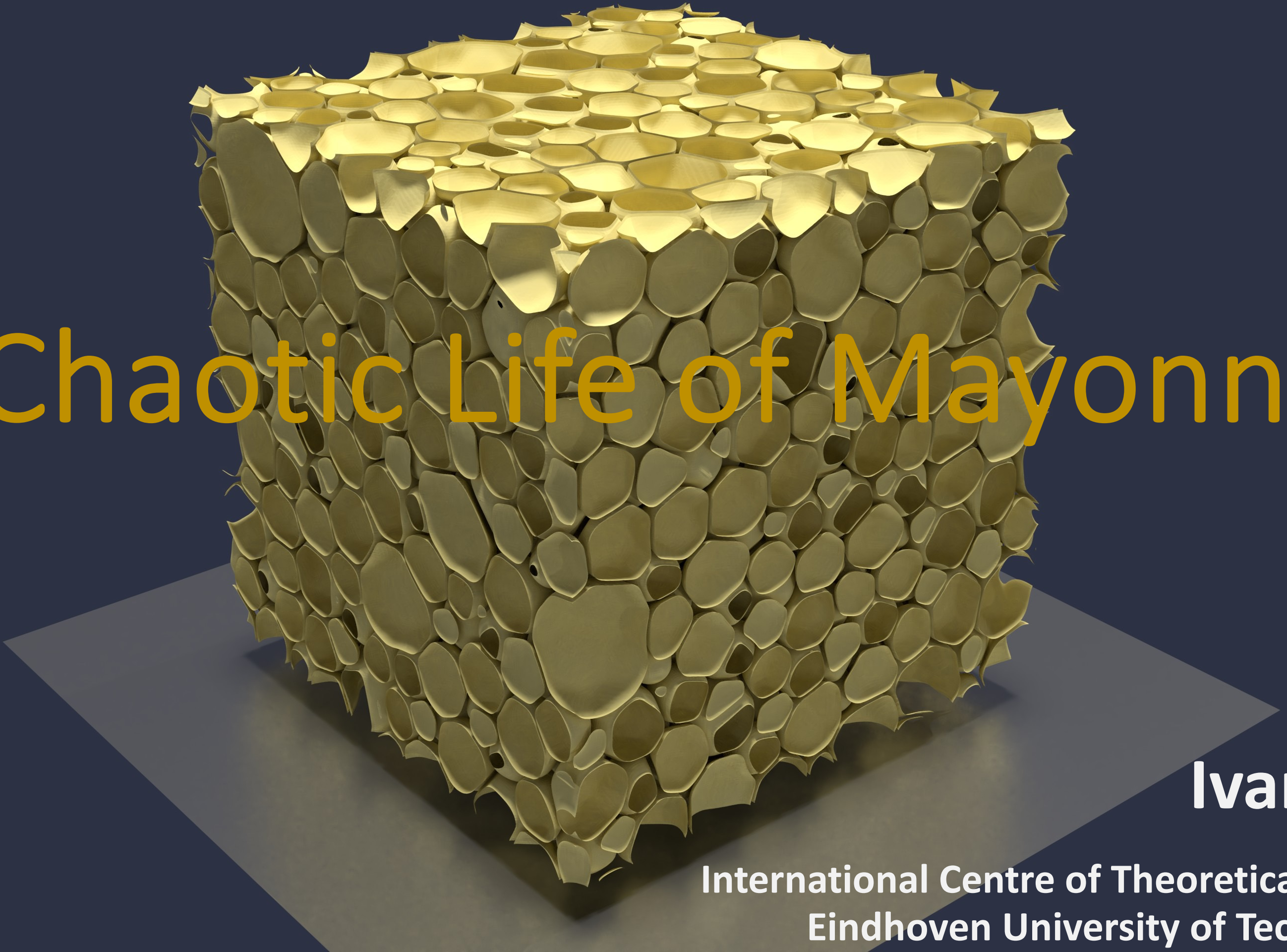
The Chaotic Life of Mayonnaise



Ivan Girotto

International Centre of Theoretical Physics (ICTP)
Eindhoven University of Technology (TU/e)

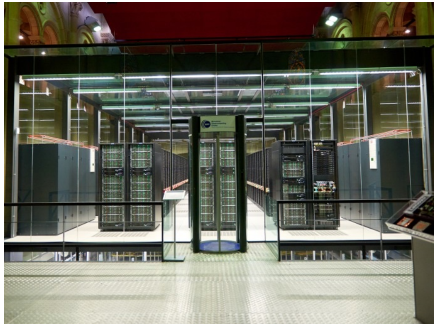
Outline

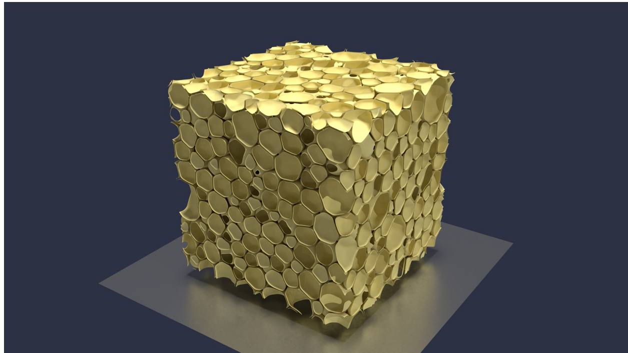
- The making of dense emulsions via large scale computer simulations

- Innovative approach for tracking droplets in dense emulsions

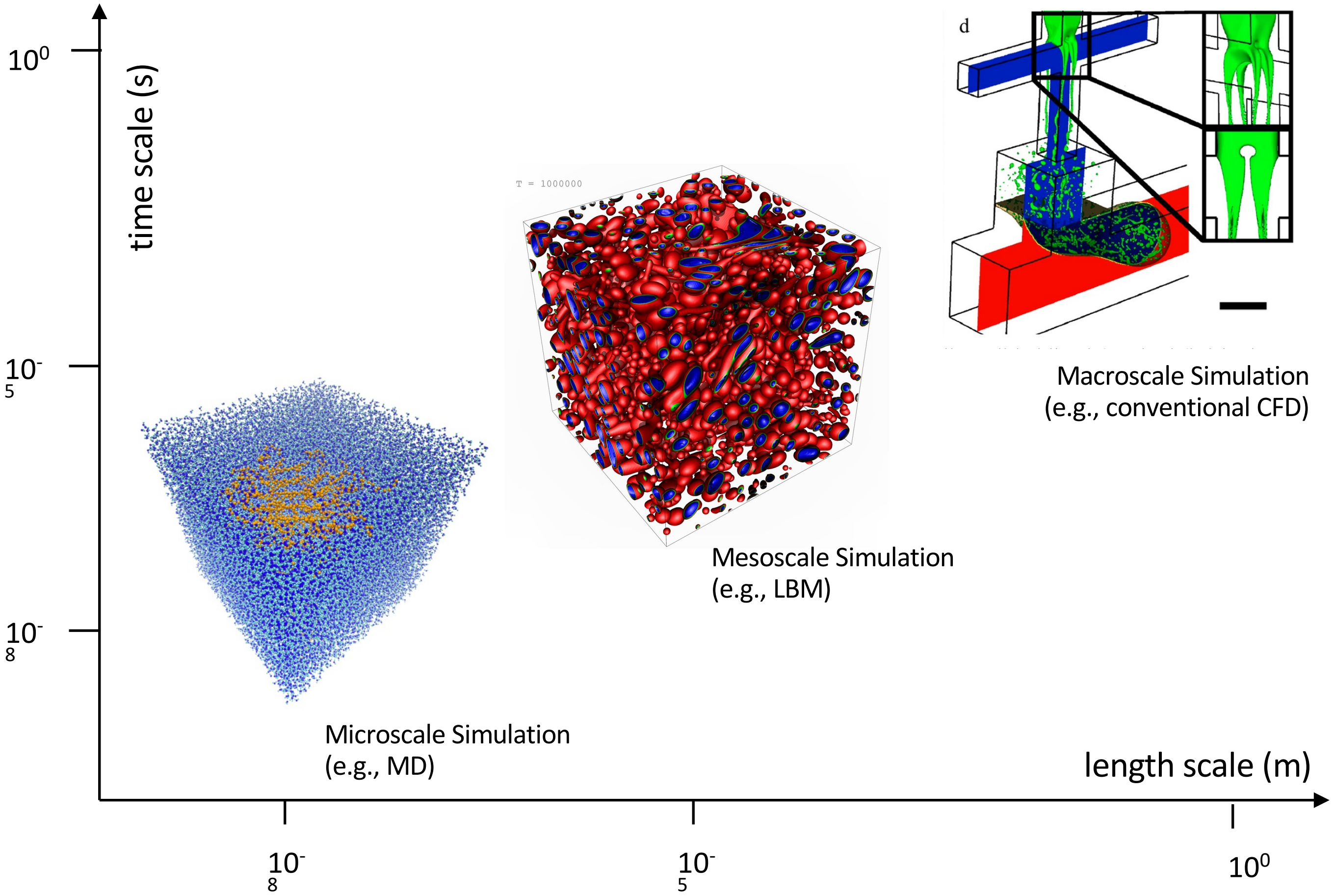
- Overview of the main results

- Conclusion and outlook





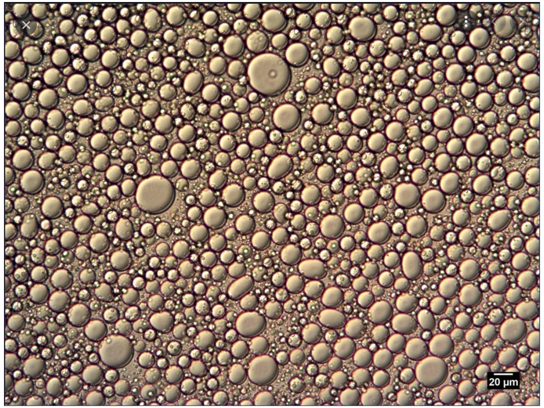
Relevant Scales in Fluid Dynamics



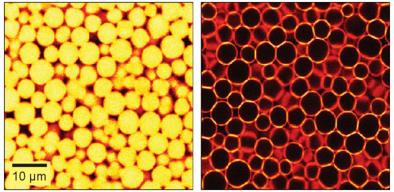
Introduction: Solid or Fluid?

2 Newtonian
simple fluids

Stirring



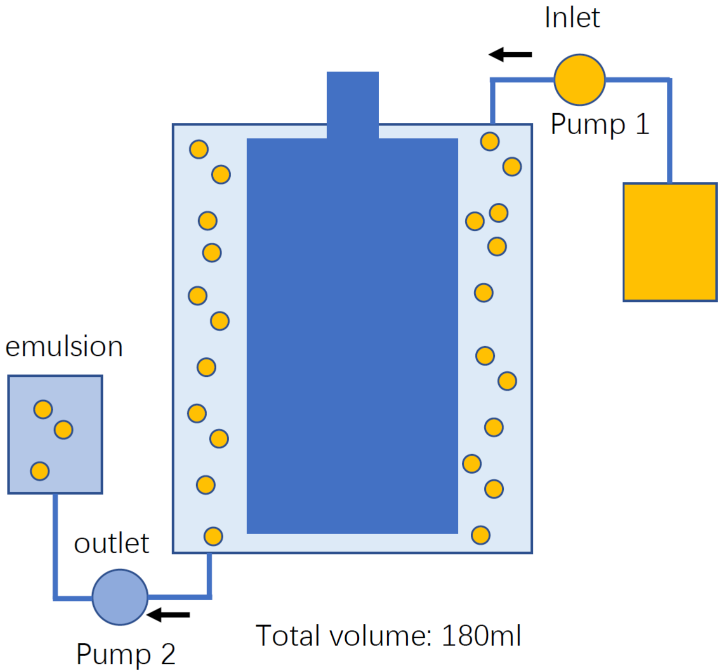
Surfactant &
(oil) Injection

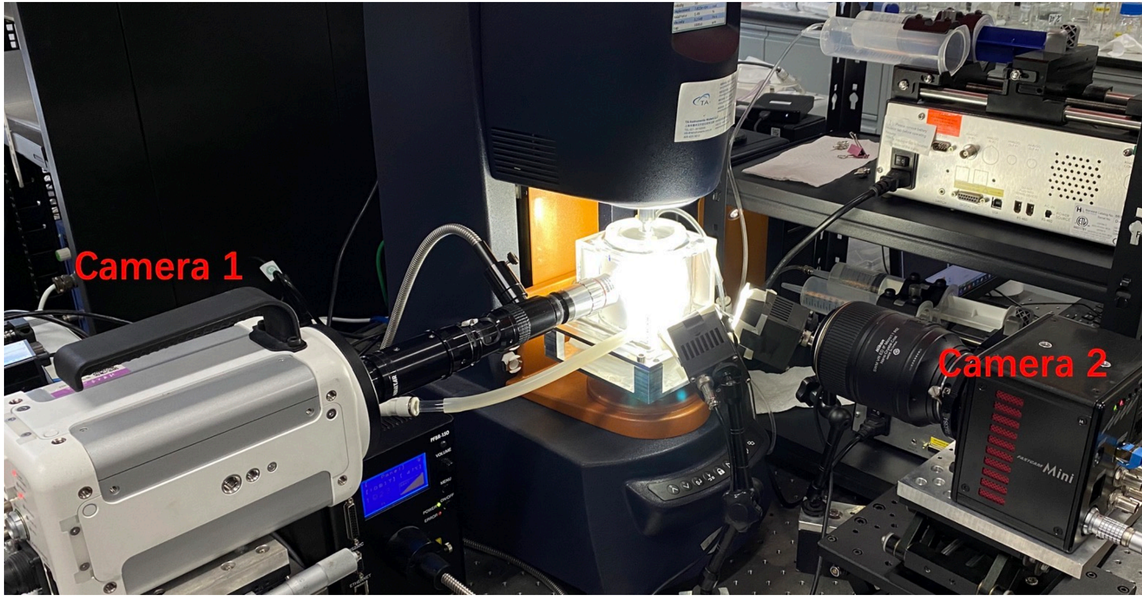


1 non-Newtonian
complex fluid

MCCLEMENTS, D. J. 2015 Food Emulsions: Principles, Practices, and Techniques. CRC press. MOIN, P. & MAHESH, K. 1998 Direct numerical simulation: a tool in turbulence research. Annu. Rev. Fluid Mech. 30 (1), 539–578.

