WP1@Spoke 2

b) Theoretical research projects in domains already using HPC solutions

5) Physics of complex systems

HPC Methods:

-Lattice Boltzmann

-Molecular dynamics

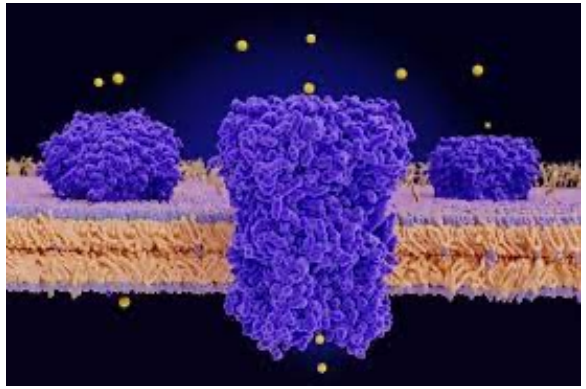
-Monte Carlo

General topics of Use Cases:

-complex fluid dynamics

-non-equilibrium statistical models

-biological models



UNIBA:

-Gonnella Giuseppe
-Suma Antonio
-Lamura Antonio
-Negro Giuseppe

UNINA:

-Milano Giuseppe
-Constantinos Siettos

UNIFE:

-Pareschi Lorenzo
-Dimarco Giacomo
-Bertaglia Giulia
-Boscheri Walter

Lattice Boltzmann Methods for complex fluids

Based on phase-space discretized form of the Boltzmann equation

$$\partial_t f + \xi_\alpha \partial_\alpha f + \frac{F_\alpha}{\rho} \partial_{\xi_\alpha} f = \Omega(f)$$

Discretizing both tin real and velocity space

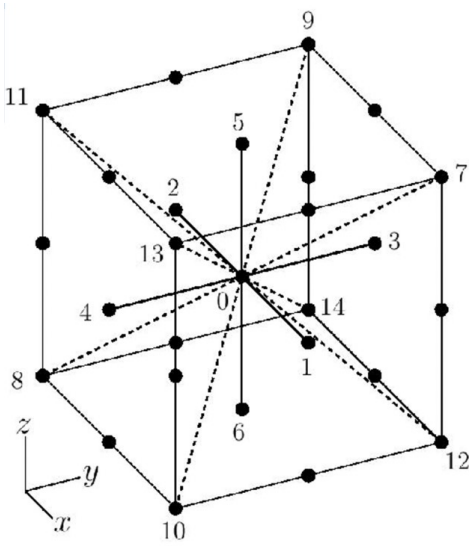
$$f_i(\vec{r} + \vec{\xi}_i \Delta t, t + \Delta t) - f_i(\vec{r}, t) = \mathcal{C}(\{f_i\}, t)$$

$$\mathcal{C}(\{f_i\}, t) = -\frac{1}{\tau}(f_i - f_i^{\mathrm{eq}})$$ BGK approximation

Mass and momentum density are defined as

$$\sum_i f_i^{eq} \xi_{i\alpha} = \rho u_\alpha \qquad \sum_i f_i^{eq} = \rho$$

$$\sum_i f_i^{eq} \xi_{i\alpha} \xi_{i\beta} = \rho u_\alpha u_\beta - \sigma_{\alpha\beta}$$



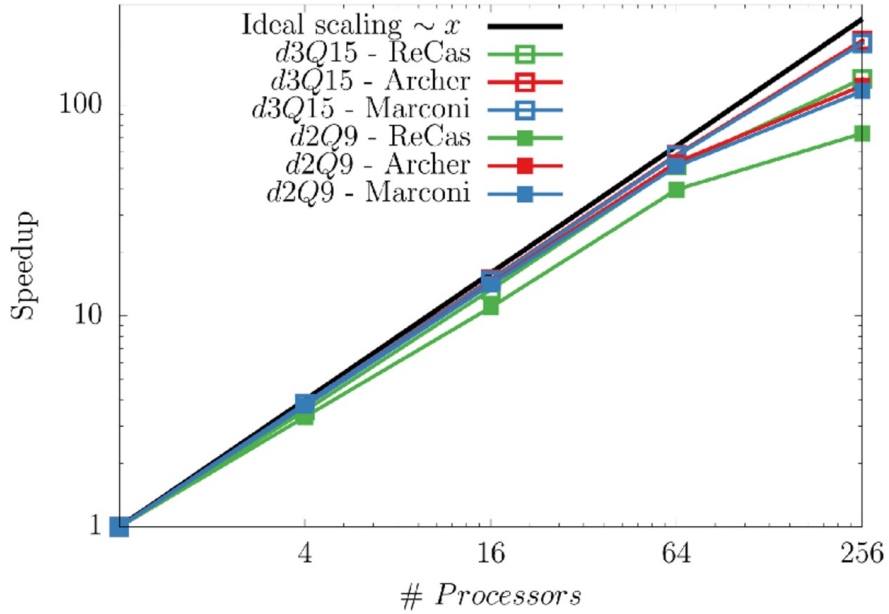
D3Q15 geometry

- The equilibrium distribution functions are expanded up to a given order in the fluid velocity u.
- The expansion coefficients are determined imposing the above constraints.
- The Navier-Stokes equations can be formally derived from the lattice Boltzmann equation in the long wave length limit through Chapman-Enskog expansion

Lattice Boltzmann Method

Numerical implementation of LBM must face some computational issues

- Memory resources
- Long processing times



"Be wise..." parallelize

- Mpi protocol
- Distributed memory system

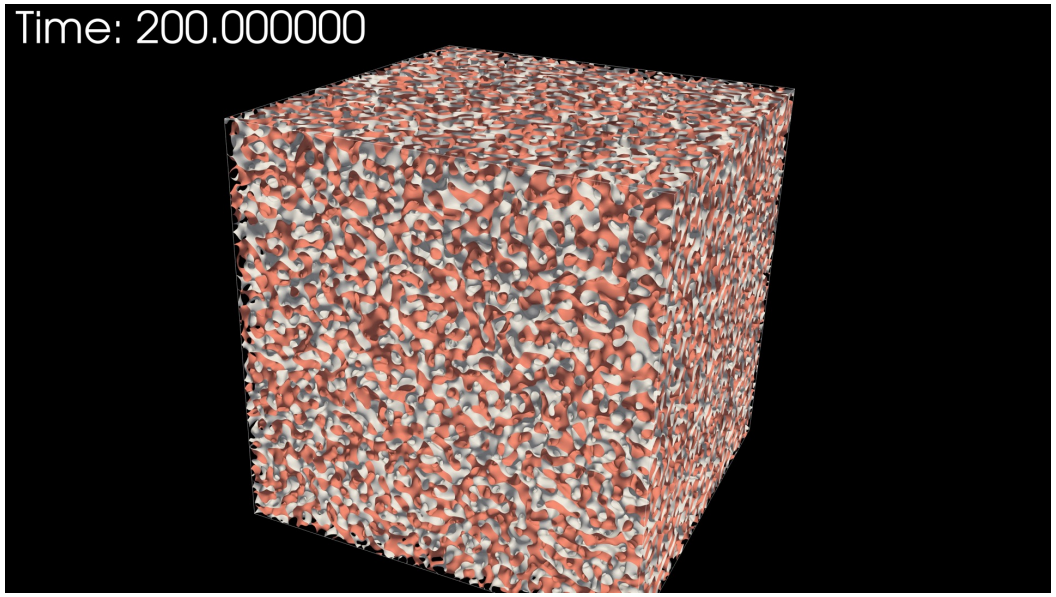
HPC facilities in Bologna, Bari and Edinburgh

Ghost cell method can be implemented to solve the problem of stencils computation on the boundaries between computational subdomains

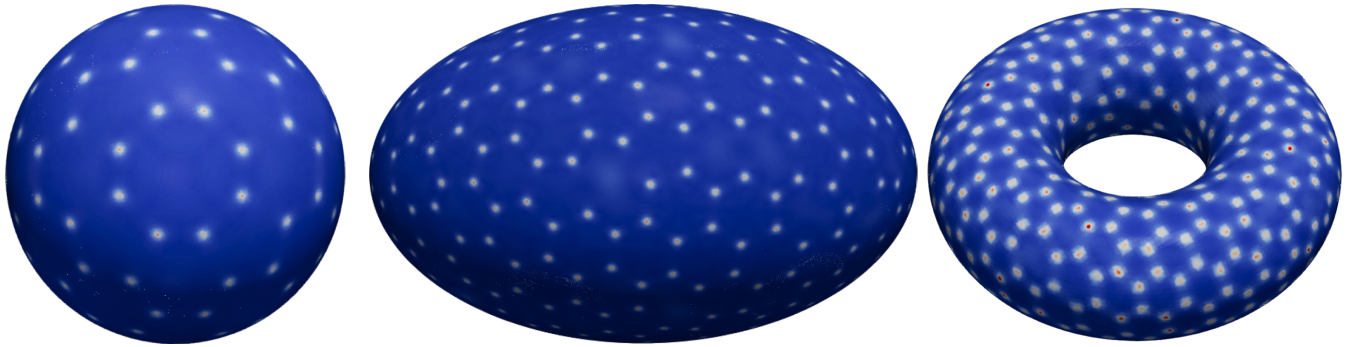
The European Physical Journal E 42 (6), 81

Complex (liquid crystals, mixtures, etc) fluids

Dynamics of multi-phase fluid mixtures



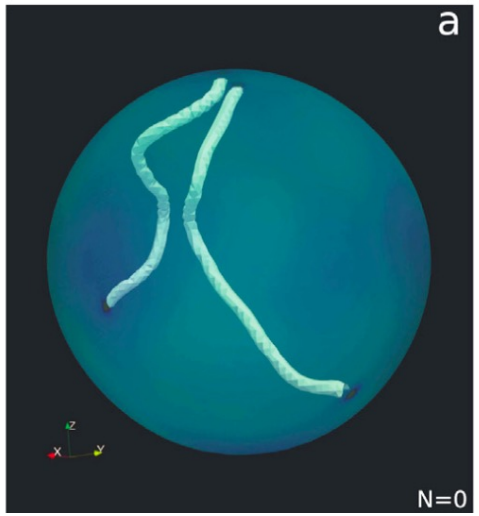
Topological properties of confined chiral liquid crystals

