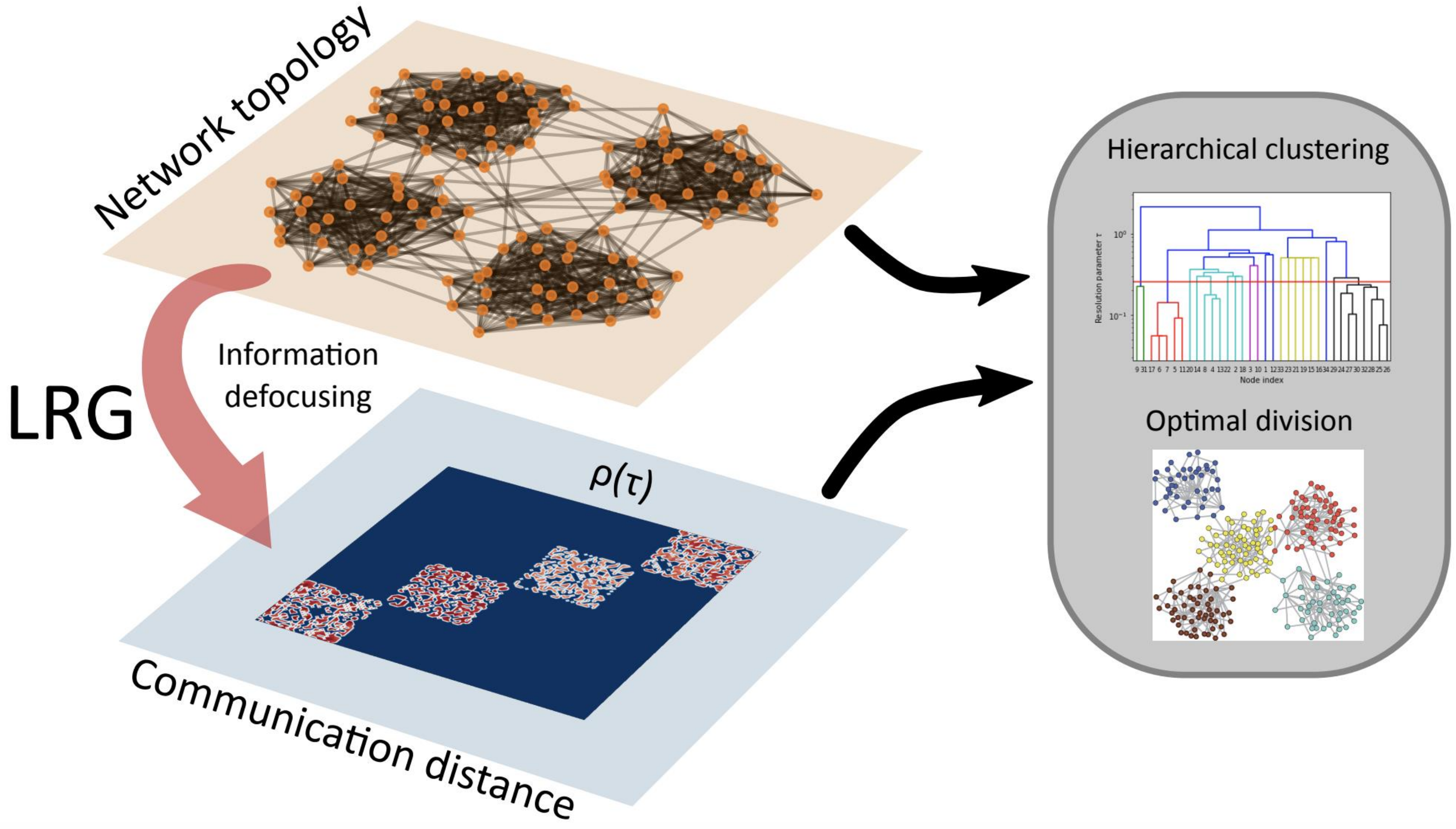
$$\dot{\theta}_i = K \left[\sum_j A_{ij}\theta_j - \sum_j \delta_{ij} \left(\sum_l A_{jl} \right) \theta_j \right] = -K \sum_j L_{ij}\theta_j,$$