Experimental set-up





* courtesy of Prof. Chao Sun and Lei Yi, Tsinghua University, Beijing, China

Scientific Challenge

- Complexity to describe these physical phenomena analytically
- Extremely challenging to be studied experimentally
- Numerically, high computational cost for modeling emulsions in three-dimensions, even at modest space and time resolution

Open Questions

- How are multi-component fluids emulsions produced via chaotic largescale stirring?
- How does the chaotic stirring and the droplets concentration influence droplets dynamics at the microscopic scale?
- How does the produced emulsion flow at the macroscopic scale, as a function of externally applied stresses?

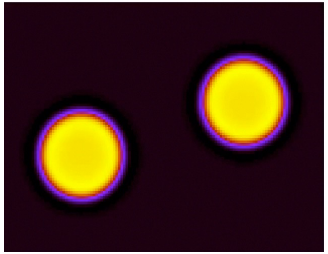
Methodology

$$F_i^{\alpha}(\boldsymbol{x},t) = A\rho^{\alpha}\sum_{j\neq i}\left[sin(k_j x_j + \Phi_k^{(j)}(t))\right]$$

Luca Biferale et al. Journal of Physics (2011)
Prasad Perlekar et al Physics of Fluids (2012)

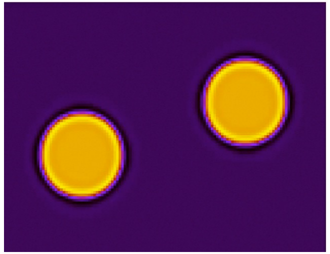
$$f_{\sigma a}(\boldsymbol{x}+\boldsymbol{c}_a, \boldsymbol{c}_a; t+1) - f_{\sigma a}(\boldsymbol{x}, \boldsymbol{c}_a; t) = -\frac{1}{\tau_{LB,\sigma}}\left(f_{\sigma a} - f_{\sigma a}^{(eq)}\right)(\boldsymbol{x}, \boldsymbol{c}_a; t) + F_{\sigma a}(\boldsymbol{x}, \boldsymbol{c}_a; t),$$

surface tension

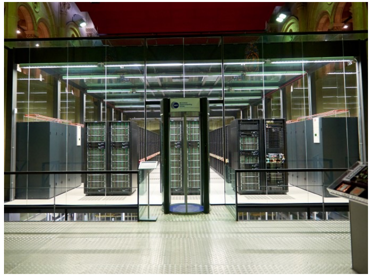


X. Shan & H. Chen, Physical Review E 47, 1815 (1993)
X. Shan & H. Chen, Physical Review E 49, 2941 (1994)
X. Shan, Physical Review E 77, 066702 (2008)
M. Sbragaglia & X. Shan, Physical Review E 84, 036703 (2011)

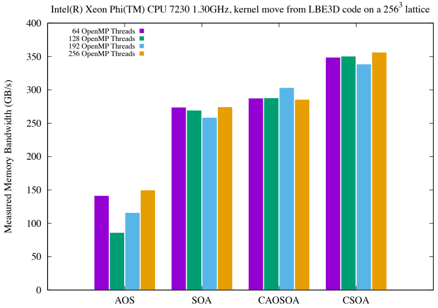
disjoining pressure



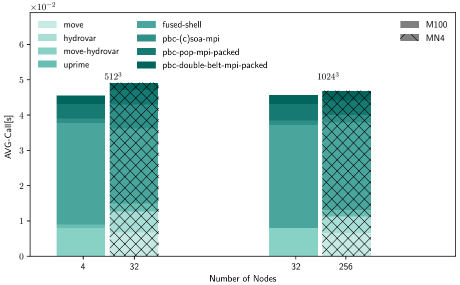
M. Sbragaglia et al. , Soft Matter, (2012)
Sbragaglia et al., Physical Review E 75, 026702 (2007)



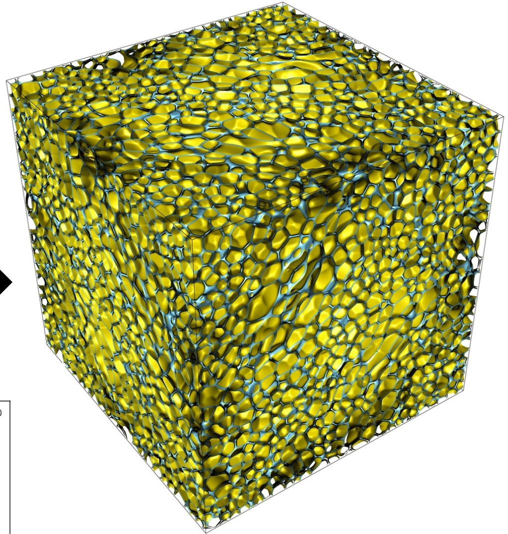
World-class Supercomputers



Marconi-100 Vs MN4



Girotto, I.; Schifano, S.F.; Calore, E.; Di Staso, G.; Toschi, F. Performance and Energy Assessment of a Lattice Boltzmann Method Based Application on the Skylake Processor. Computation 2020, 8, 44.

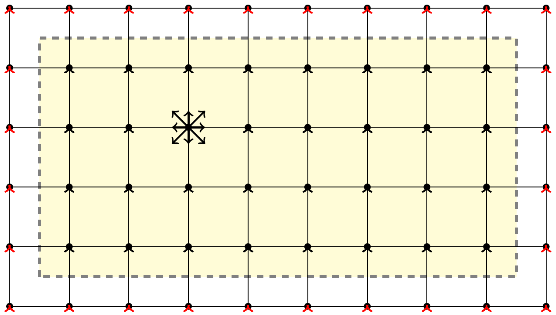


The Multicomponent Lattice Boltzmann

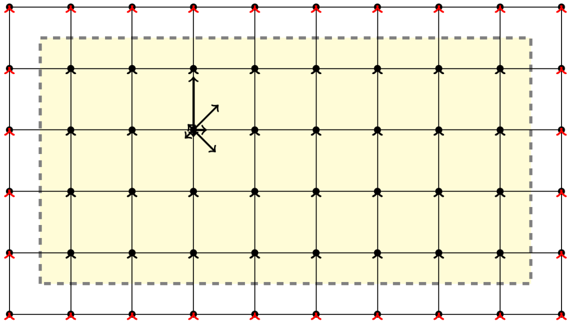
$$f_{\sigma a}(\boldsymbol{x} + \boldsymbol{c}_a, \boldsymbol{c}_a; t+1) - f_{\sigma a}(\boldsymbol{x}, \boldsymbol{c}_a; t) = -\frac{1}{\tau_{LB,\sigma}}\left(f_{\sigma a} - f_{\sigma a}^{(eq)}\right)(\boldsymbol{x}, \boldsymbol{c}_a; t) + F_{\sigma a}(\boldsymbol{x}, \boldsymbol{c}_a; t),$$

- f_a *is* probability distribution function for LBM populations of the the σ component
- $a = 0, \ldots, N$ indexes the population streaming with velocity c_a
- $\sigma =$ A or B component
- F_a is the interaction force, including short range attraction and long range repulsion
- The Lattice Boltzmann scheme is composed by two steps:

Streaming: only memory-to-memory copies



Collision: only (local) floating point operations



Lattice Boltzmann Method (LBM)

- Populations are first moved from lattice-site to lattice-site applying the propagate operator, and then are modified through a collisional operator changing their values according to the local equilibrium condition.

Equilibrium distribution

Time step

Discrete velocities

$$f_i(\mathbf{x}+\mathbf{c}_i\delta_t, t+\delta_t) = f_i(\mathbf{x},t) - \frac{f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)}{\tau}$$

Lattce Boltzmann equation

i=0,1,…,8 in a **D3Q19 lattice**

Relaxation time

```
for all time step do
    < Set boundary conditions >
    for all lattice site do
            < Move >
    for all lattice site do
            < Hydrovar >
  for all lattice site do
            < Equili >
  for all lattice site do
            < Collis >
    end for
end for
```

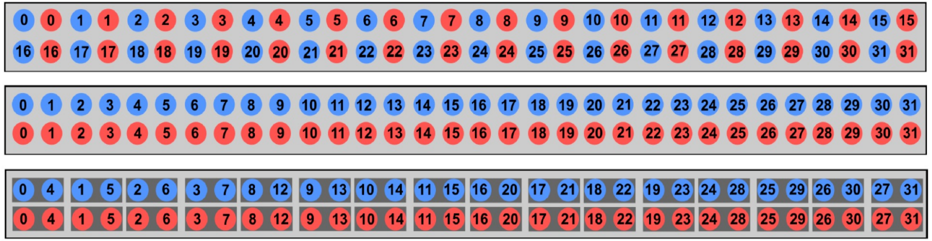
```
for all time step do
    < Set boundary conditions >
    for all lattice site do
            < Move >
    for all lattice site do
            < COLLIDE_FUSED >
    end for
end for
```

```
for all time step do
    < Set boundary conditions >
    for all lattice site do
            < FULLY_FUSED>
    end for
end for
```

Loop compression and better data locality!!

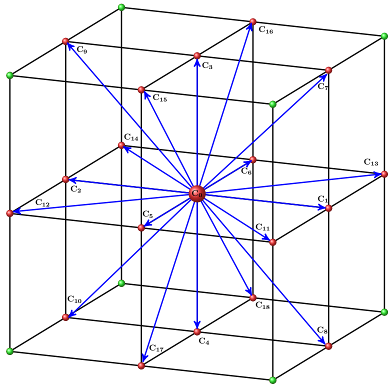
LBM Kernels Optimization

Lattice 4 x 8 (blue and red) population per site



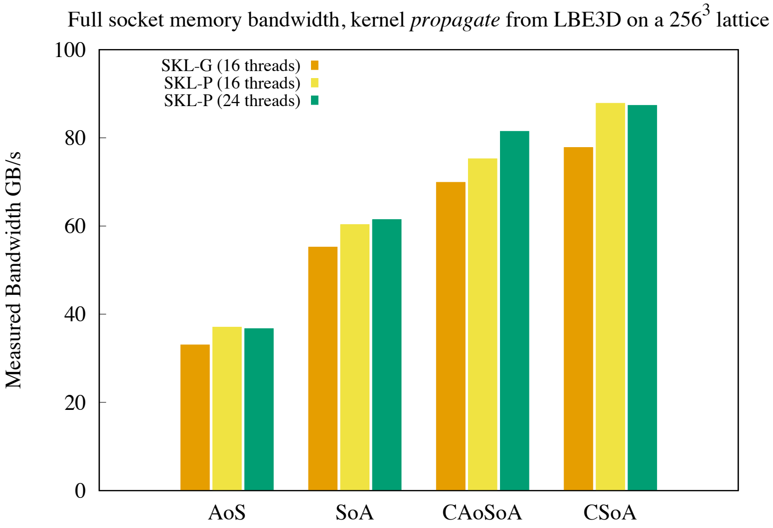
Girotto, I.; Schifano, S.F.; Calore, E.; Di Staso, G.; Toschi, F. Performance and Energy Assessment of a Lattice Boltzmann Method Based Application on the Skylake Processor. Computation 2020, 8, 44.

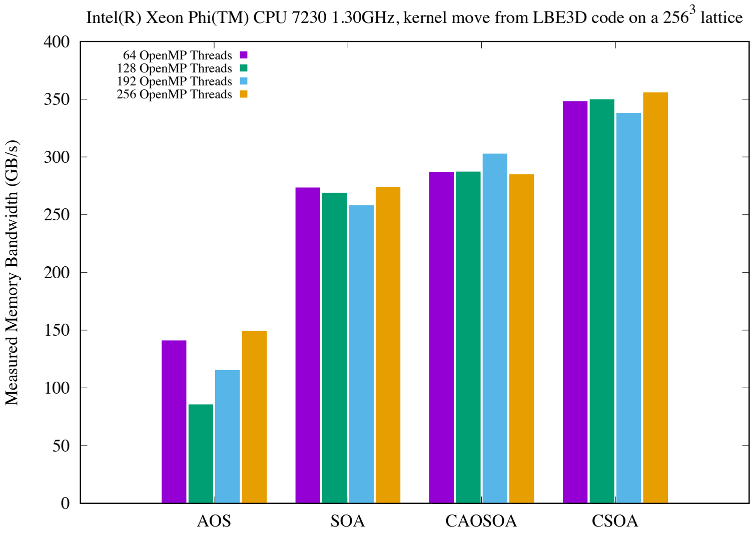
1 lattice point



1 population

256^3, 512^3, 1024^3 & 2048^3 lattice points!