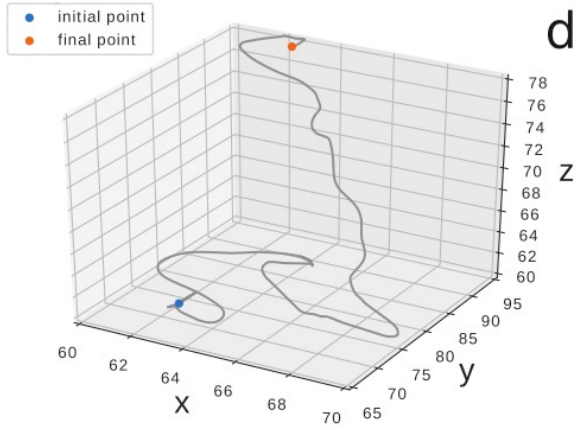


Cholesteric shells: two-dimensional blue fog and finite quasicrystals
LN Carenza, G Gonnella, D Marenduzzo, G Negro, E Orlandini
Physical Review Letters 128 (2), 027801 (2022)

Active fluids

Self-motility of active droplets

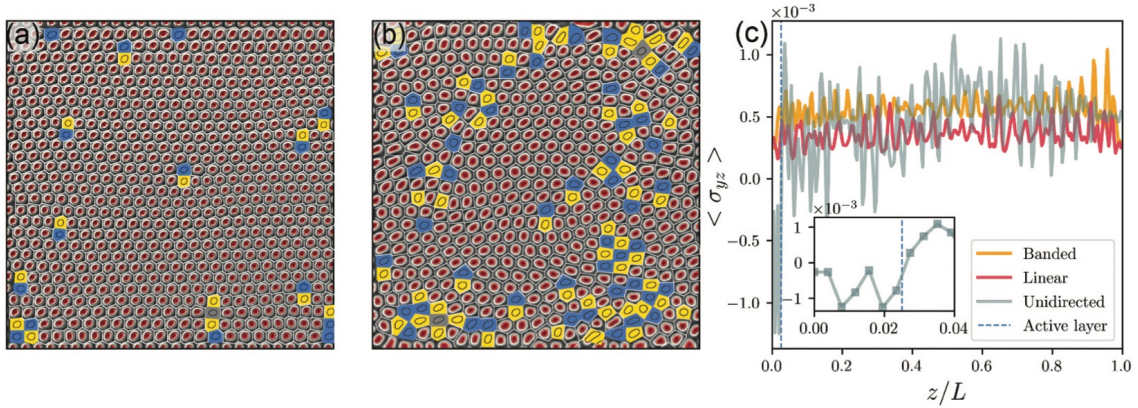




[Rotation and propulsion in 3D active chiral droplets](#)LN Carenza, G Gonnella, D Marenduzzo, G Negro
Proceedings of the National Academy of Sciences 116 (44), 22065-22070, (2020)

[Chaotic and periodical dynamics of active chiral droplets](#)LN Carenza, G Gonnella, D Marenduzzo, G Negro
Physica A: Statistical Mechanics and its Applications 559, (2020)

Morphology and rheology of active fluids

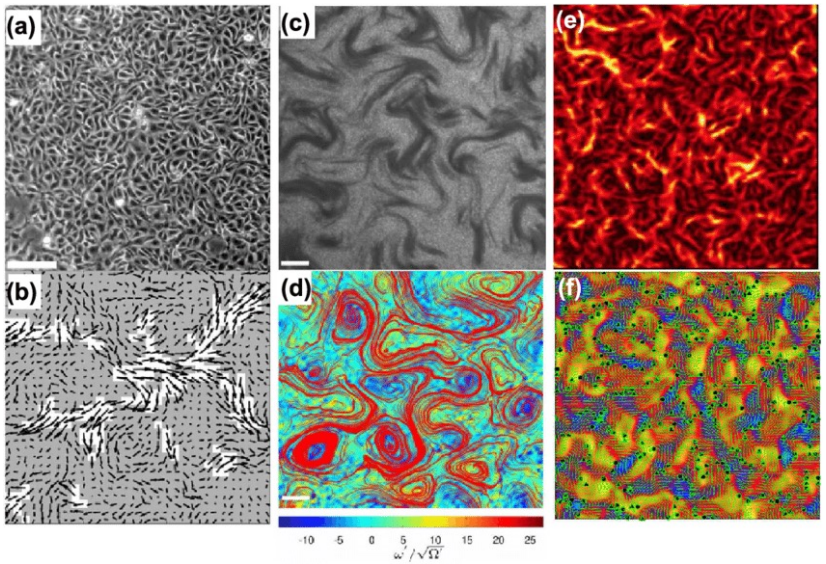


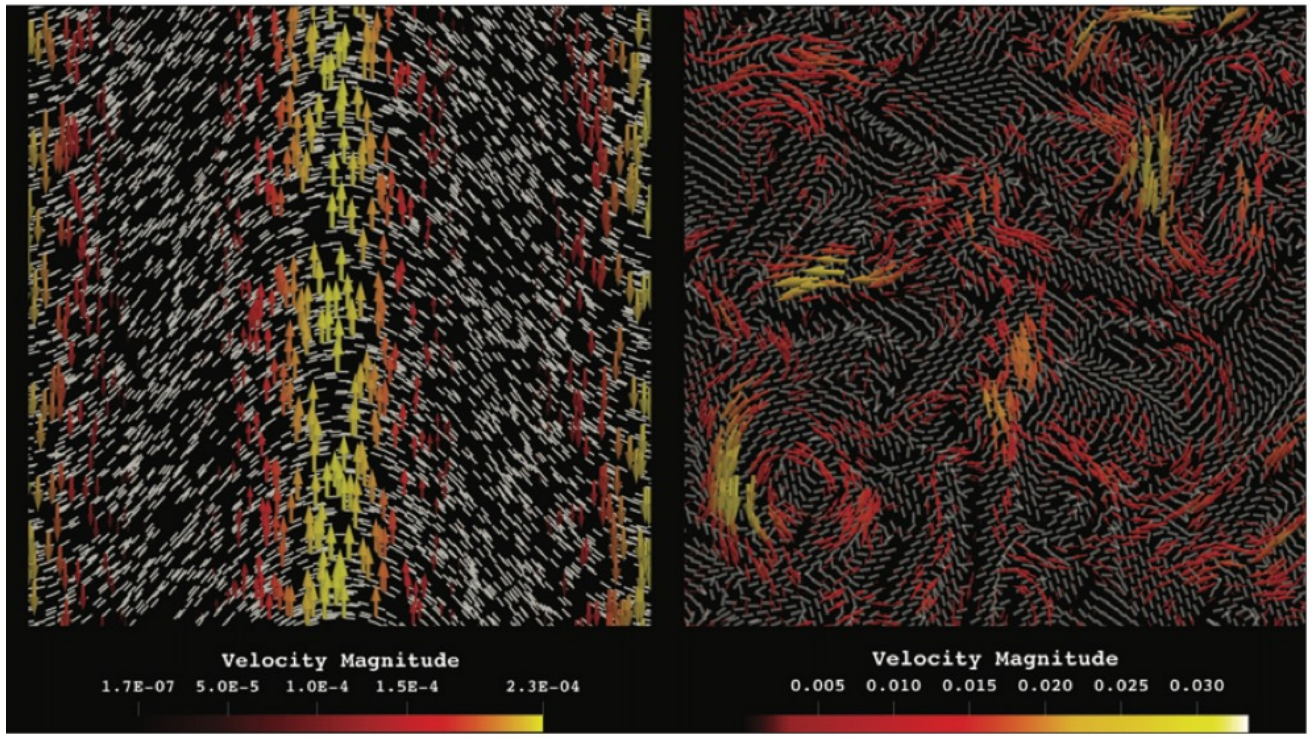
Emergence of negative viscosity states in active polar emulsions

[Activity-induced isotropic-polar transition in active liquid crystals](#)MG Giordano, F Bonelli, LN Carenza, G Gonnella, G Negro
Europhysics Letters 133 (5), 58004

Active fluids

Active Turbulence





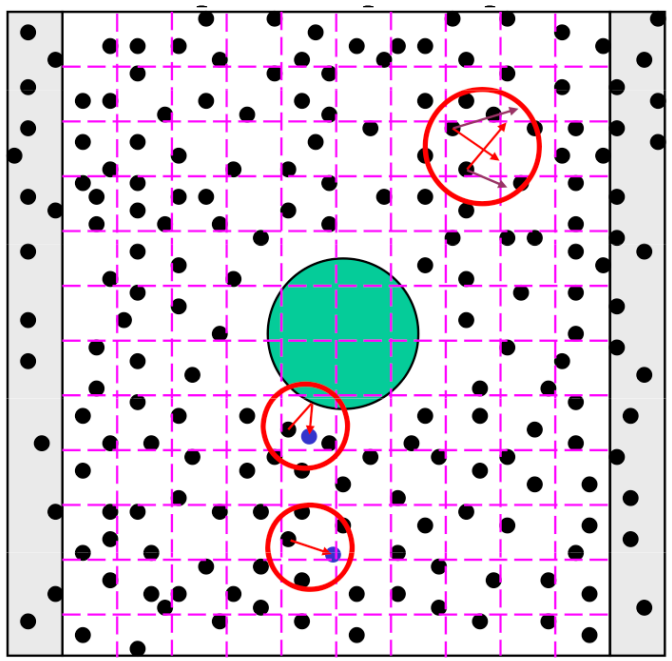
No signal of non-linear hydrodynamical transfer and turbulent cascades in active nematic gels