It is a common feature of many models as we know from statistical field theory



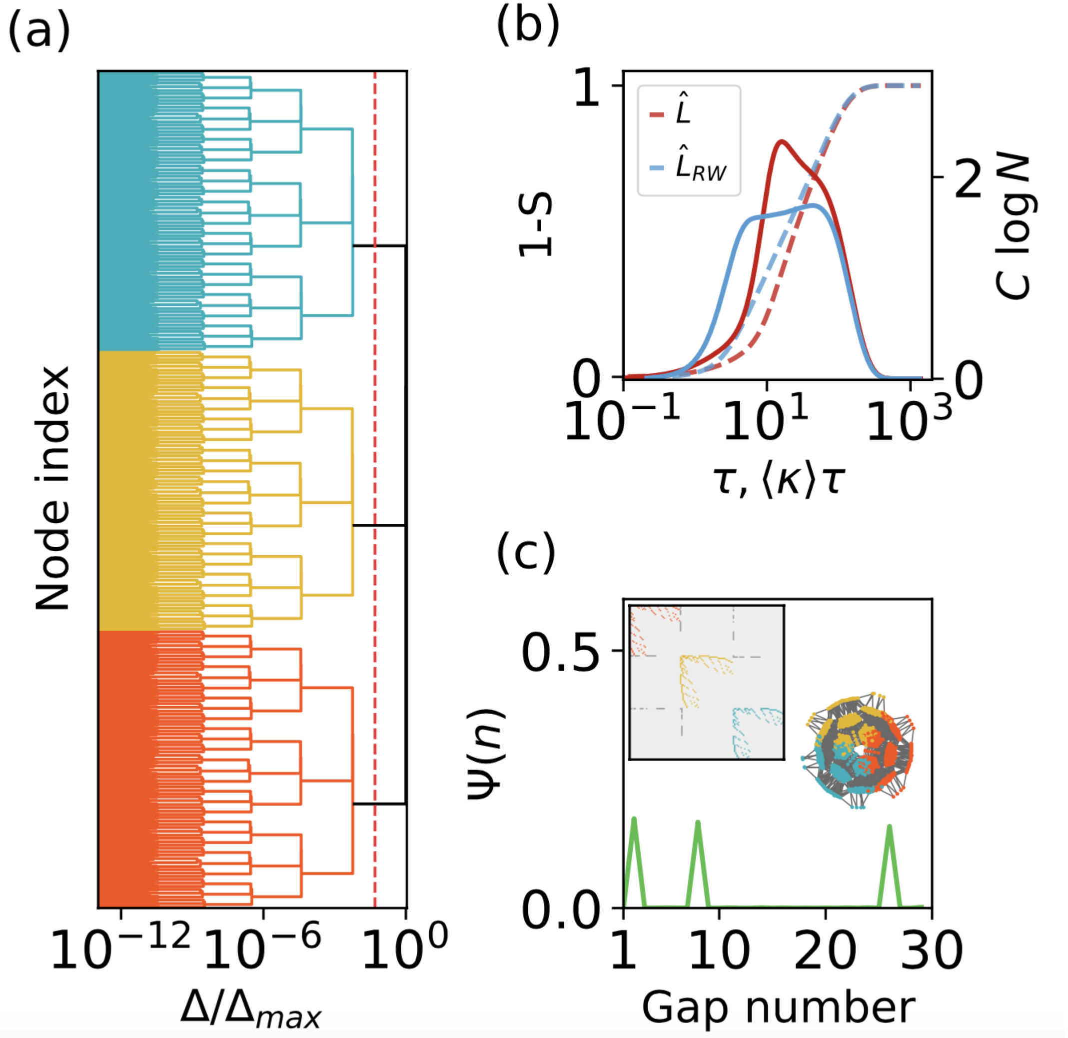
THE NEXT CHALLENGE: A *PHYSICAL* FORMULATION OF COMMUNITY DETECTION

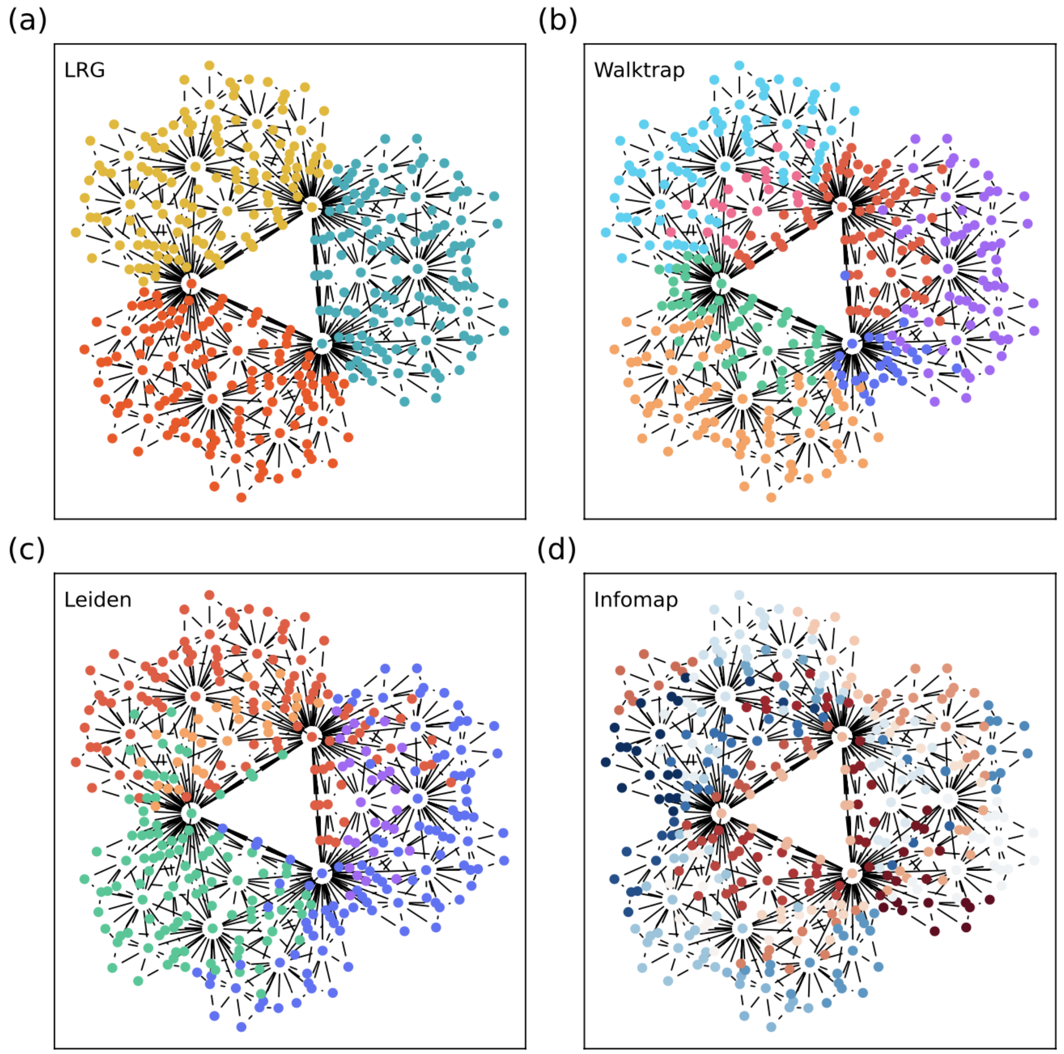
- At each t the matrix $\rho_{ij}(t)$ permits to build a dendrogram for clustering nodes.
- The most stable partition (largest step in the dendrogram) is the optimal partition at the diffusion scale t: informational stability
- At different t there can be one or more most stable partitions in time