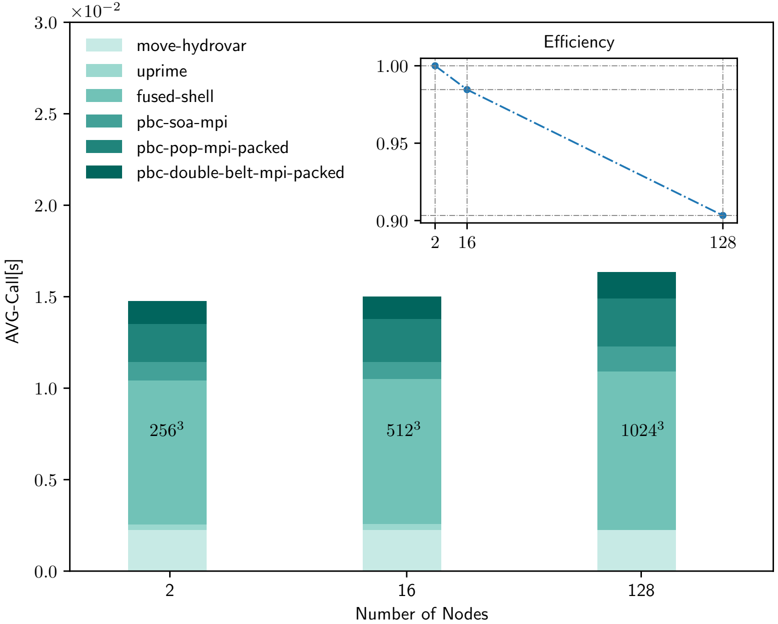
3D cartesian topology

```
MPI_Cart_create (MPI_COMM_WORLD, 3, dims, periods, 0, &MPI_COMM_CART);


/* Build the sub-communicators along X and Y */
coords[0] = 1; coords[1] = 0; coords[2] = 0;
MPI_Cart_sub (MPI_COMM_CART, coords, &MPI_COMM_ALONG_X);
coords[0] = 0; coords[1] = 1; coords[2] = 0;
MPI_Cart_sub (MPI_COMM_CART, coords, &MPI_COMM_ALONG_Y);
coords[0] = 0; coords[1] = 0; coords[2] = 1;
MPI_Cart_sub (MPI_COMM_CART, coords, &MPI_COMM_ALONG_Z);

/*! logical mapping of neighbour tasks ONLY for cartesian grid (using mpi functions) */
MPI_Cart_shift (MPI_COMM_ALONG_X, 0, 1, &pxm, &pxp);
MPI_Cart_shift (MPI_COMM_ALONG_Y, 0, 1, &pym, &pyp);
MPI_Cart_shift (MPI_COMM_ALONG_Z, 0, 1, &pzm, &pzp);
```

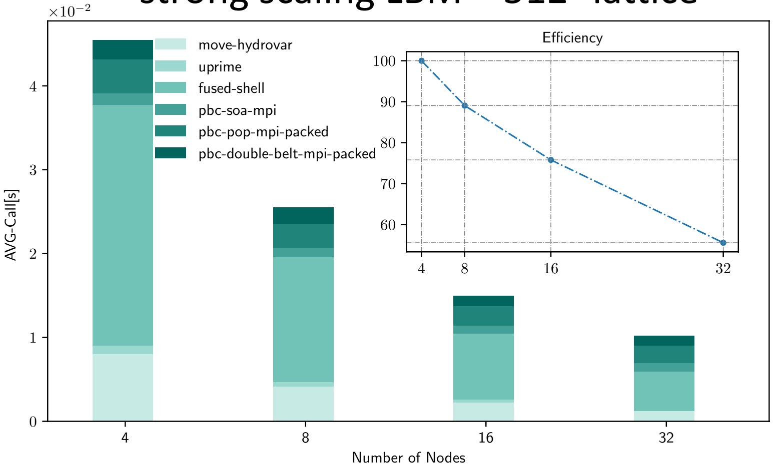
3D cartesian topology: comm pattern

```
MPI_Sendrecv( field + NZP2*NYP2*NX + NZP2+1, 1, MPI_X_RhoPlane, pxp, 20,
              field + NZP2+1 ,  1, MPI_X_RhoPlane, pxm, 20, MPI_COMM_ALONG_X, &status1);
MPI_Sendrecv( field + NZP2*NYP2 + NZP2+1, 1, MPI_X_RhoPlane, pxm, 21,
              field + NZP2*NYP2*(NX+1) + NZP2+1 , 1, MPI_X_tytpe, pxp, 21, MPI_COMM_ALONG_X, &status1);


MPI_Sendrecv( field + NZP2*(NY) + 1, 1, MPI_Y_RhoPlane, pyp, 22,
              field + 1,  1, MPI_Y_RhoPlane, pym, 22, MPI_COMM_ALONG_Y, &status1);
MPI_Sendrecv( field + NZP2 + 1, 1, MPI_Y_RhoPlane, pym, 23,
              field + NZP2*(NY+1) + 1, 1, MPI_Y_type, pyp, 23, MPI_COMM_ALONG_Y, &status1);


MPI_Sendrecv( field + NZ,  1, MPI_Z_type, pzp, 24,
              field,  1, MPI_Z_type, pzm, 24, MPI_COMM_ALONG_Z, &status1);
MPI_Sendrecv( field + 1, 1, MPI_Z_RhoPlane, pzm, 25,
              field + NZ+1, 1, MPI_Z_RhoPlane, pzp, 25, MPI_COMM_ALONG_Z, &status1);
```

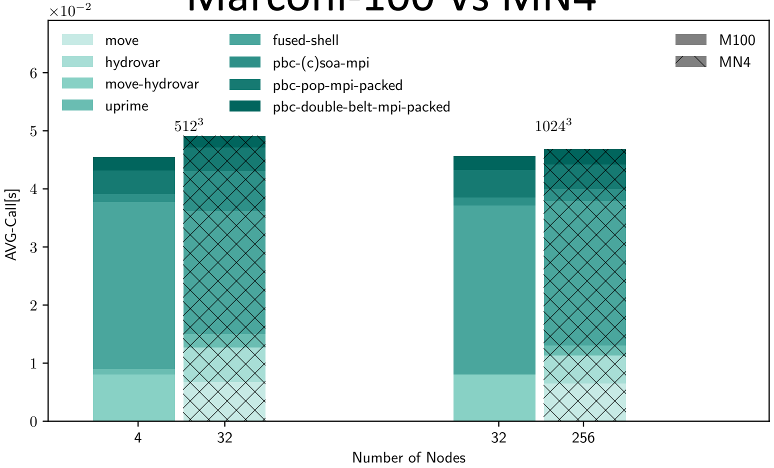
Multicomponent LBM for distributed multi-GPU (results on Marocni-100)



strong scaling LBM – 512^3 lattice



Marconi-100 Vs MN4

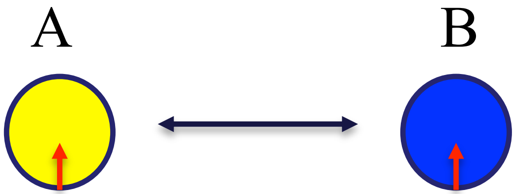


Motivations

- From two simple fluids, to one complex fluid (yield-stress)
- Validate state-of-the-art computational models in 3D
- Study the process of turbulent emulsification in details
- Explore the physics of fluid emulsions
- Make via computer simulation what experiments can't do

MCCLEMENTS, D. J. 2015 Food Emulsions: Principles, Practices, and Techniques. CRC press. MOIN, P. & MAHESH, K. 1998 Direct numerical simulation: a tool in turbulence research. Annu. Rev. Fluid Mech. 30 (1), 539–578.

Modeling disjoining pressure



X. Shan & H. Chen, Physical Review E 47, 1815 (1993)
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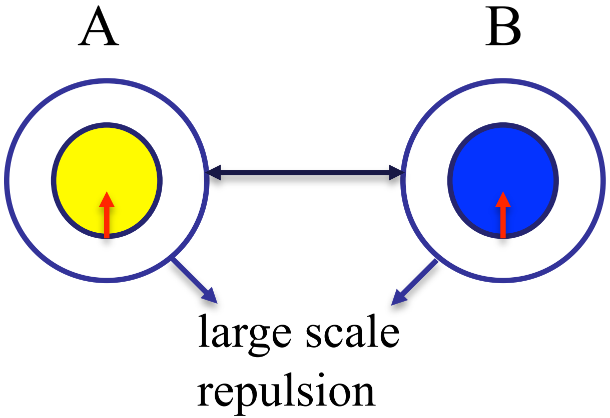
M. Sbragaglia & X. Shan, Physical Review E 84, 036703 (2011)



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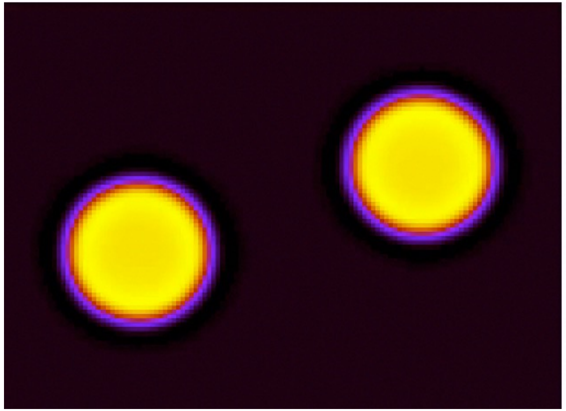
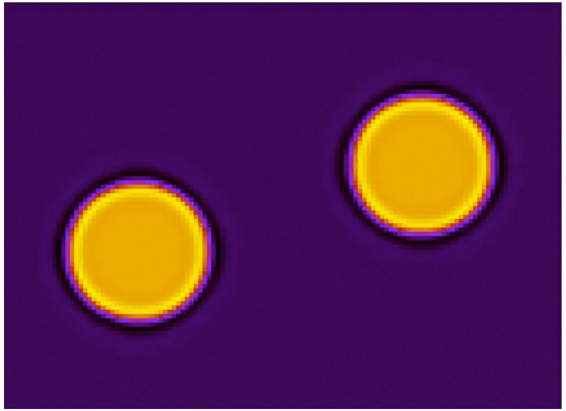
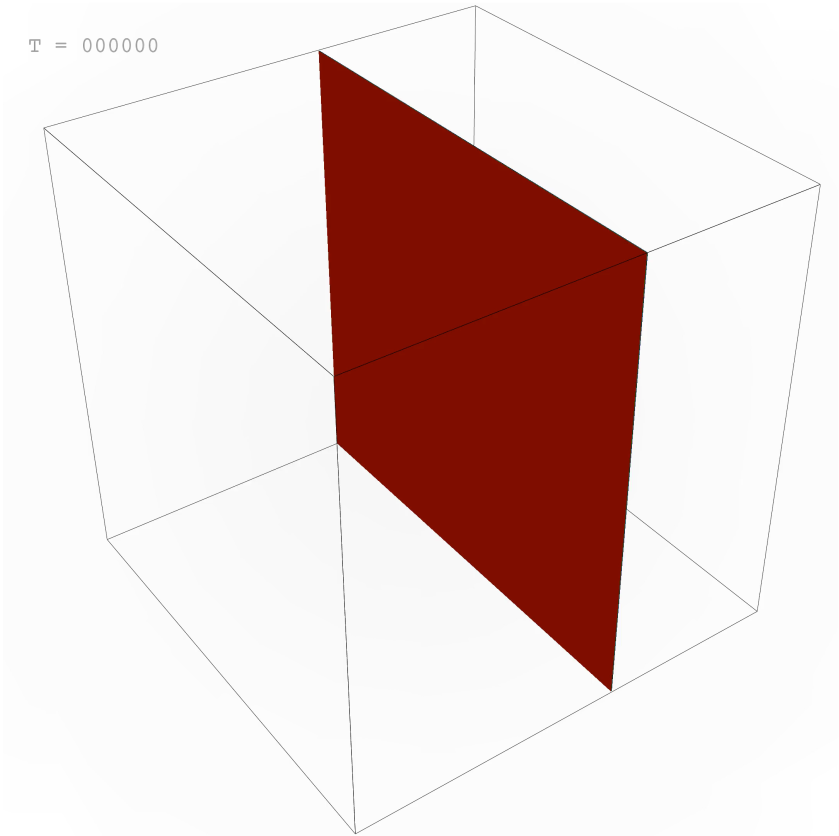
Sbragaglia et al., Physical Review E 75, 026702 (2007)