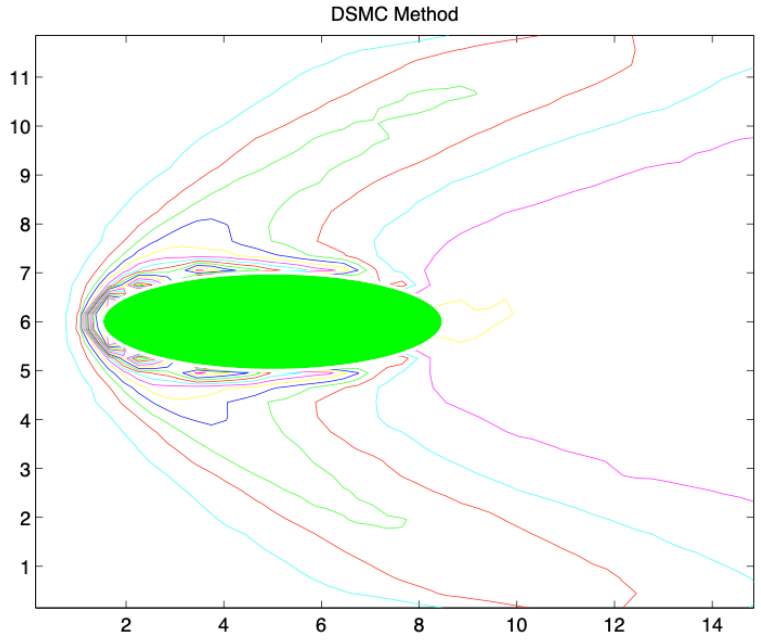
Cascade or not cascade? Energy transfer and elastic effects in active nematics
LN Carenza, L Biferale, G Gonnella
Europhysics Letters 132 (4), 44003 (2021)

Multiscale control of active emulsion dynamics
LN Carenza, L Biferale, G Gonnella
Physical Review Fluids 5 (1), 011302 (2020)

General complex systems methods

Introducing an intermediate step between particle systems and fluid models: the so-called kinetic level. These models, characterized by Boltzmann equations, deal with a quantity, the distribution function, which is the density of particles in phase-space (say position and velocity).
The essential idea of Monte Carlo or particle simulations for the Boltzmann equation is to return to the particle description with a number of particles small enough to make the situation computationally treatable but ”sufficiently close” to the physical situation.

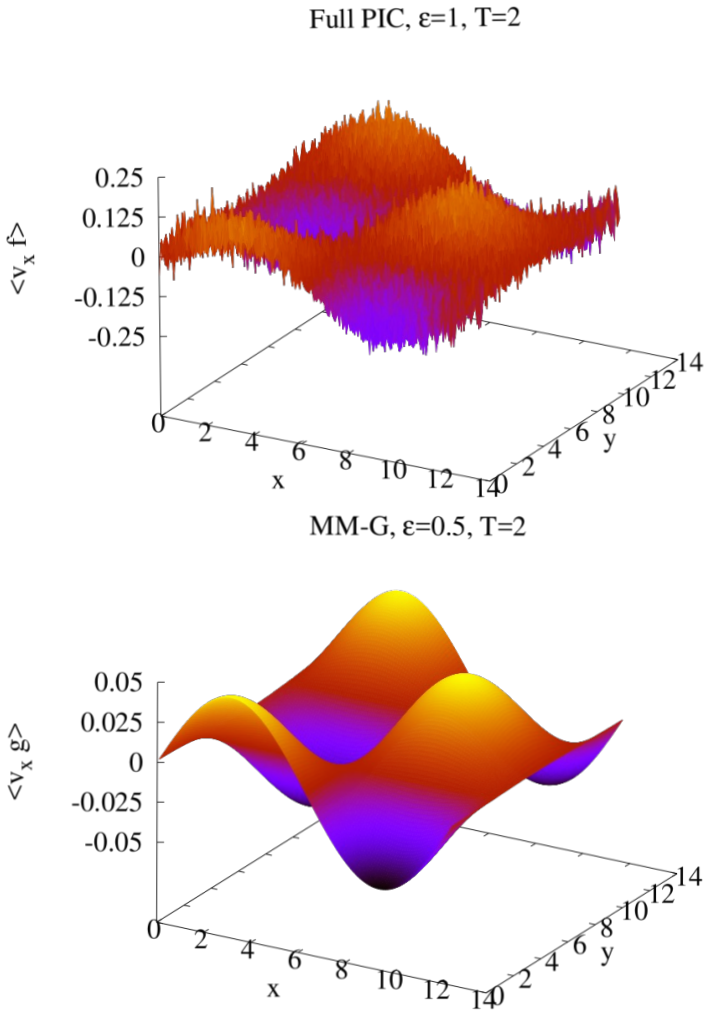




General complex systems methods

Fluid dynamics and rarefied flows

Monte Carlo methods for fluid dynamics and rarefied flows. We plan to develop new stochastic based methods for the resolution of flows out of equilibrium. In particular we will address the resolution of the Boltzmann and of the Fokker-Planck equations. The focus is on efficiency and low variance methods by coupling the solution of deterministic equilibrium flows with non equilibrium stochastic solvers.



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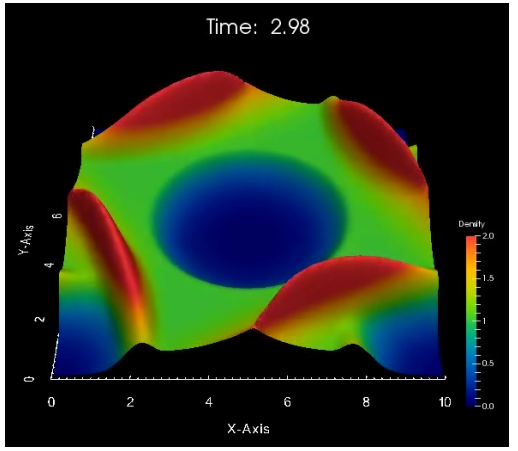
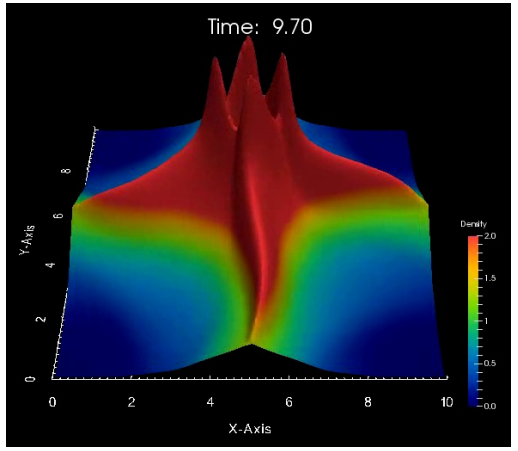
- Time diminishing schemes (TDS) for kinetic equations in the diffusive scaling. A Crestetto, G. Dimarco, N. Crouseilles, M. Lemou. Journal of Computational Physics 394, pp. 243-262 (2019).
- A new deviational Asymptotic Preserving Monte Carlo method for the homogeneous Boltzmann equation. A. Crestetto, N. Crouseilles, G. Dimarco, M. Lemou. Communications in Mathematical Sciences 18, pp. 2305-2339 (2020).

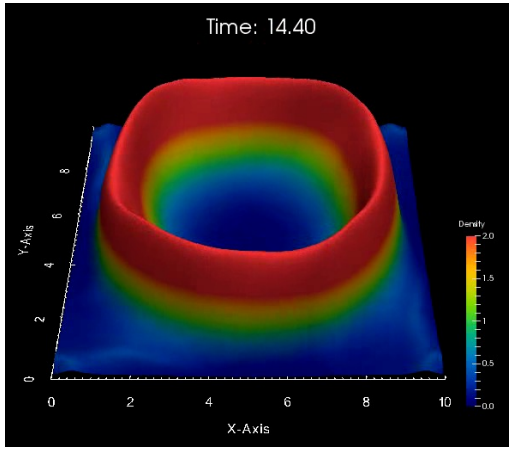
General complex systems methods

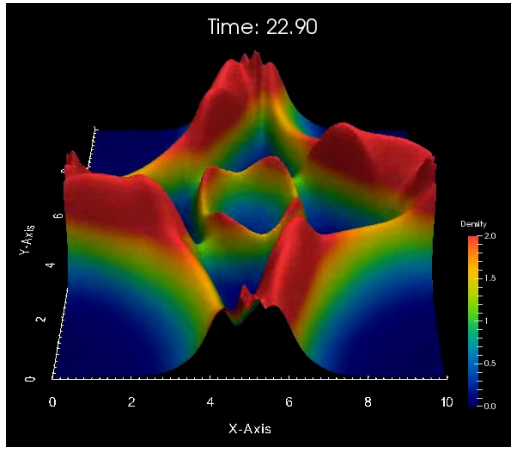
Emergence behavior in living biological systems

Understanding of the emergence behavior in living biological systems and humanity. The focus here is in the description of complex systems such as organisms, human behaviors and economics. Knowledge, social stratification, opinion dynamics and spread of fake news will considered as prototypes of complex dynamics. The capability of dealing with large amount of data and to infer about these dynamics will be out of the main goal of this WP. We will also consider data-driven approaches in which experimental information measured from real-world systems will be inserted into the model to calibrate the parameters.