P.Villegas, A. Gabrielli, A. Poggialini, T. Gili, https://arxiv.org/abs/2301.04514

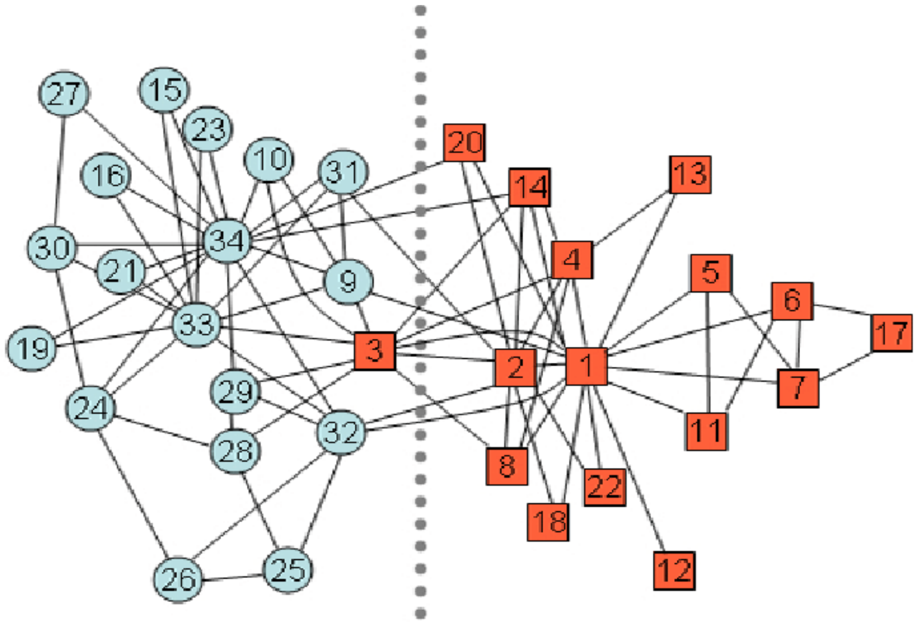
Dorogotsev-Goltsev-Mendes graph

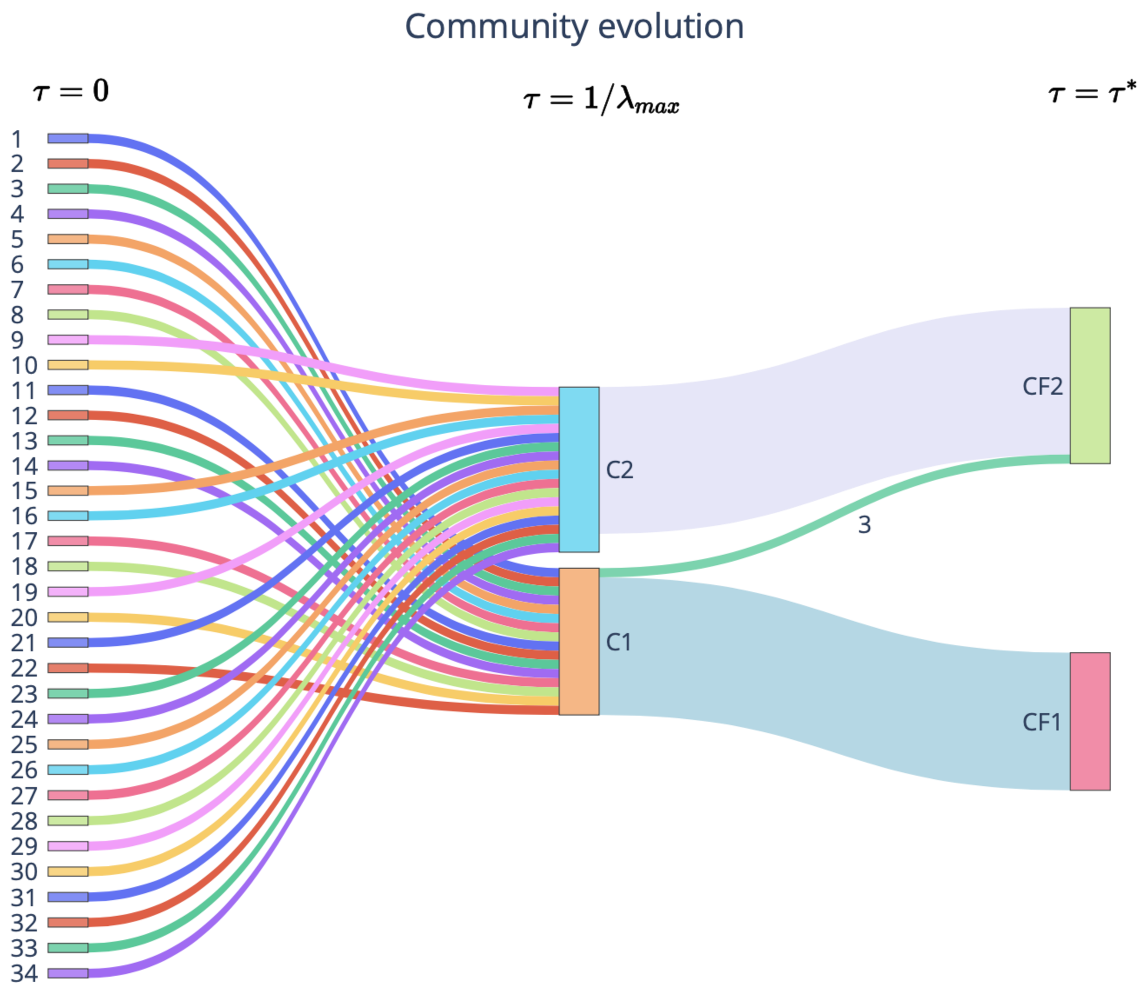




Metastable nodes

- Sankey diagram and the *metastable* nodes
- Fundamental bridges between communities.
- They guarantee the information flow between different communities





Zachary's karate club

SUMMARY

Take home messages:

(i) The informational entropy related to the homogeneous (per link) diffusion on graphs can be used to detect network *information cores, communities* and structural transitions in strict analogy with statistical physics critical phenomena;

(ii) It is also a natural way to define a coarse graining procedure of the network and embedded processes which is a direct generalization of the usual coarse graining in homogeneous spaces defined in the usual RG scheme in statistical physics

Perspectives

- Extend statistical mechanics analogy to explore structural organization of the network: Fluctuation Dissipation Theorem and Community Detection
- Generalizing the Wilson RG approach to statistical models (e.g. Contact processes, Kuramoto) for homogeneous systems to heterogeneous networks can shed light on the appearence of hierarchical phase transitions (e.g. Griffits phases) for this kind of systems

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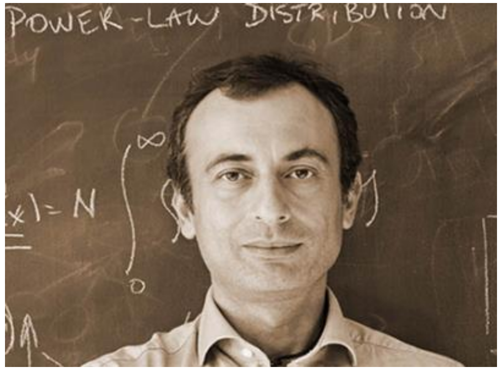

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