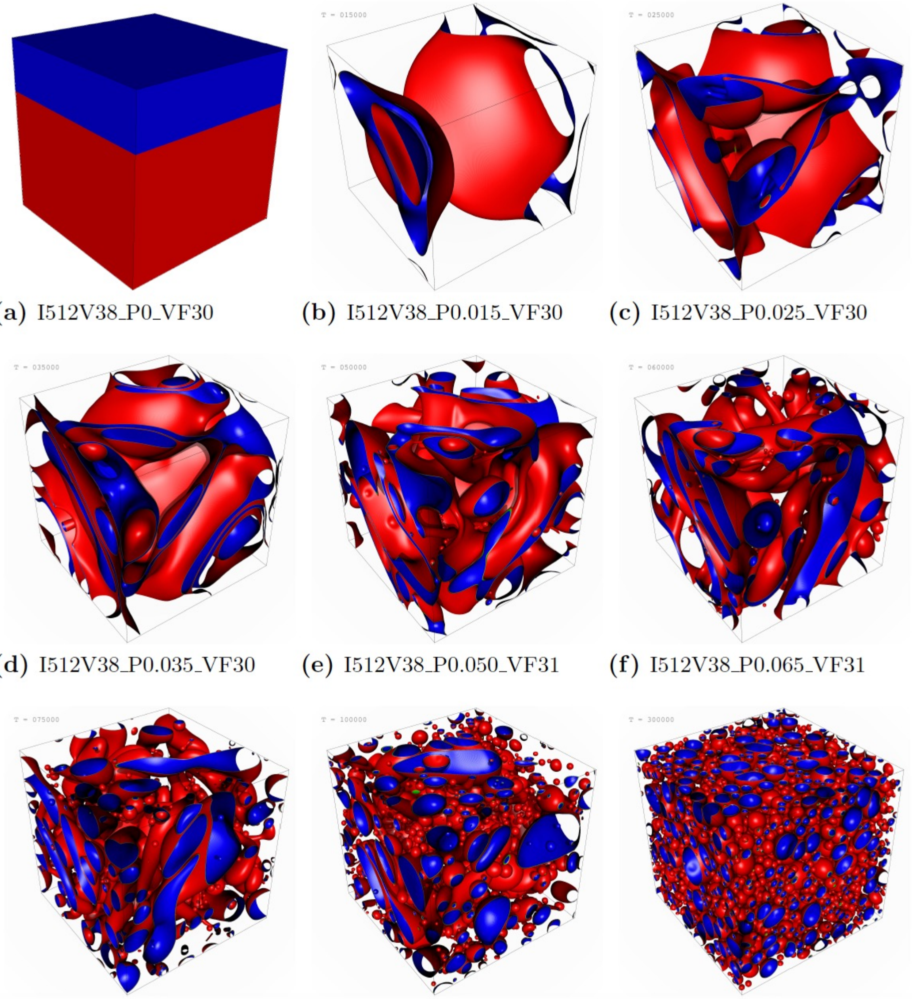




Parameters set from:
R. Benzi et al 2010 EPL 91 14003

Interface Fragmentation



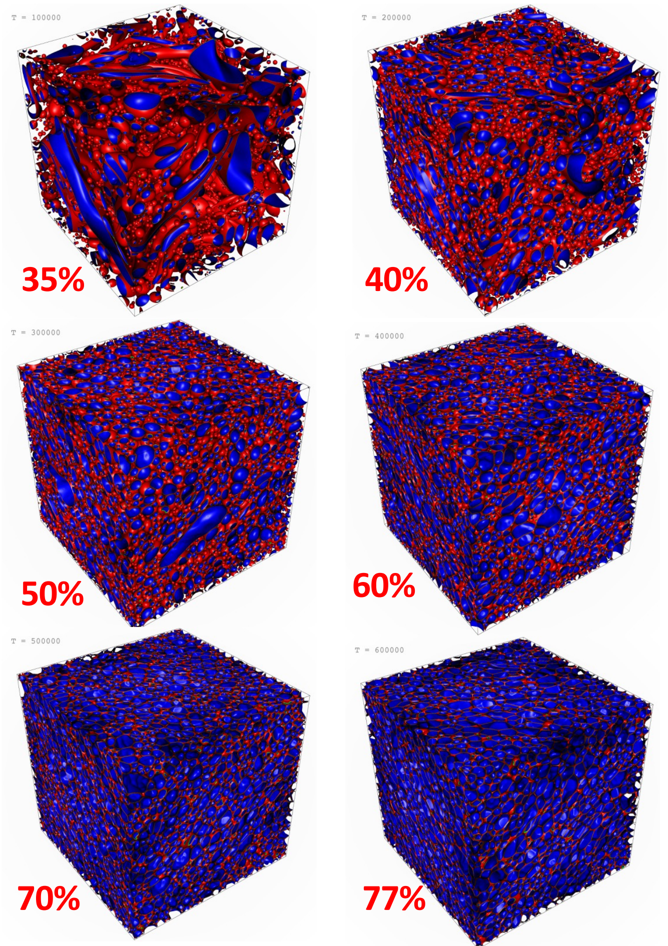


(a) I512V38_P0_VF30 (b) I512V38_P0.015_VF30 (c) I512V38_P0.025_VF30

(d) I512V38_P0.035_VF30 (e) I512V38_P0.050_VF31 (f) I512V38_P0.065_VF31

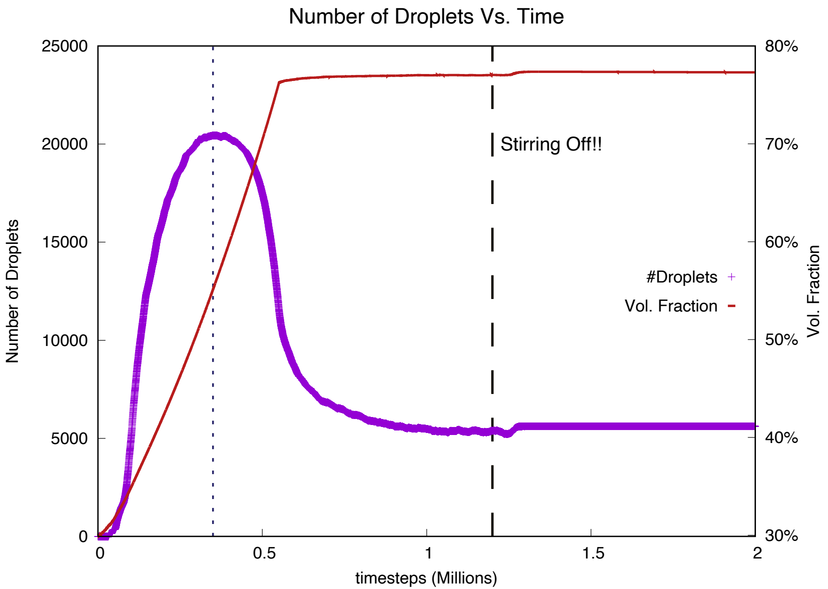
(g) I512V38_P0.075_VF32 (h) I512V38_P0.1_VF34 (i) I512V38_P0.3_VF38

The Making of Dense Emulsions



We slowly inject/remove mass of fluid such that :

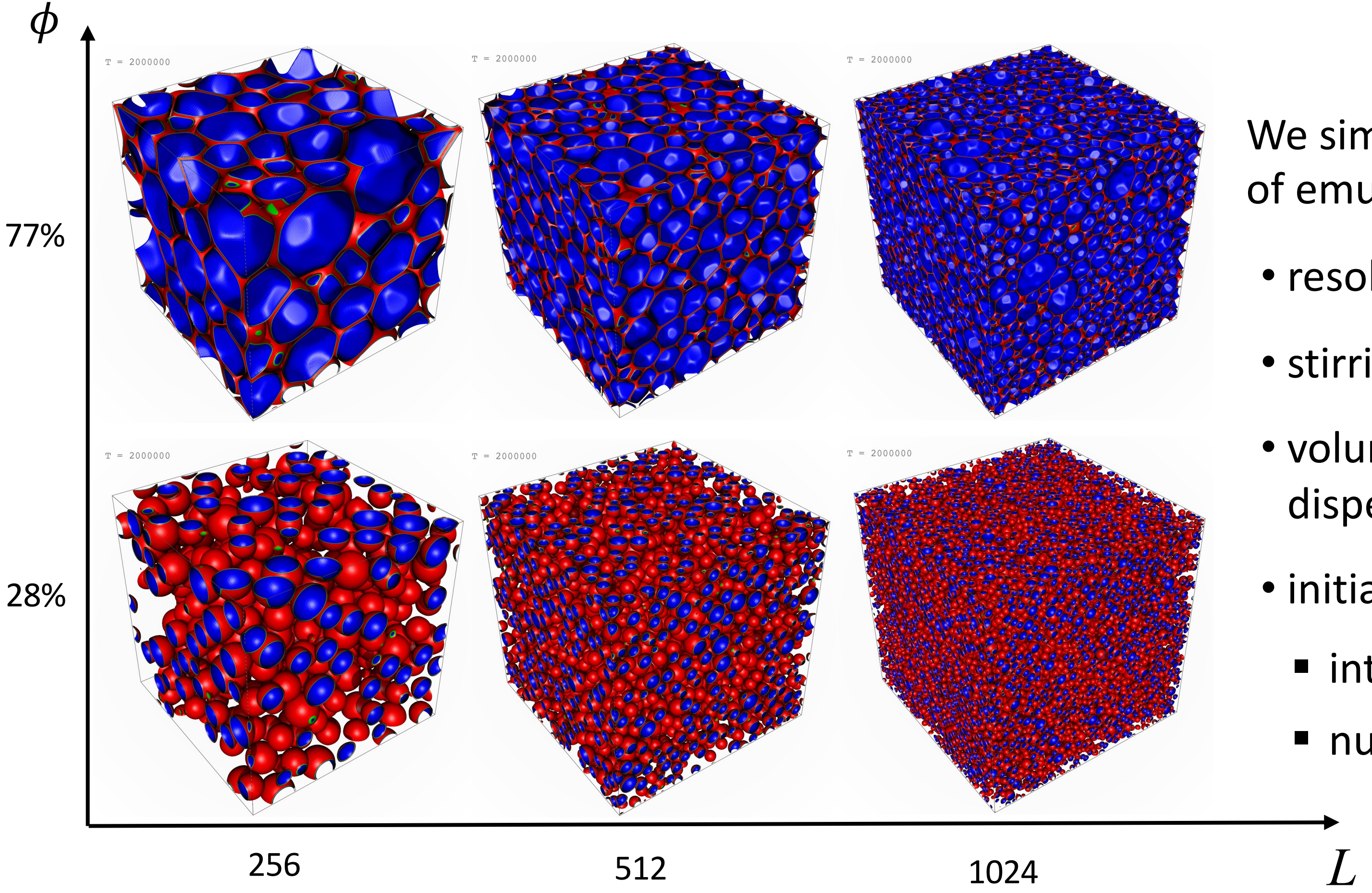
1. the total mass of the fluid component is preserved
2. the system adiabatically adjust to the new mechanical equilibrium



The emulsion is stirred via a large scale forcing, mimicking a classical stirring often used in spectral simulation of turbulent flows, as in:

- Prasad Perlekar, Luca Biferale, Mauro Sbragaglia, Sudhir Srivastava, and Federico Toschi. Droplet size distribution in homogeneous isotropic turbulence. Physics of Fluids, 24(6):065101, 2012.

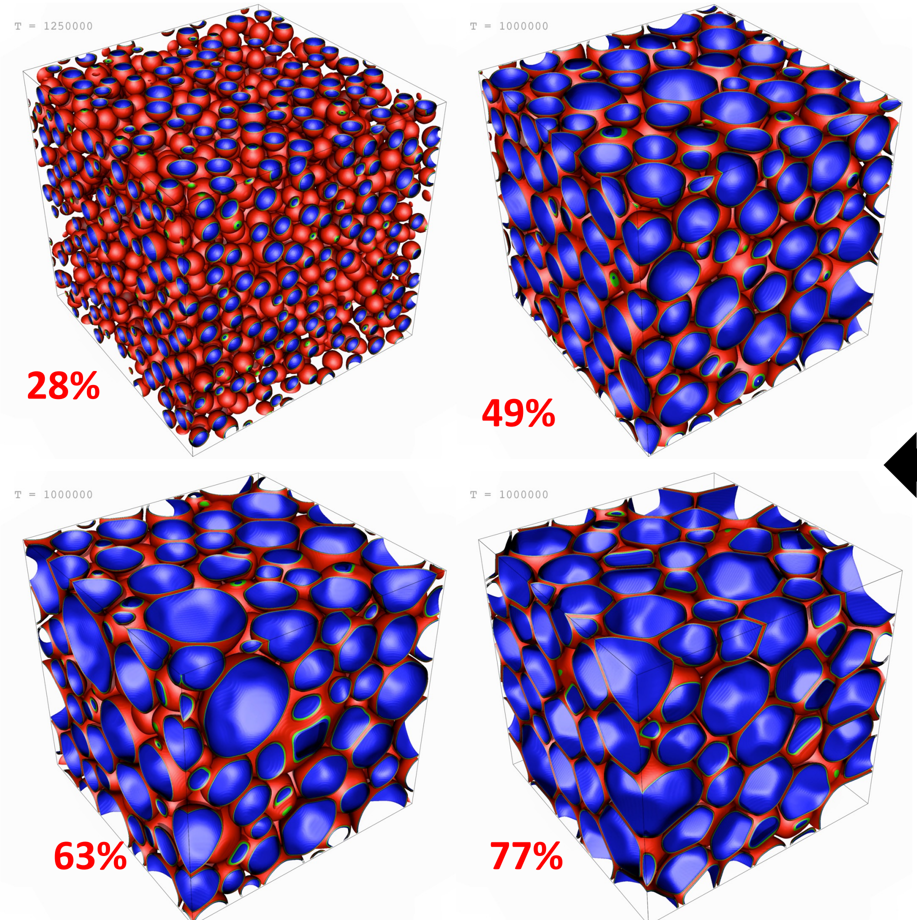
Exploration of the of the Parameter Space of Emulsions



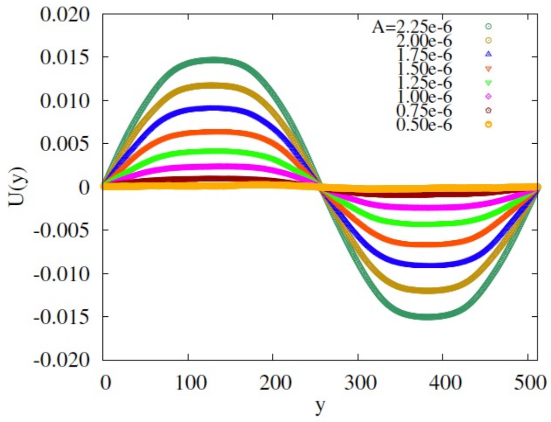
We simulated a large number of emulsions varying:

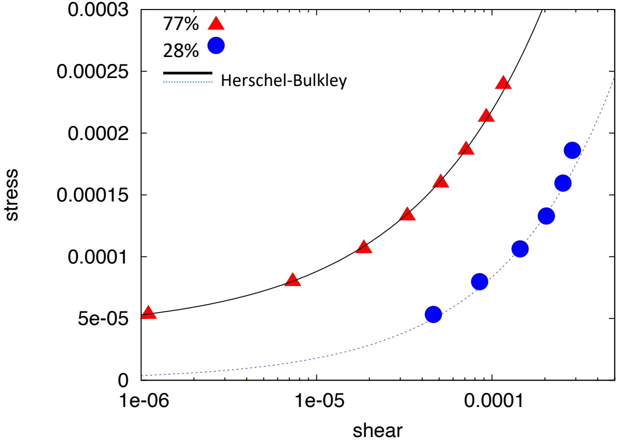
- resolutions (up to 2048^3)
- stirring amplitude
- volume fraction of the dispersed phase (ϕ)
- initial conditions:
  - interface fragmentation
  - nucleation

Is the final emulsion really dense and Jammed?