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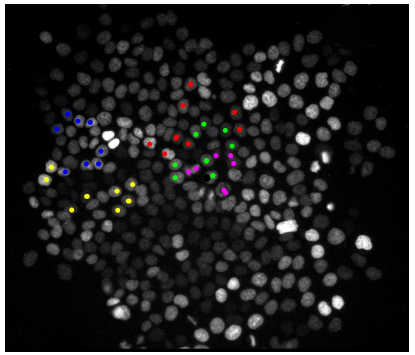
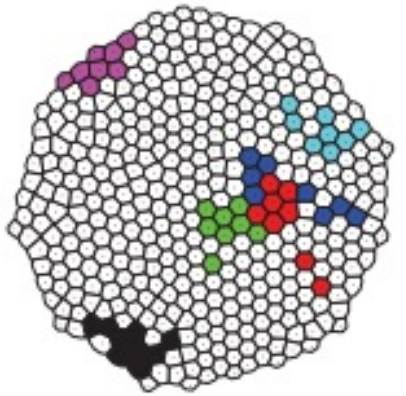
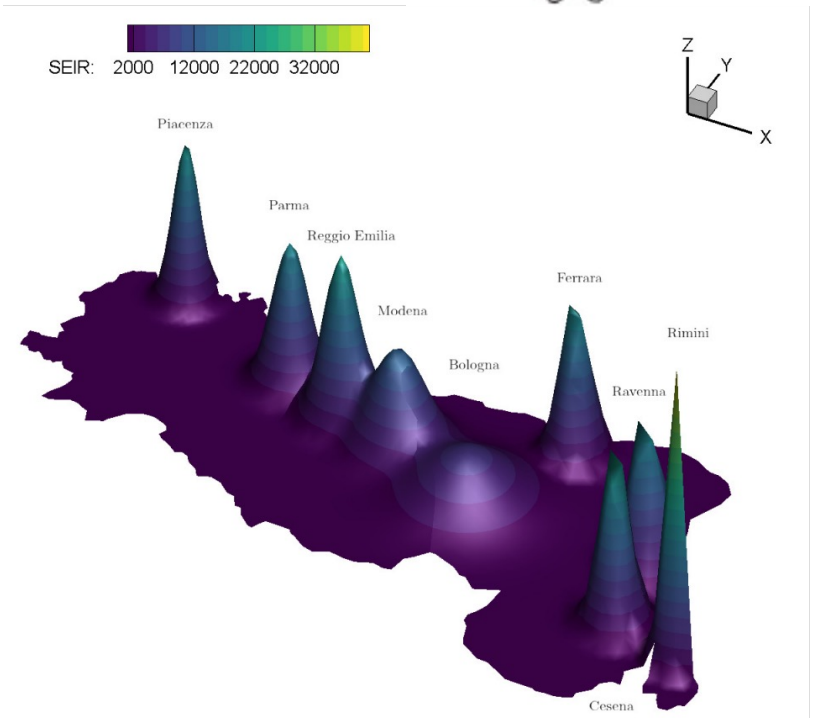
- Kinetic modeling of alcohol consumption. G. Dimarco, G. Toscani. Journal of Statisical Physics 177, pp. 1022-104 2(2019).
- Social climbing and Amoroso distribution. G. Dimarco, G. Toscani. Mathematical Models and Methods in Applied Sciences 30, pp. 2229-2262 (2020).
- Wealth distribution under the spread of infectious diseases. G. Dimarco, L. Pareschi, G. Toscani, M. Zanella. Physical Review E 102, 022303 (2020).

Medical applications

Medical applications such as modeling and simulations of the spread of viruses (Covid-19) through spatially dependent multiscale approaches will be addressed. An important role will be played by the contact dynamics analysis and modeling. The growth, the spread and the control of tumor cells will be studied. For these new models, particle methods and fitting with the data will be also considered. The role of uncertainty in the data will be also discussed and addressed for the construction of reliable models.







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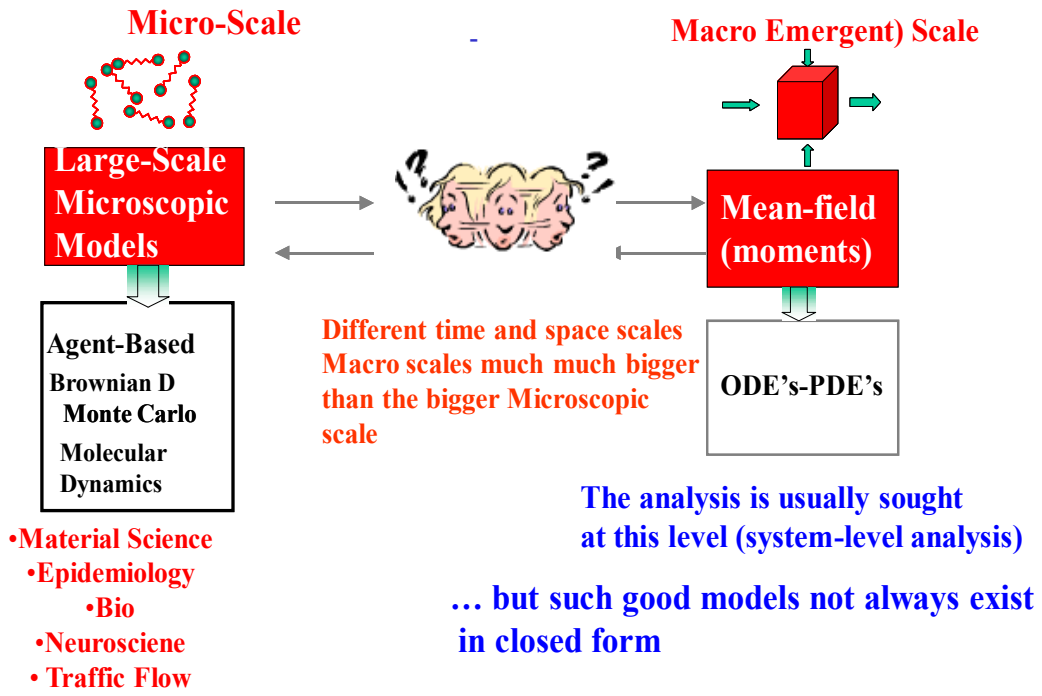
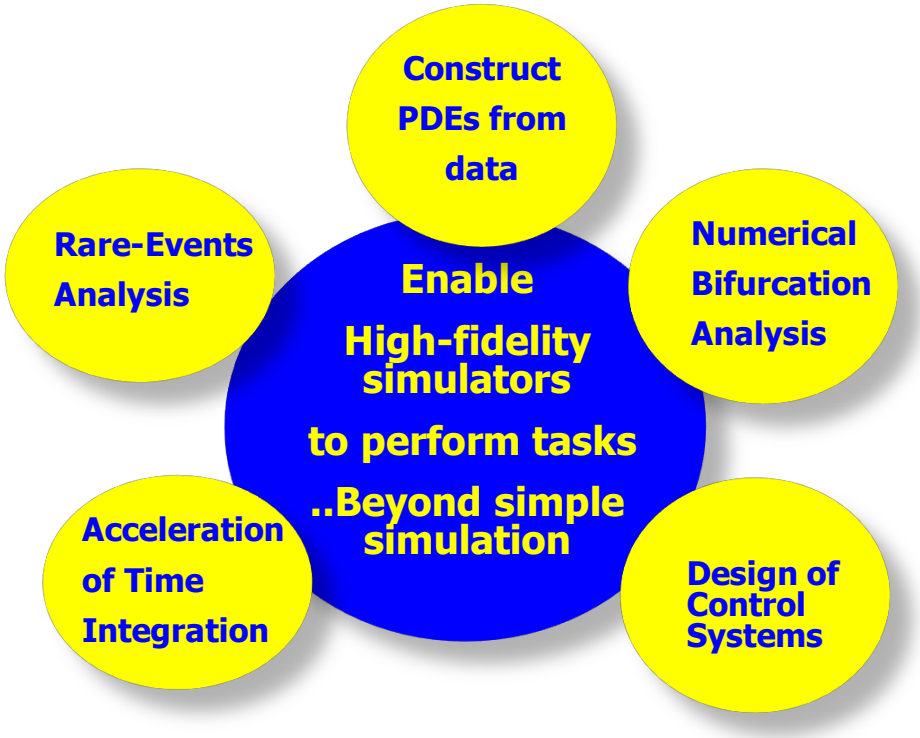
- Spatial spread of COVID-19 outbreak in Italy using multiscale kinetic transport equations with uncertainty. G. Bertaglia, W. Boscheri, G. Dimarco, L. Pareschi. Math. Biosci. Eng. 18 (2021) 7028-7059.
- A data-driven epidemic model with social structure for understanding the COVID-19 infection on a heavily affected Italian Province. M. Zanella, C. Bardelli, G. Dimarco, S. Deandrea, P. Perotti, M. Azzi, S. Figini, G. Toscani. Mathematical Models and Methods in Applied Sciences 12, 2533-2570 2021.
- Kinetic models for epidemic dynamics with social heterogeneity. G. Dimarco, B. Perthame, G. Toscani, M. Zanella. Journal of Mathematical Biology 83(1),4 (2021).

Bridge the gap between micro and macro scales of Complex Systems

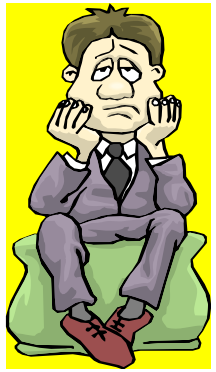


constantinos.siettos@unina.it

Objectives



What if physics are known in a more detailed (microscopic) level?