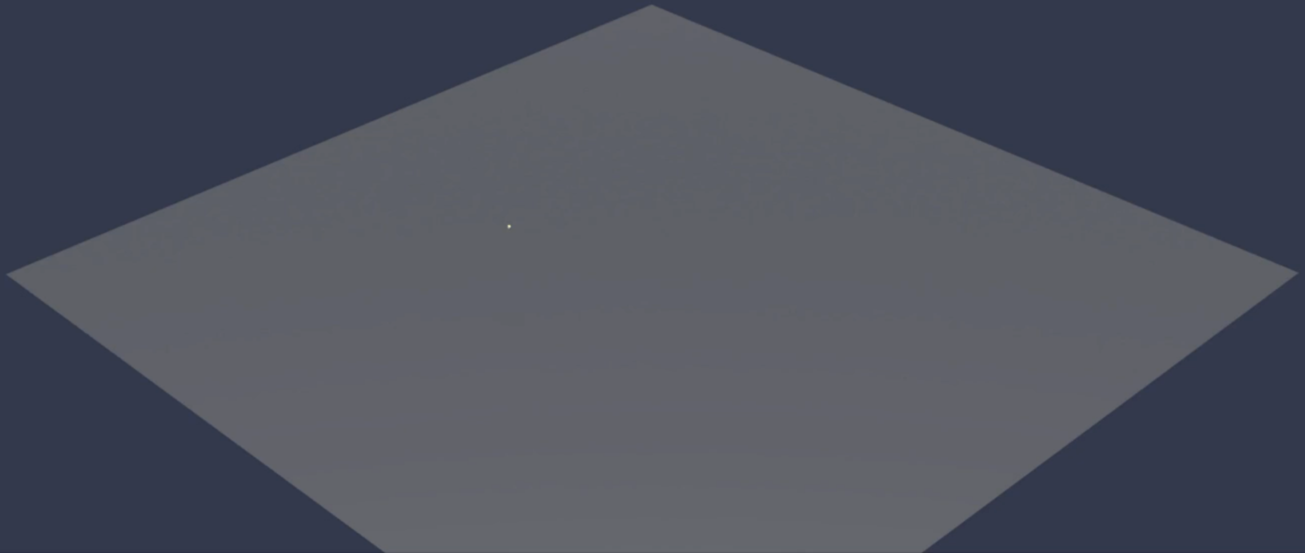
A = 1.0e-6





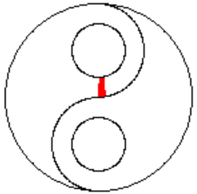
R. Benzi, M. Bernaschi, M. Sbragaglia, and S. Succi. Herschel-bulkley rheology from lattice kinetic theory of soft glassy materials. EPL (Euro-physics Letters), 91(1):14003, jul 2010.

The chaotic life of mayonnaise: DOI: https://doi.org/10.1103/APS.DFD.2019.GFM.V0032

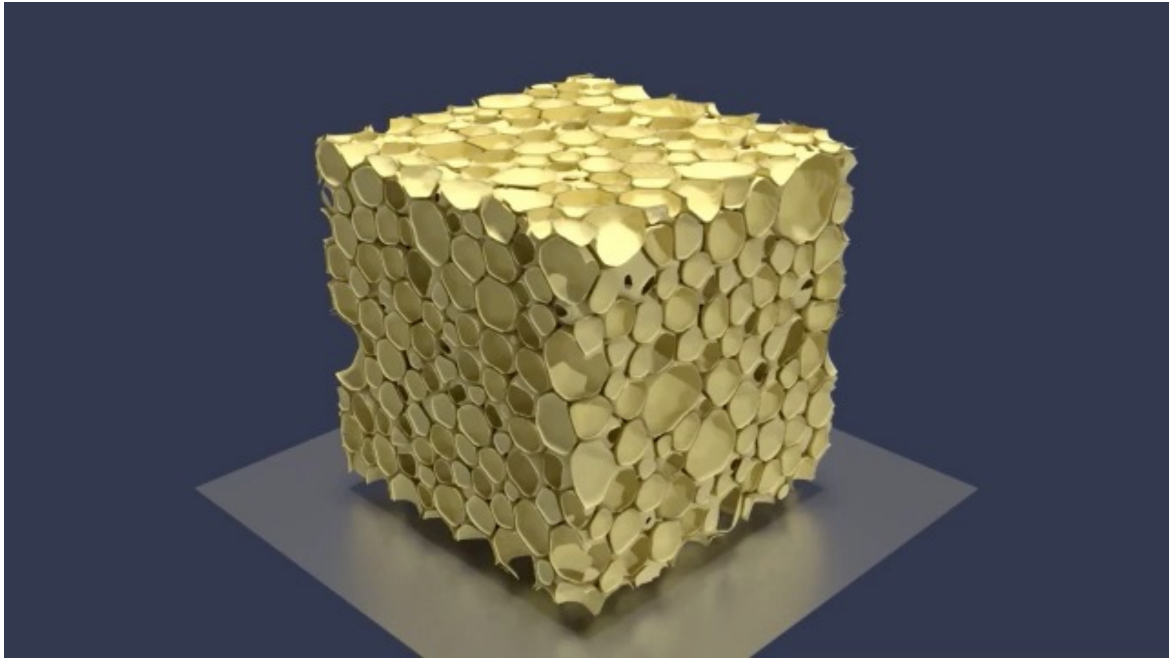


Droplets Coloring Algorithm

Via a flood fill parallel algorithm* we can intercept and provide a quantitative descriptions of all droplets in the system



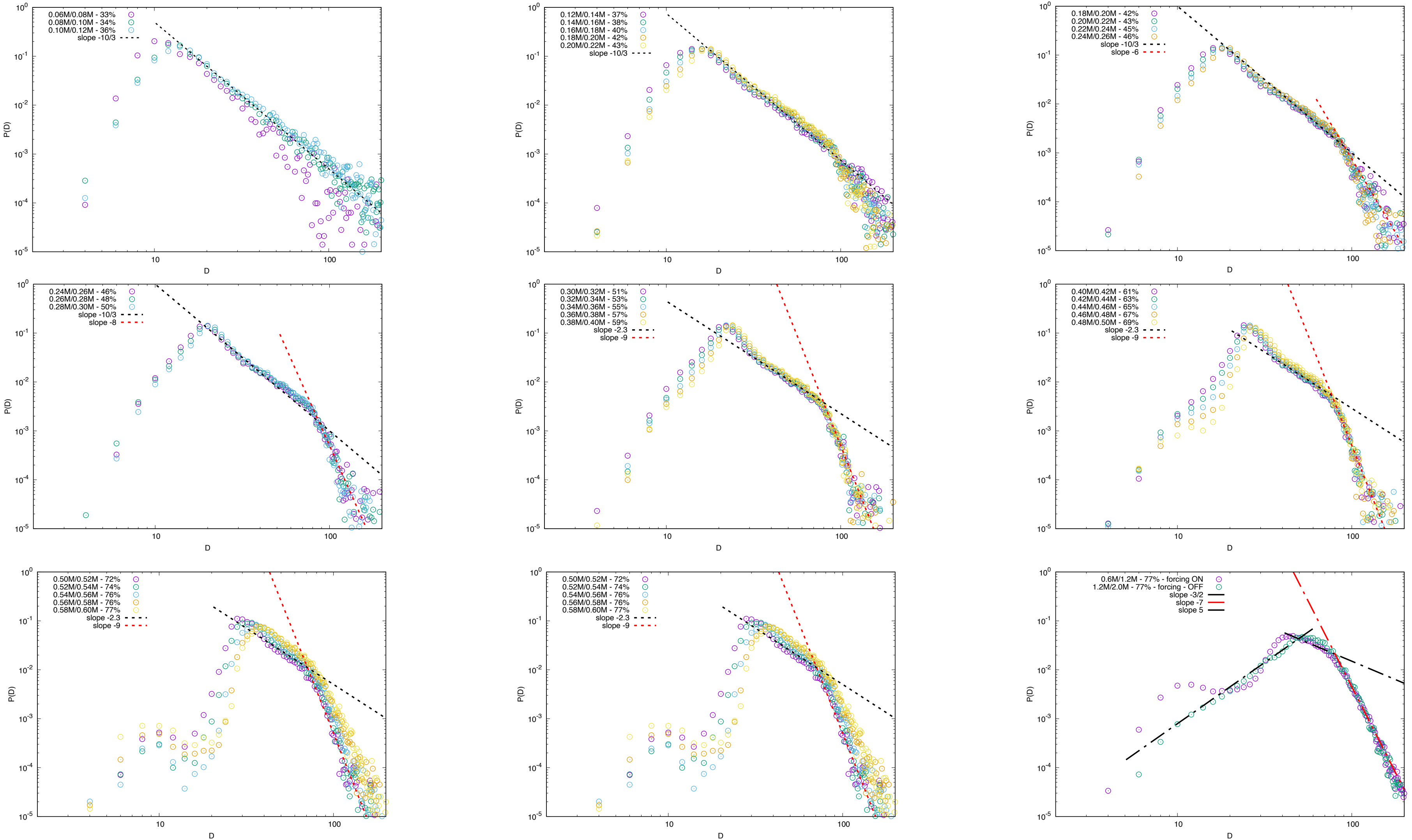
https://en.wikipedia.org/wiki/Flood_fill



The chaotic life of mayonnaise

DOI: https://doi.org/10.1103/APS.DFD.2019.GFM.V0032

***S. Frijters, T. Krueger, and J. Harting, "Parallelised Hoshen-Kopelman algorithm for lattice-Boltzmann simulations", CPC**


0.06M/0.08M - 33%
0.08M/0.10M - 34%
0.10M/0.12M - 36%
slope -10/3
0.12M/0.14M - 37%
0.14M/0.16M - 38%
0.16M/0.18M - 40%
0.18M/0.20M - 42%
0.20M/0.22M - 43%
slope -10/3
0.18M/0.20M - 42%
0.20M/0.22M - 43%
0.22M/0.24M - 45%
0.24M/0.26M - 46%
slope -10/3
slope -6
0.24M/0.26M - 46%
0.26M/0.28M - 48%
0.28M/0.30M - 50%
slope -10/3
slope -8
0.30M/0.32M - 51%
0.32M/0.34M - 53%
0.34M/0.36M - 55%
0.36M/0.38M - 57%
0.38M/0.40M - 59%
slope -2.3
slope -9
0.40M/0.42M - 61%
0.42M/0.44M - 63%
0.44M/0.46M - 65%
0.46M/0.48M - 67%
0.48M/0.50M - 69%
slope -2.3
slope -9
0.50M/0.52M - 72%
0.52M/0.54M - 74%
0.54M/0.56M - 76%
0.56M/0.58M - 76%
0.58M/0.60M - 77%
slope -2.3
slope -9
0.50M/0.52M - 72%
0.52M/0.54M - 74%
0.54M/0.56M - 76%
0.56M/0.58M - 76%
0.58M/0.60M - 77%
slope -2.3
slope -9
0.6M/1.2M - 77% - forcing ON
1.2M/2.0M - 77% - forcing - OFF
slope -3/2
slope -7
slope 5
P(D)
D

Droplets Tracking Algorithm

- In the domain at time t_1 there are N_1 droplets and at (an immediately later dump) t_2 there are N_2. We first round the continuum density field to a 0 or 1 values. This is achieved by the following operation:

$$\rho_k(\boldsymbol{x}, t_1) = \theta(\rho_k^{(c)}(\boldsymbol{x}, t) - \rho_t)$$

- The *initial* state of a single droplet k_1 at time t_1 is represented in the bra-ket notation from quantum mechanics as $| k_1, t_1 \rangle$ and the *final* state is represented by the following bra notation: $\langle k_2, t_2 |$
- We want to define a transition probability in order to track droplets in time, including coalescence and breakup events. The transition probability is give by the following bra-ket expression:

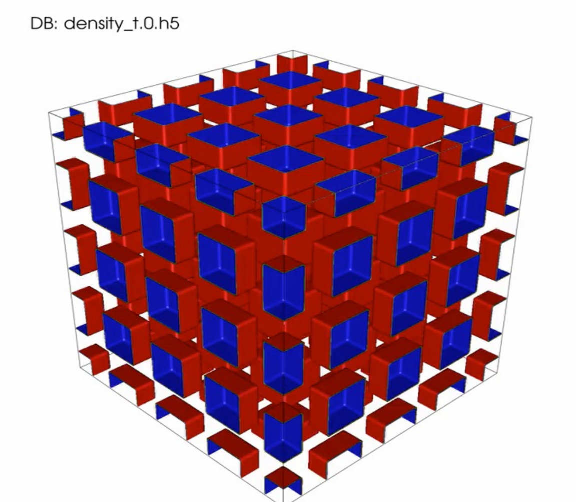
$$P_{k_1 \to k_2} = \langle k_2, t_2 | k_1, t_1 \rangle = \frac{1}{V} \int \rho_{k_2}(\boldsymbol{x}, t_2) \rho_{k_1}(\boldsymbol{x}, t_1) d^3 x$$

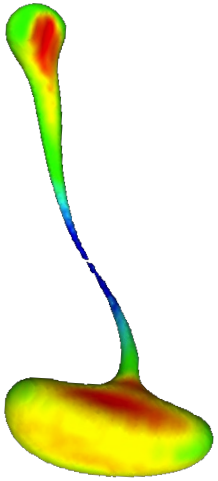
- We apply the Kalman filtering, for considering the initial (t_1) velocity field of a given droplet
- By construction $\langle k, t | k, t \rangle = 1$. What happens if a droplet is just translating with uniform velocity? We expect that the maximal correlation will occur for:

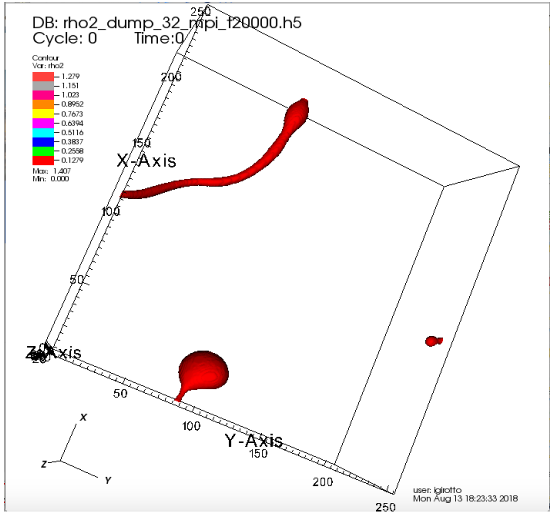
$$\langle shift(k, v \cdot dt), t + \delta t | k, t \rangle = \frac{1}{V} \int \rho_k(\boldsymbol{x} - \boldsymbol{v} \cdot dt, t + \delta t) \rho_k(\boldsymbol{x}, t) d^3 x$$

Real Time Monitoring Implementation

- Monitor droplets during the simulation for N timesteps to collect physical statistics
  - only post run analysis is not convenient at the target scale
- Droplets could be really big, of unpredictable shape and, distributed across the grid of processes

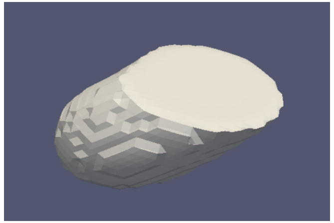






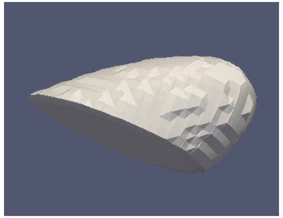
Parallel Flood Fill Algorithm

- The problems are:
  - identify all droplets’ chunks in a density field
  - identify whether a chunk is a single droplet or a chunk of a droplet composed of multiple chunks
  - droplet chunks can be spread among the processes
  - Periodic Boundaries Conditions are applied



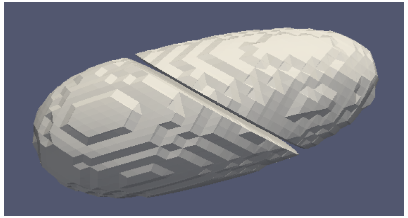
Process (X, Y, Z)

+

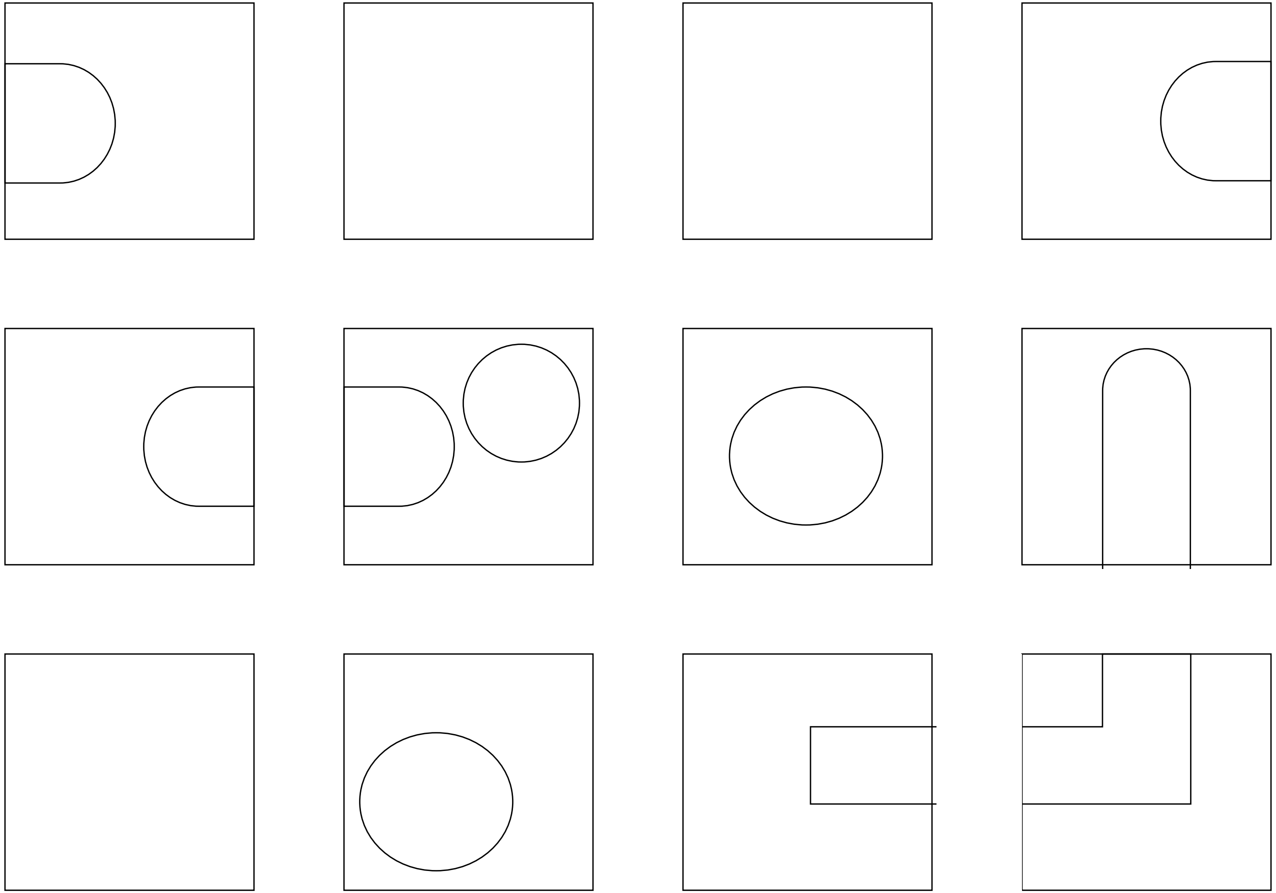


Process (X^1, Y^1, Z^1)

=



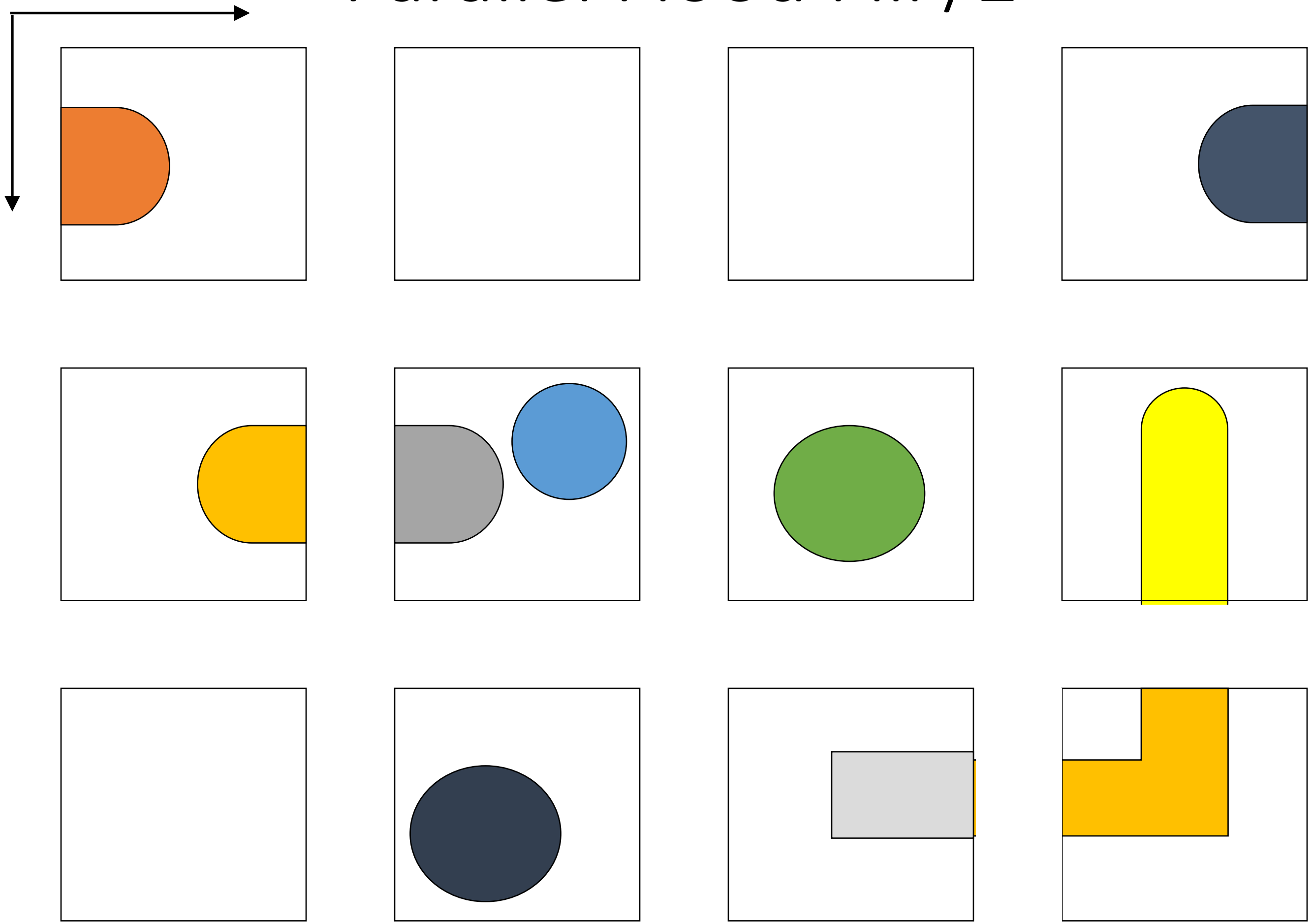
Parallel Flood Fill /1



Parallel Flood Fill Description /2

```
Set <- density lattice

//First Phase: all droplets point are somehow colored
For all element ∊ Set do
    If element >= threshold then
        If( check_all_neighbors_colors == 0) Then
            color <- create_new_color
            flag[ element ] <- color
            flag_all_neighbors_above_threshold
        Else
            color <-
find_minimum_colorId_among_neighbors
            flag[ element ] <- color
            flag_all_neighbors_above_threshold(color)

End For
//assign to all distributed colors a unique and progressive
Id
Parallel Global Color Naming
```