…but there is no description (in moments of distribution) of the macroscopic behavior;

SIMULATION: LIKE EXPERIMENTS

MICRO-scopic

MACRO-scopic

EQUATION-FREE METHODS

Physics-Informed Machine Learning

CONTROL

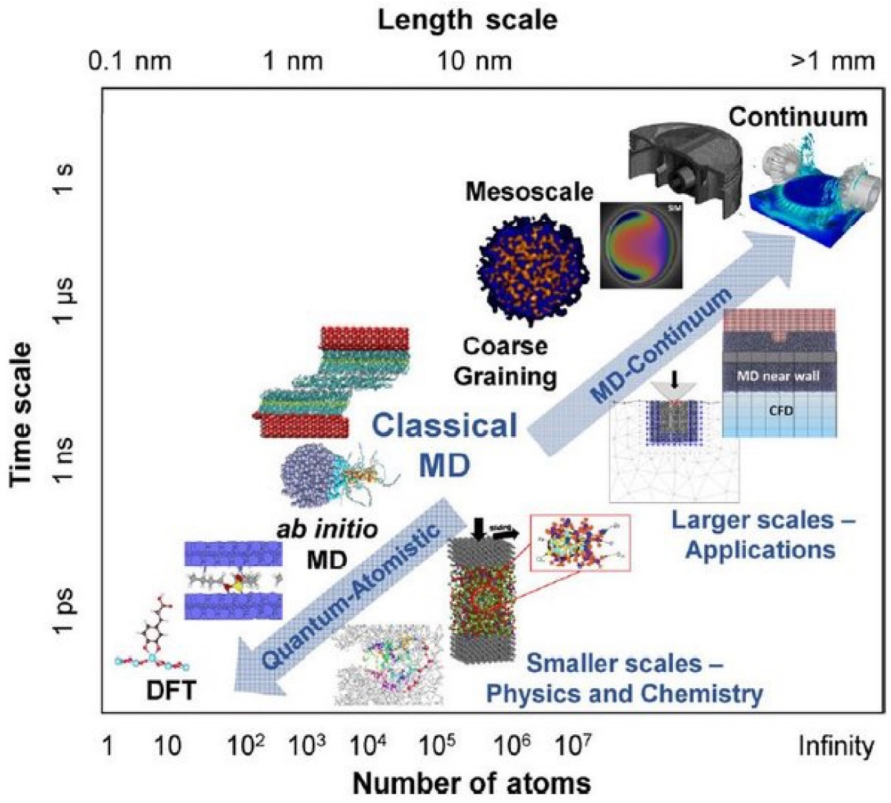
OPTIMIZATION

i.e. run atomistic-based models for many units (atoms, agents etc) and for different parameters and for long time to get macroscopic (system-level) information

AIM: Systematically bridge the gap between Micro-scopic and Macro-scopic (system-level) World

But good macroscopic models do not always exist in closed form ….

Molecular Dynamics Methods

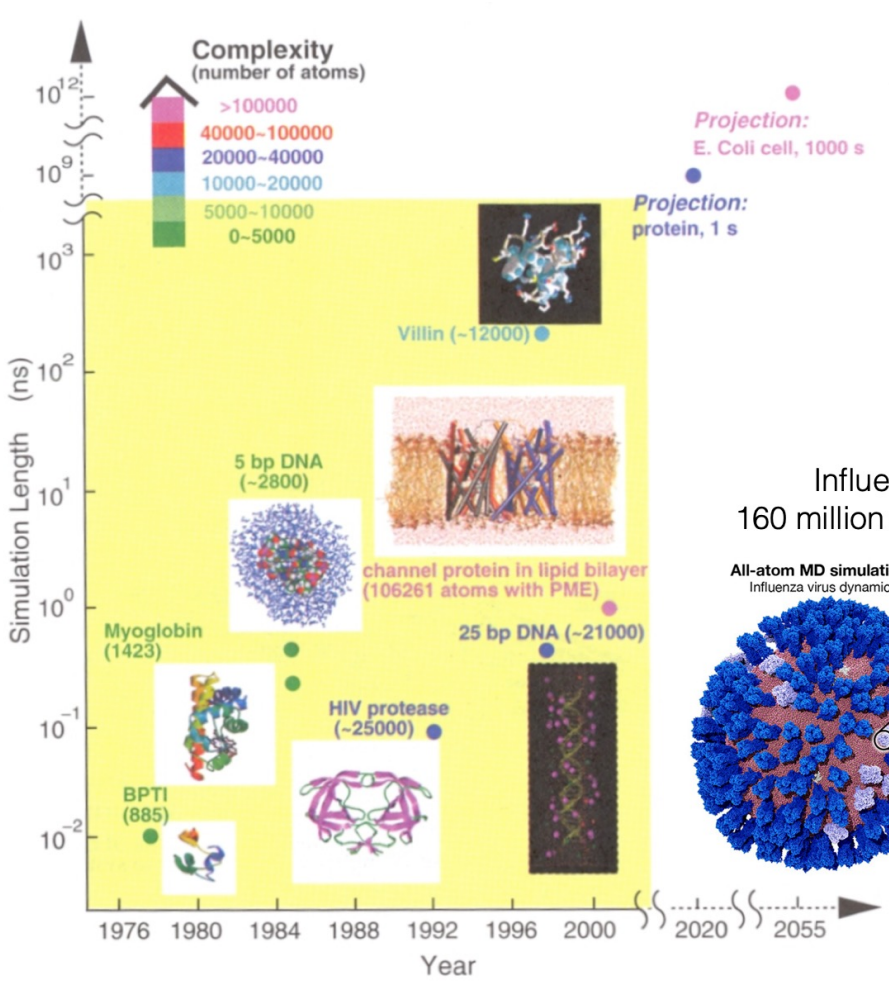


Basic elements are atoms (as a whole, no electrons, protons) or group of atoms in more coarse-grained systems

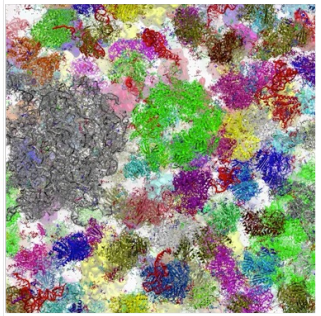
They are considered as classical objects
(no quantum mechanics involved, only Newton's equation of motions.)

Molecular Dynamics Methods

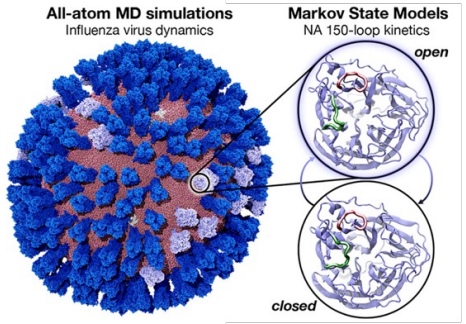
General outlook of MD by system's dimension (for biological structures)



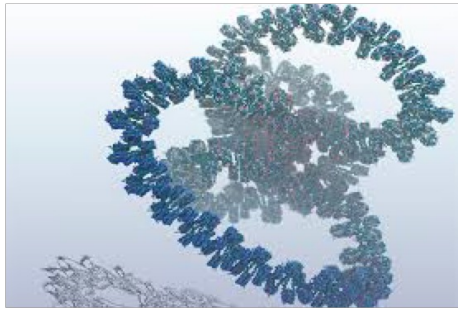
Bacterial cytoplasm
103million atoms ~100ns



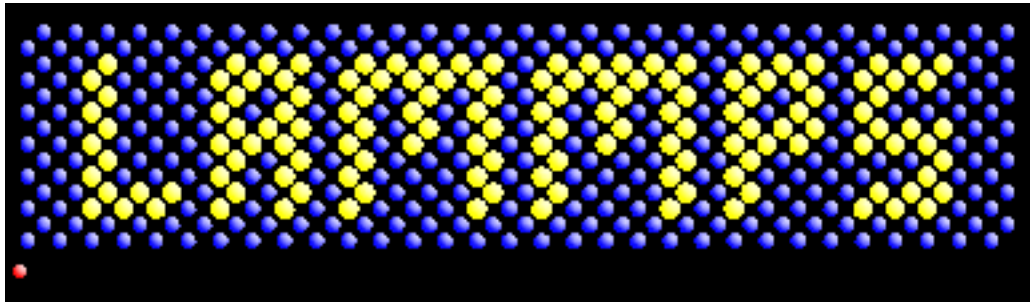
Influenza virus
160 million atoms ~100ns



Chromatin
1 billion atoms 130000cores



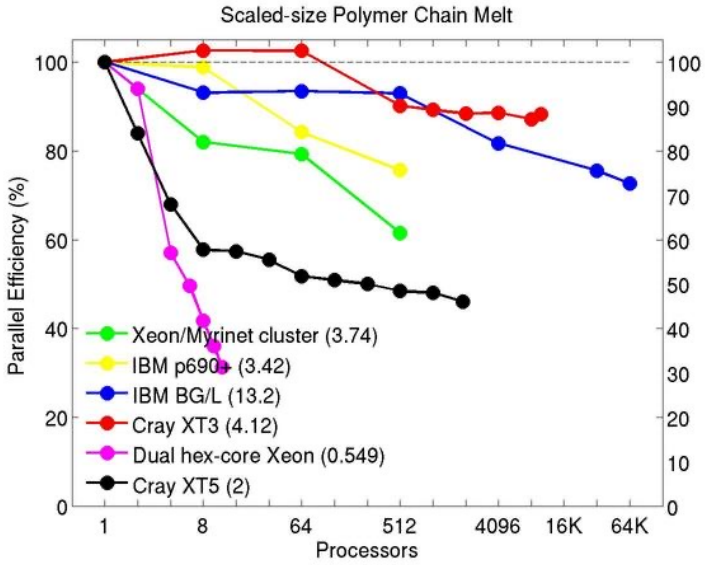
Molecular Dynamics Methods



LAMMPS is a classical molecular dynamics code with a focus on materials modeling.

It's an acronym for **Large-scale Atomic/Molecular Massively Parallel Simulator**.