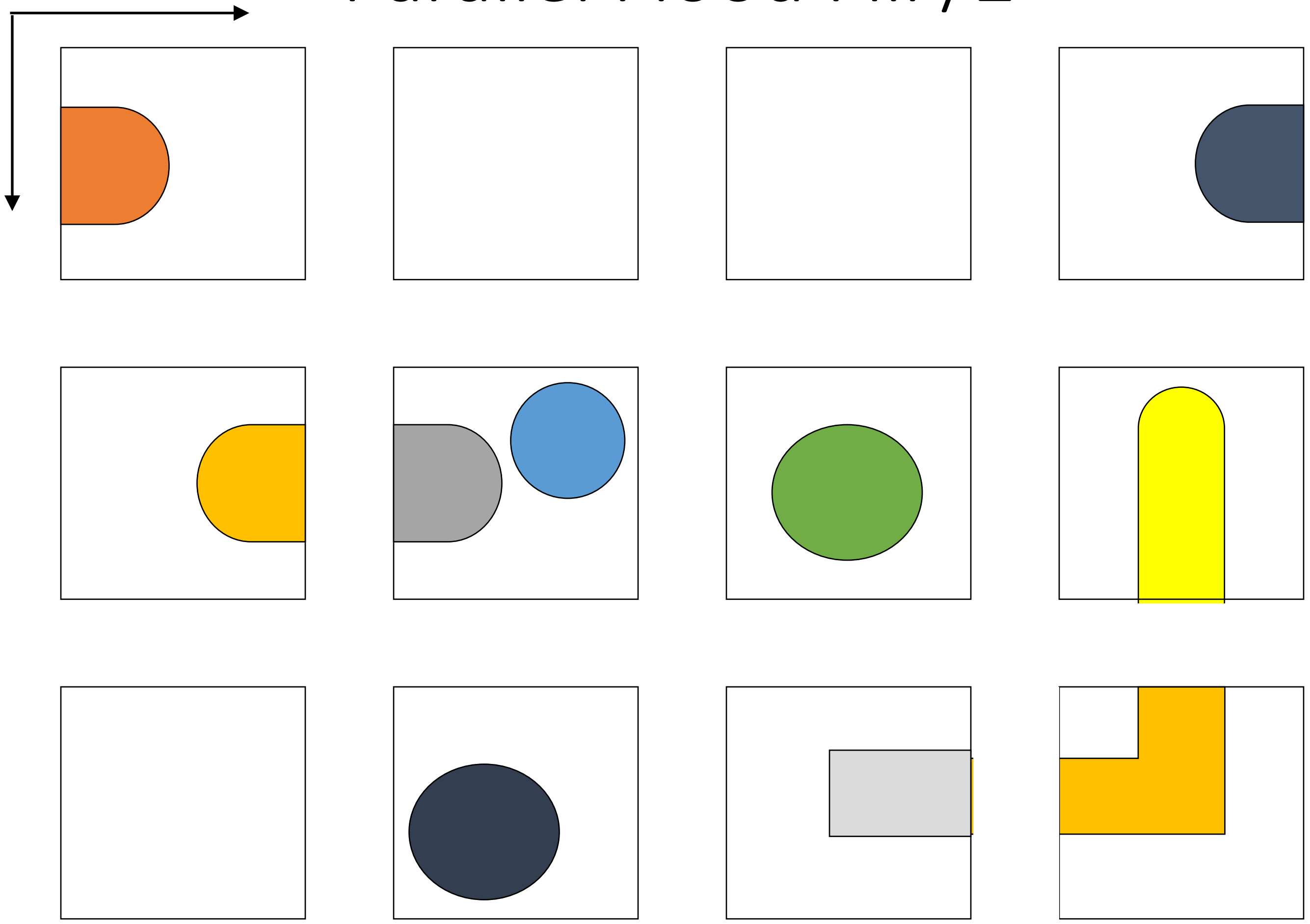
Parallel Flood Fill /2



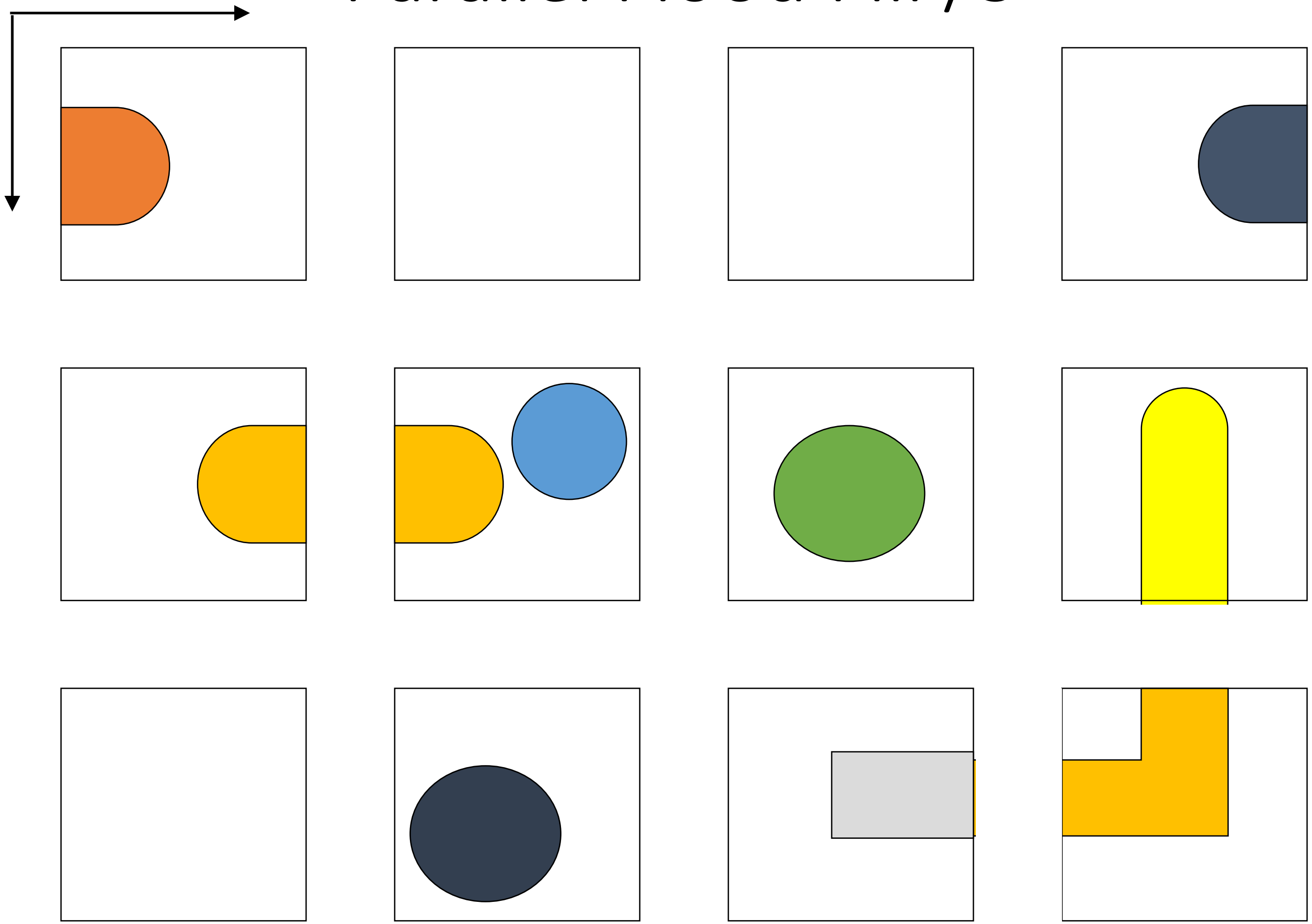
Parallel Flood Fill Description /3

```
//Second Phase: propagate the colors among the processes
Set <- flag // colors lattice

Do  check <- 0
   For all element ∈ flag do

        If ( element is a color )  Then

            color <- find_minimum_colorId_among_neighbors
            flag_all_neighbors_elements(color)
            check <- 1
    End For
    For all element ∈ flag do in reverse order

        If ( element is a color )  Then

            color <- find_minimum_colorId_among_neighbors
            flag_all_neighbors_elements(color)
            check <- 1
    End For

    All_reduce_check_value_among_processes

While( check != 0)
```