It can be used with multiple CPUs and with a GPU



Bead-spring polymer melt with 100-mer chains and FENE bonds:

- 32,000 atoms for 100 timesteps
- reduced density 0.8442 (liquid)
- force cutoff of 2^(1/6) sigma
- neighbor skin = 0.4 sigma
- neighbors/atom = 5 (within force cutoff)
- NVE time integration

OCCAM: Hybrid Particle-Field Parallel MD Simulations

-Development of coarse-grained models based on Field Theory for soft matter simulations
-High Performance Large Scale Molecular Dynamics parallel simulations

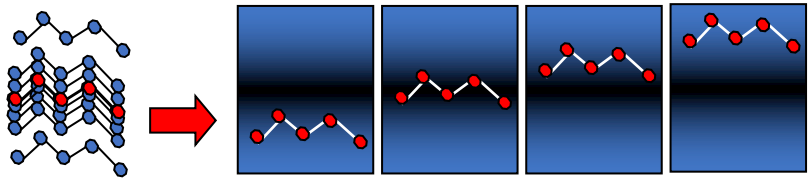
giuseppe.milano@unina.it

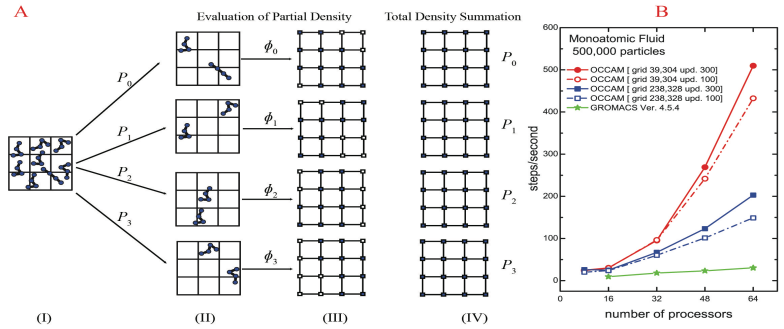
Parallel OCCAM for distributed memory (Implementation of MPI interface for CPU, multi GPU in progress)

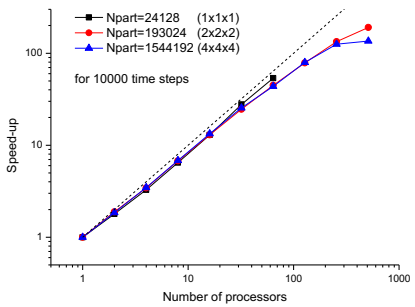
OCCAM
Molecular Dynamics

https://sites.google.com/view/occammd

Complex Molecular Architectures using Field Theory

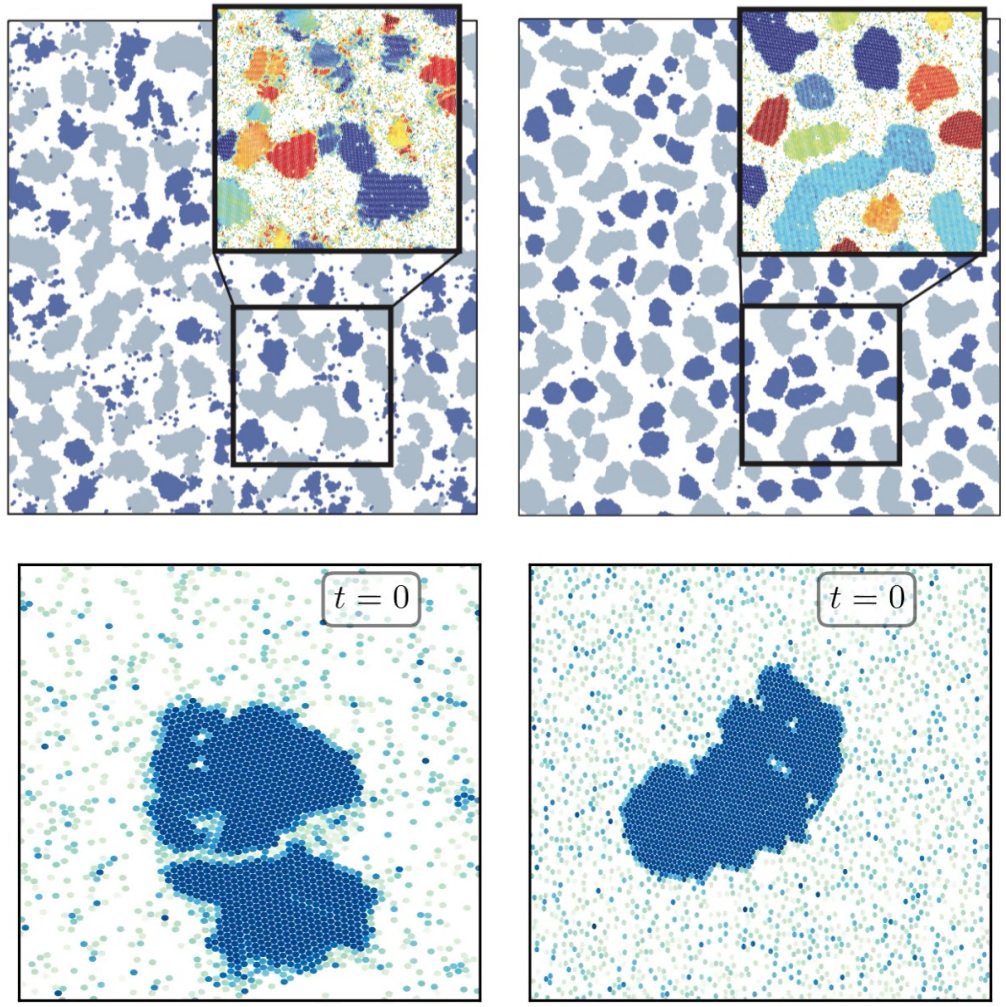




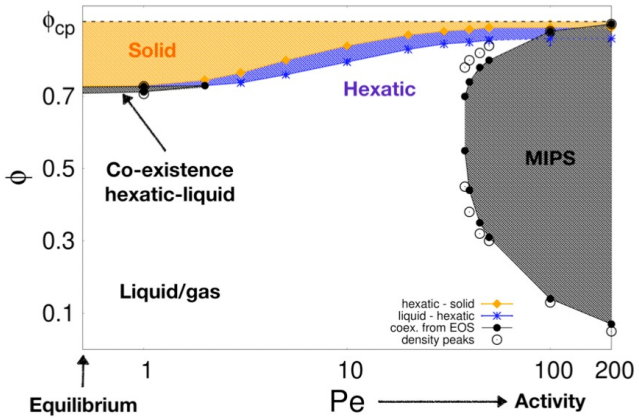


Active self-propelled particles

Active (with repulsion) **Passive (with attraction)**



- Micro and macro phase separation of active systems
- Self-organization and dynamics of active clusters
- Phase diagram

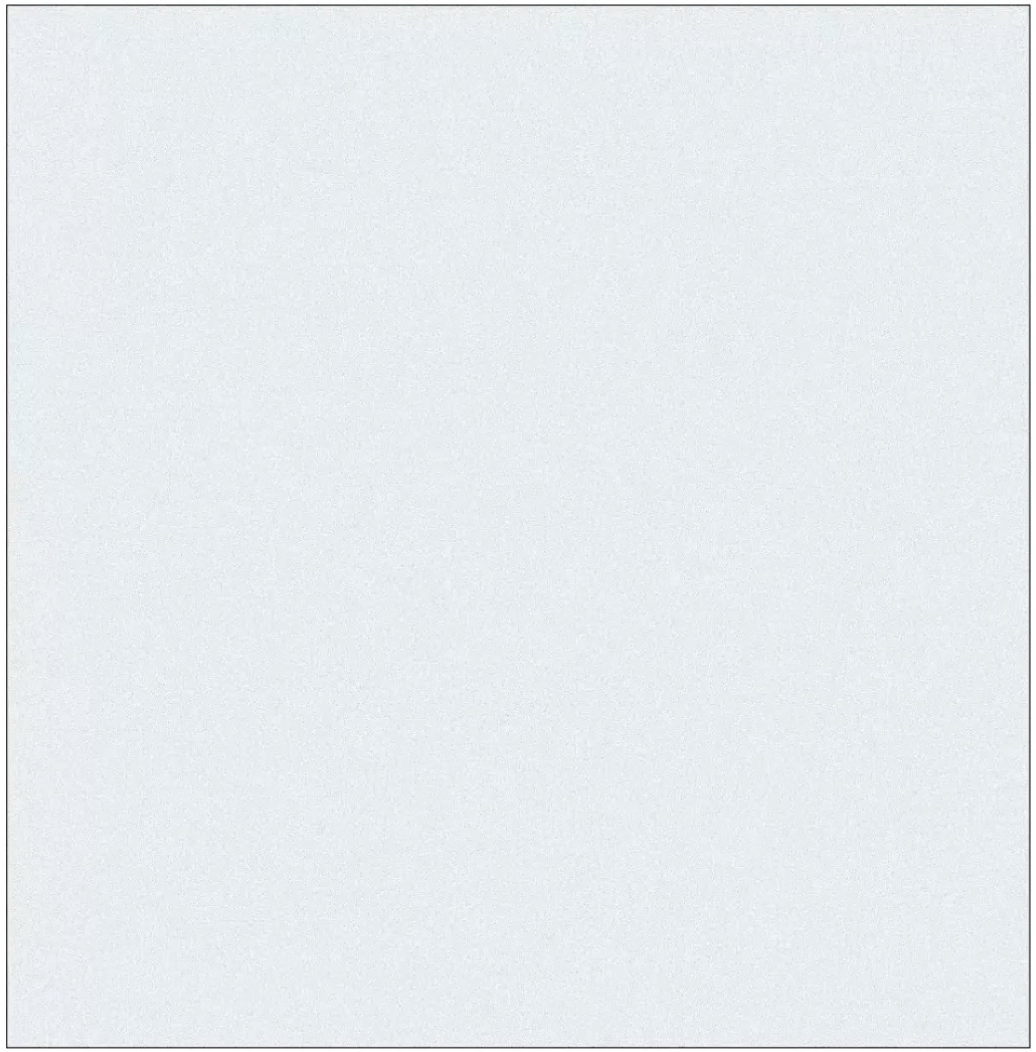


Cugliandolo et al. PRL 119 (26), 268002 2017

Digregorio et al. PRL 121, 098003 2018

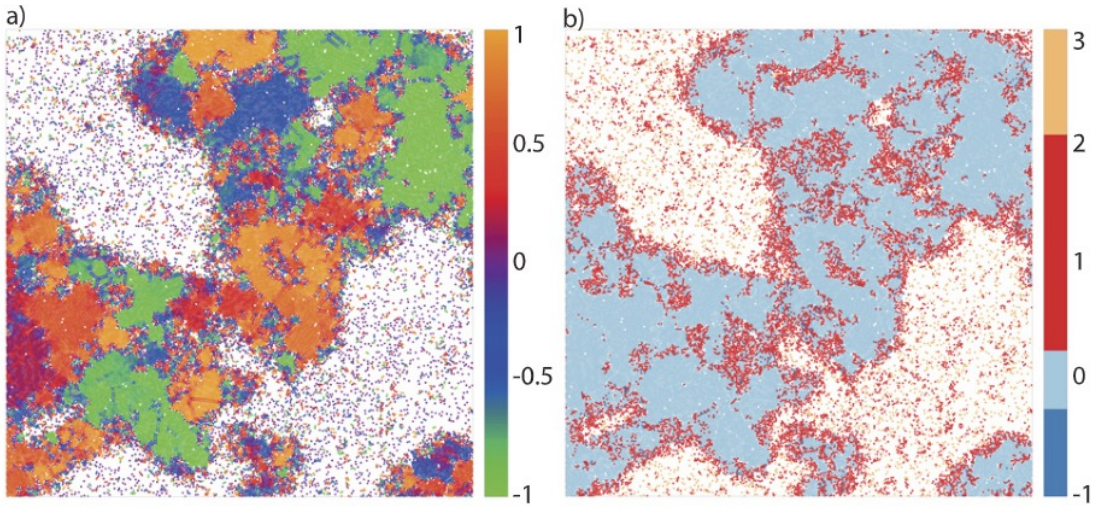
Caporusso et al. PRL 125 (17), 178004 2020

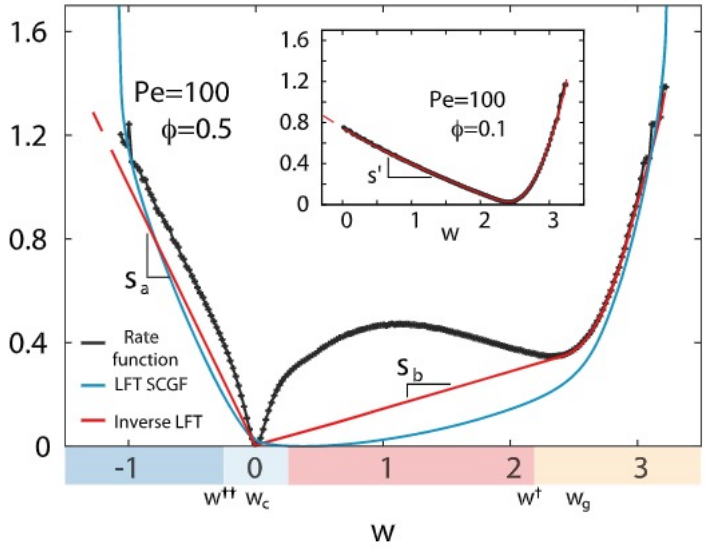
Active self-propelled particles



Cluster tracking for 1024^2 particles using clustering algorithms

Non-equilibrium statistical mechanics





- Analytical and numerical evaluation of the Active Work distributions for active particles
- Study of Fluctuation Relations

Semeraro et al., J Stat Mech, 12 2021

Cagnetta et al. PRL 119 (15), 158002 2018

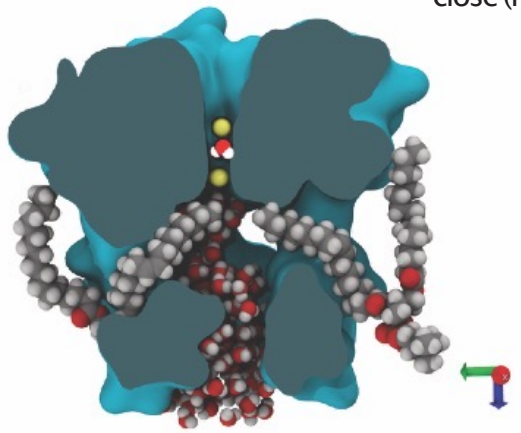
Chiarantoni et al. Journal of Physics A 53 (36), 36LT02 2020

Petrelli et al. 102 (1), 012609 2020

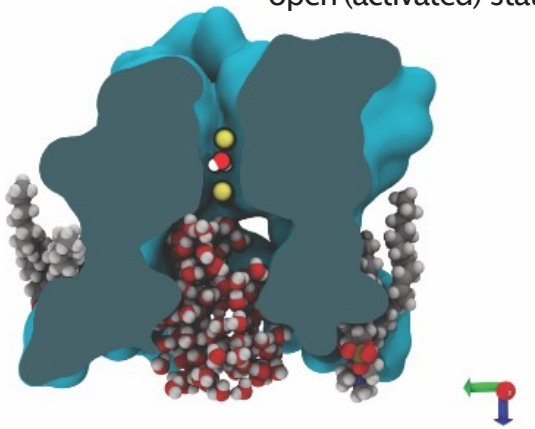
Model for lipid bilayers and ion channels

Atomistic

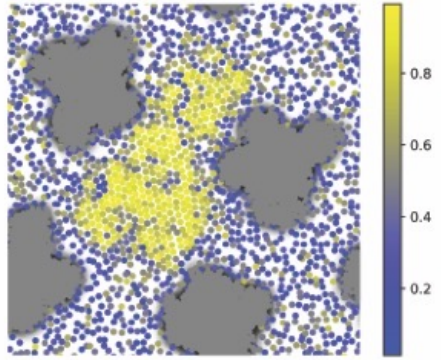
close (resting) state

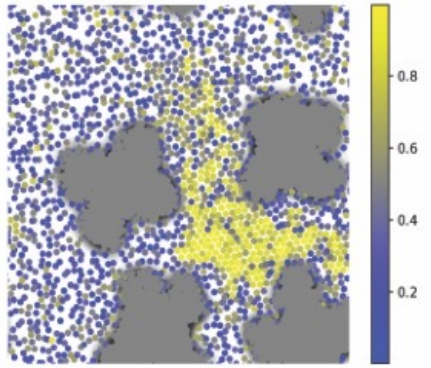


open (activated) state order promoting

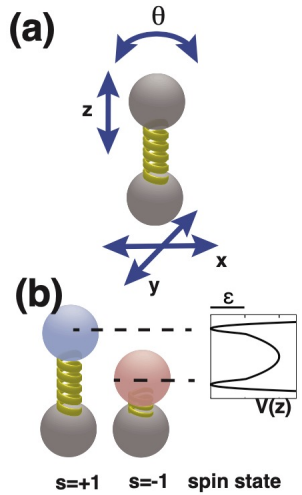


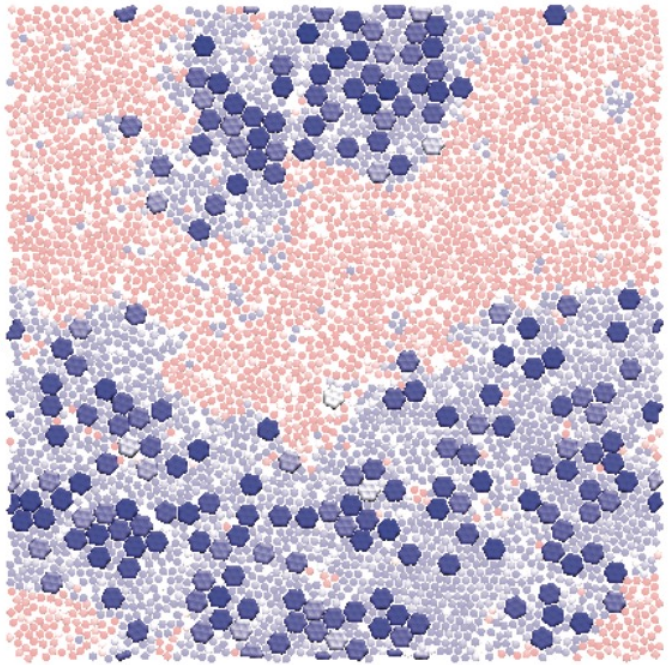
Mesoscopic





Coarse-grained





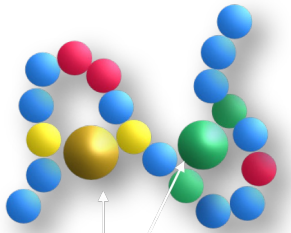
Model for chromatin

POLYMER MODEL FOR GENE ORGANIZATION AND TRANSCRIPTION

Neutral

Binding sites (TU)

3Mbp-> 1000 beads (each 30nm in diameter->3Kbp)

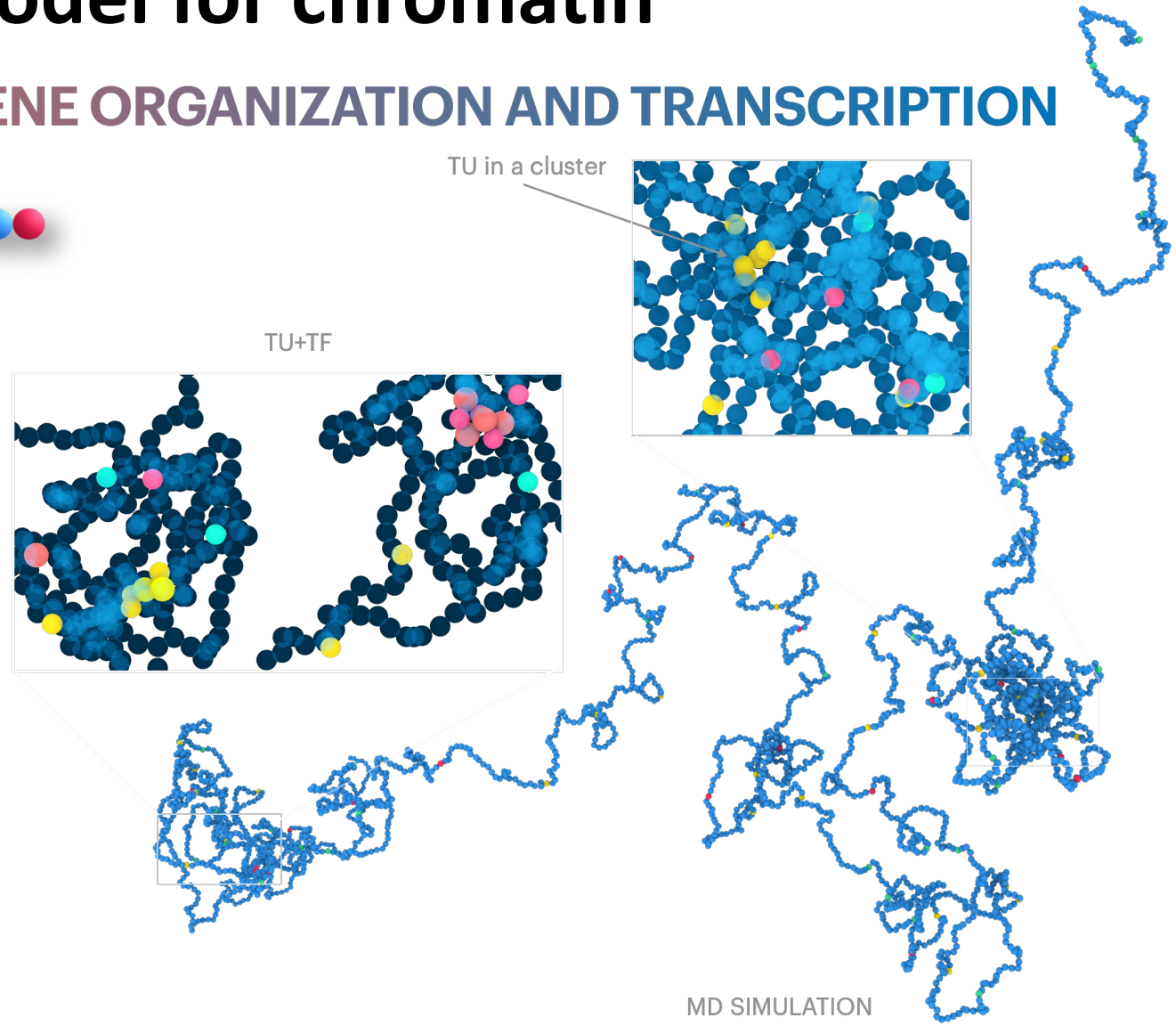


Binders (TF) Weakly with all others

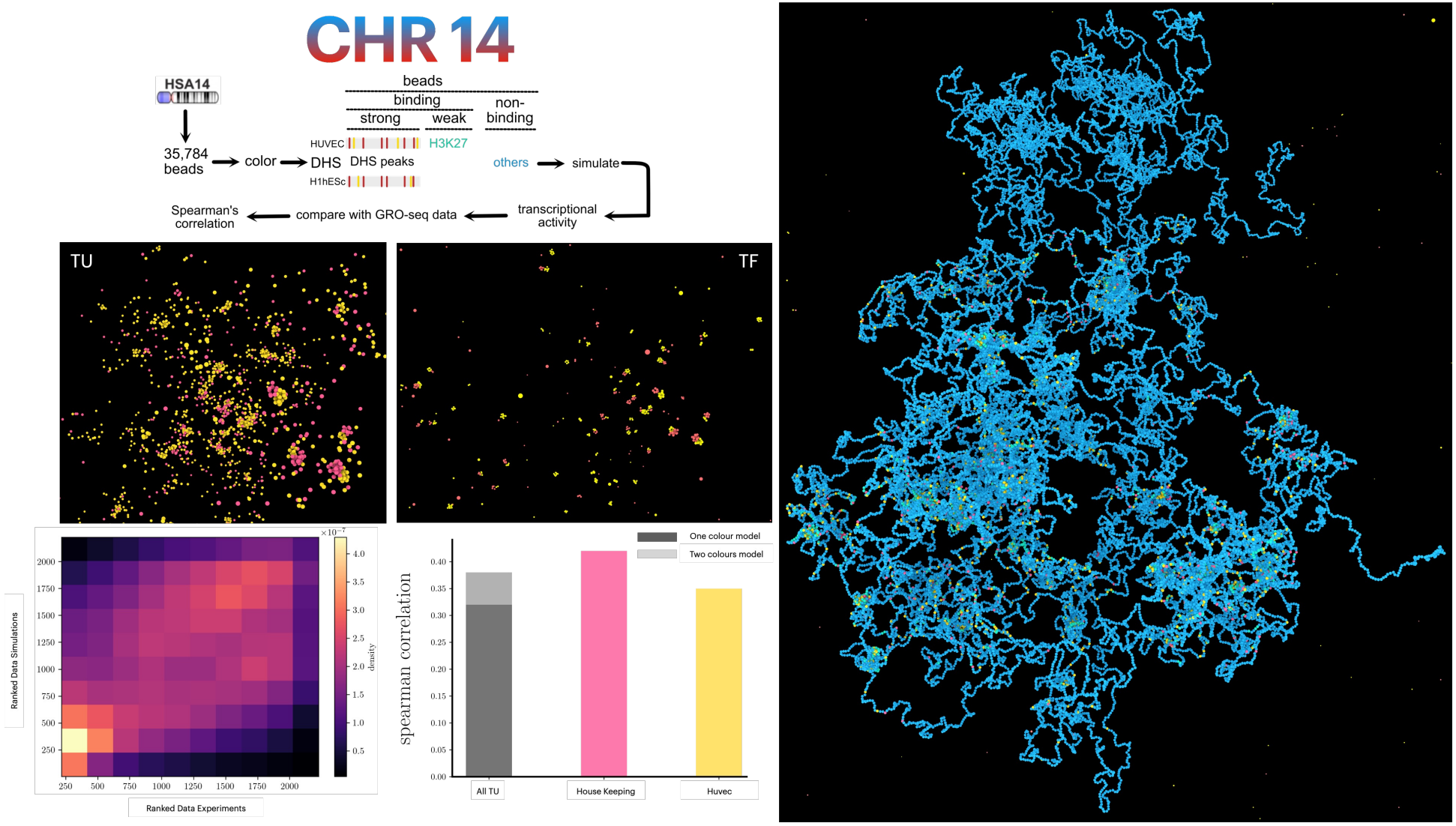
TF SWITCH BETWEEN ACTIVE AND INACTIVE STATES

Rapid exchange of factors and polymerases between bound and free states seen in photobleaching experiments

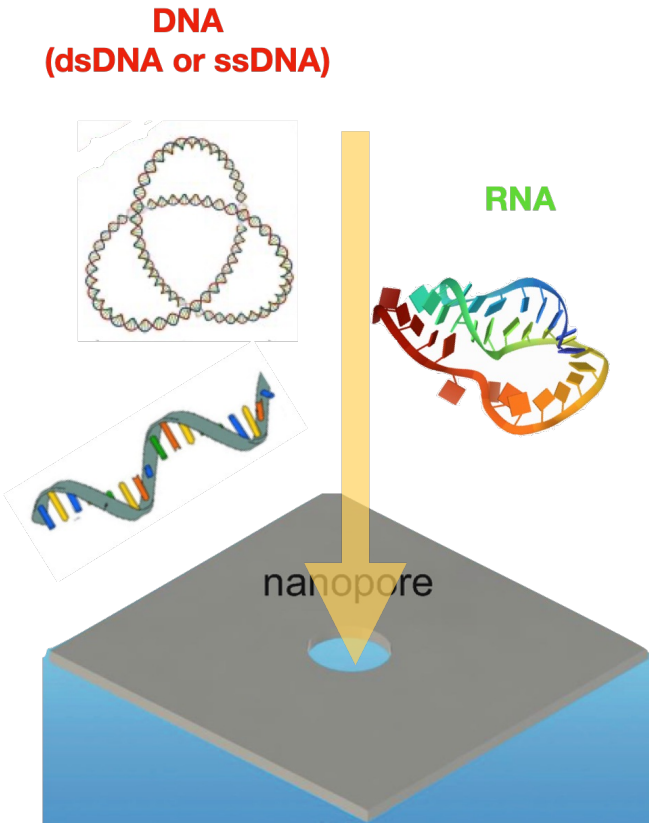
C. A. Brackley et al, Nat. Comm. (2021)

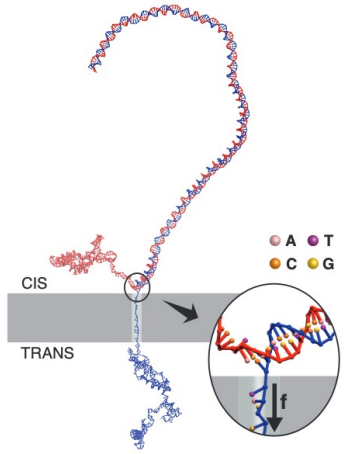


Model for chromatin



Translocation of biopolymers





Detection of knots and other topological structures
Study the impact of different topologies on translocation
See how topological structures are exploited by nature

Suma et al. Nature communications 11 (1), 1-9 2020
Suma et al. NAR gkaa080 2020
Suma et al. PNAS 114 (15), E2991-E2997 2017

Thank You