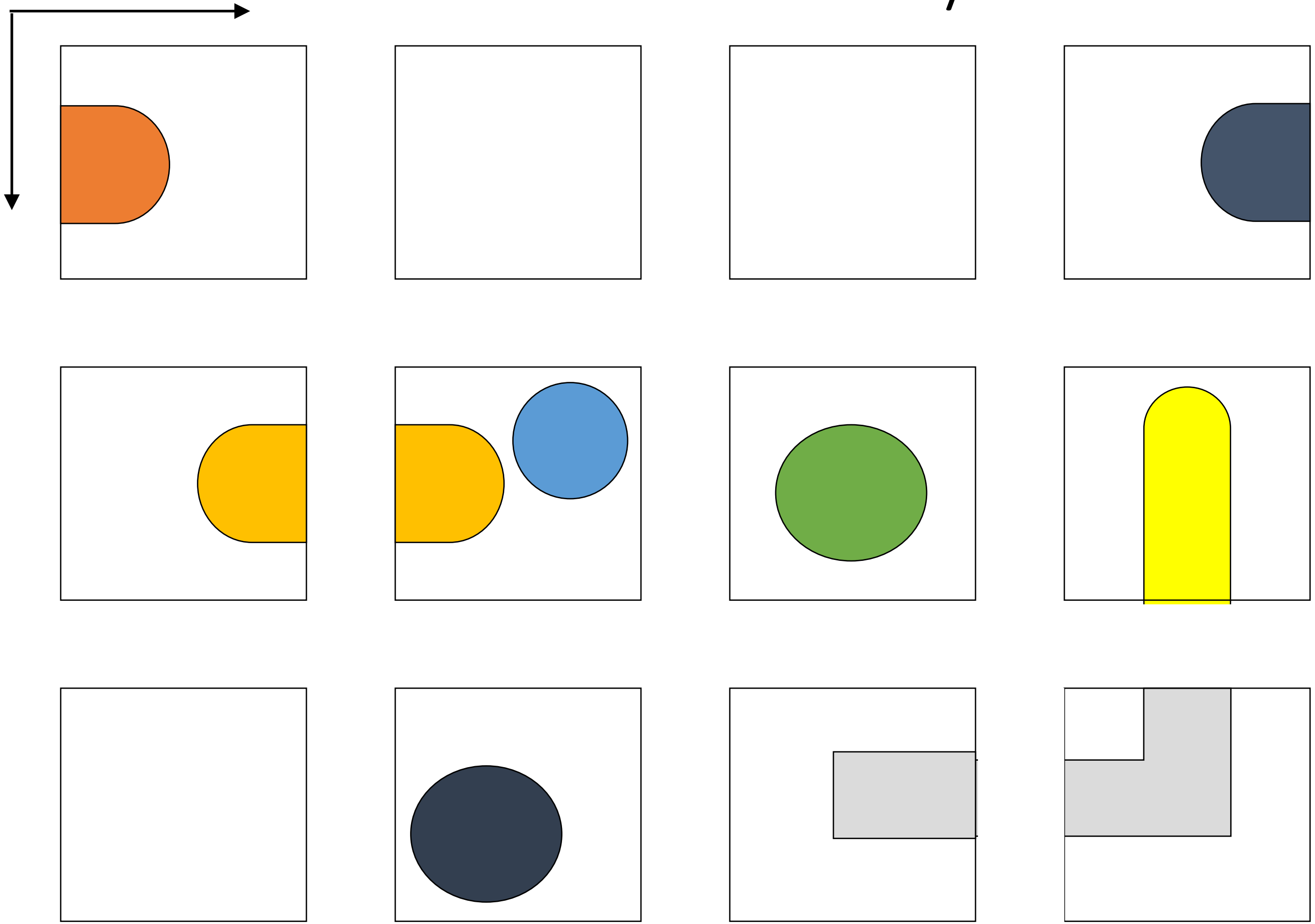
Parallel Flood Fill /2



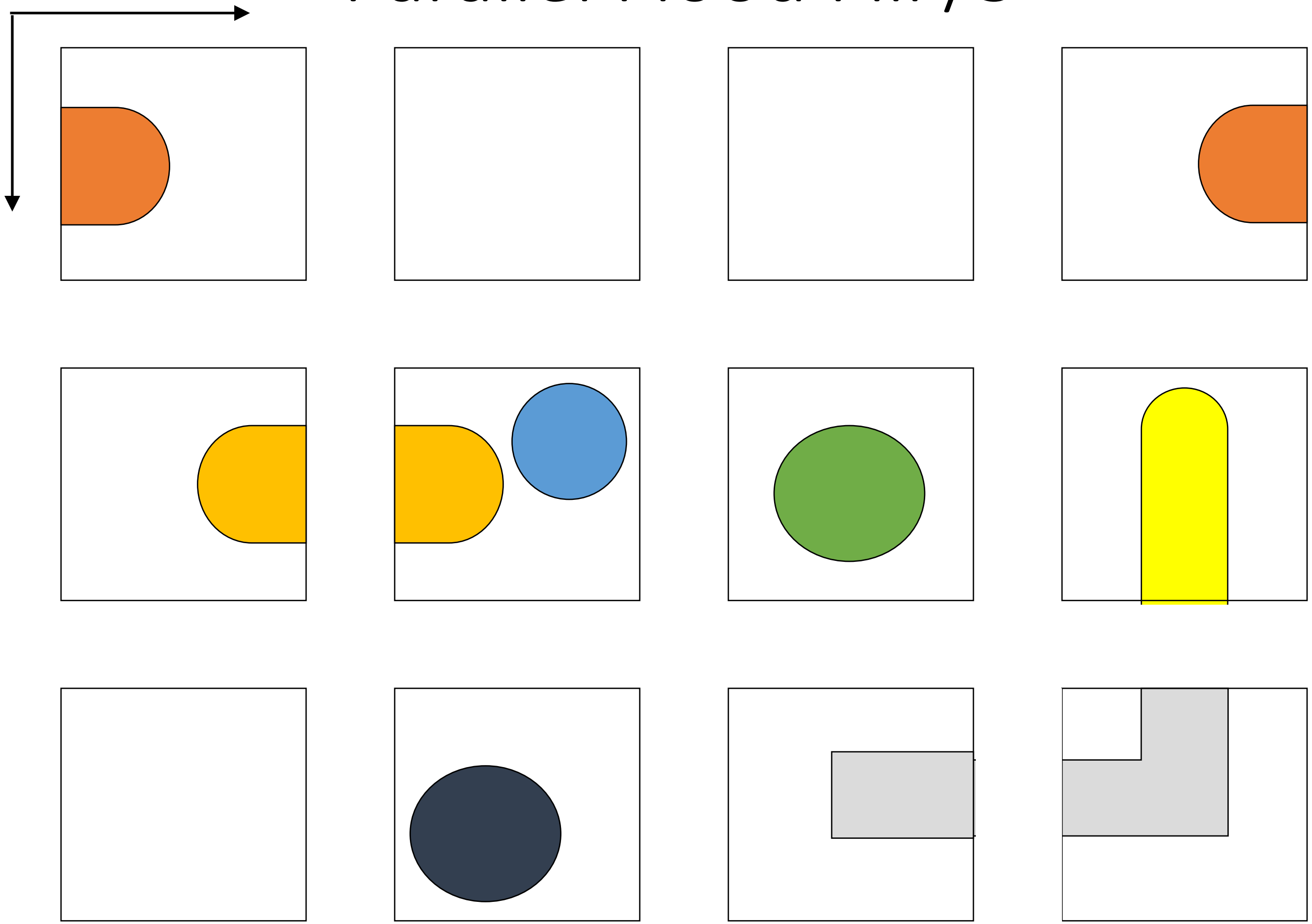
Parallel Flood Fill /3



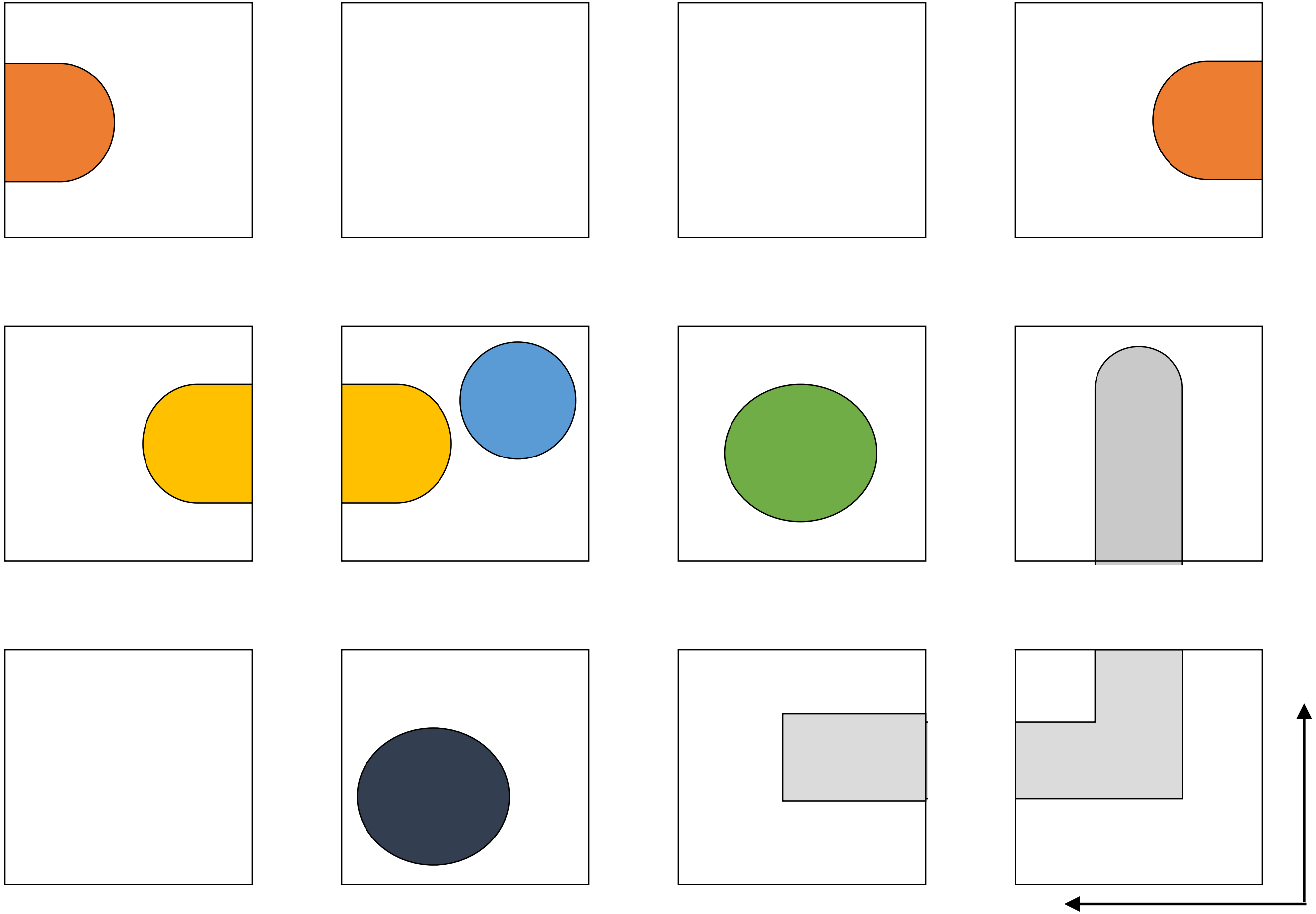
Parallel Flood Fill /4



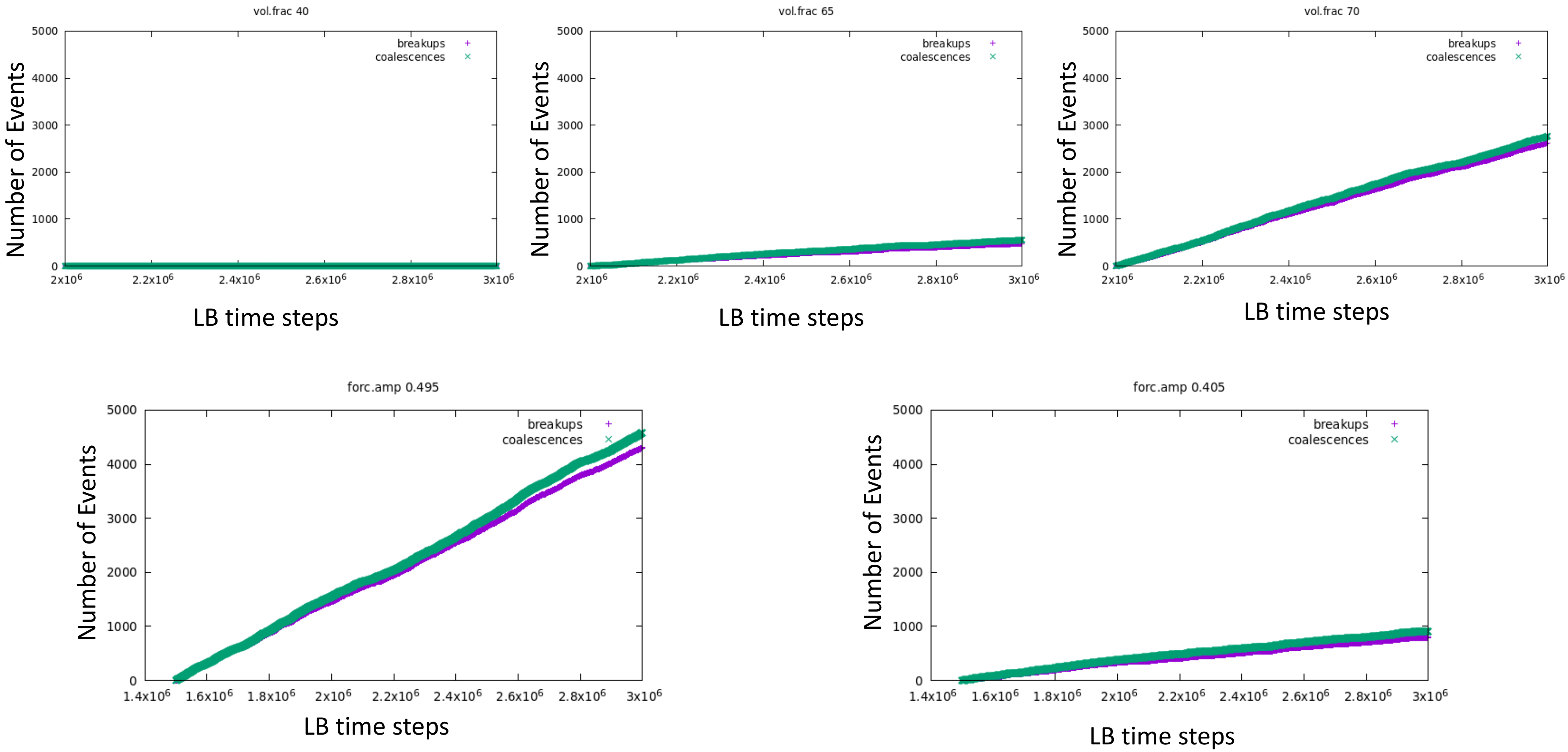
Parallel Flood Fill /5



Parallel Flood Fill /6



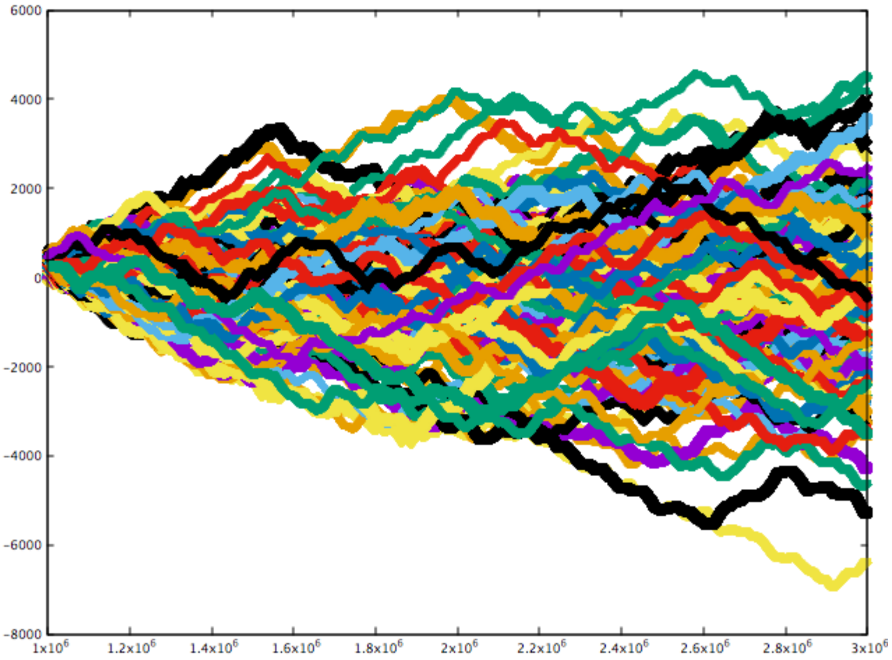
Droplets Dynamics



Droplets Dynamics

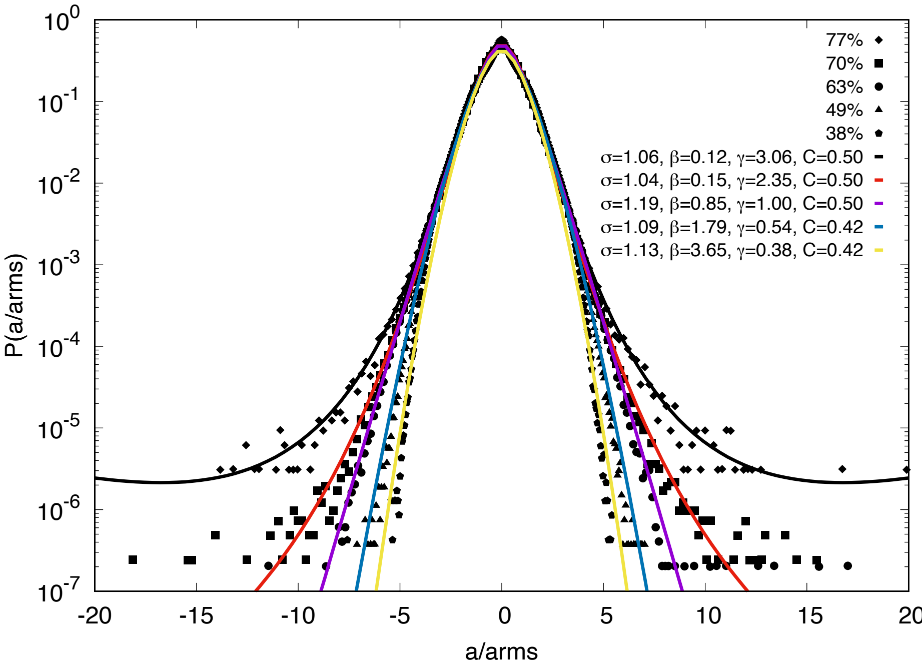
Girotto, I., Scagliarini, A., Benzi, R., & Toschi, F. (2024). Lagrangian statistics of concentrated emulsions. *Journal of Fluid Mechanics*, *986*, A33. doi:10.1017/jfm.2024.364

Absolute trajectories of all droplets existing througouth a simulation of 2M time steps on a 512^3 box



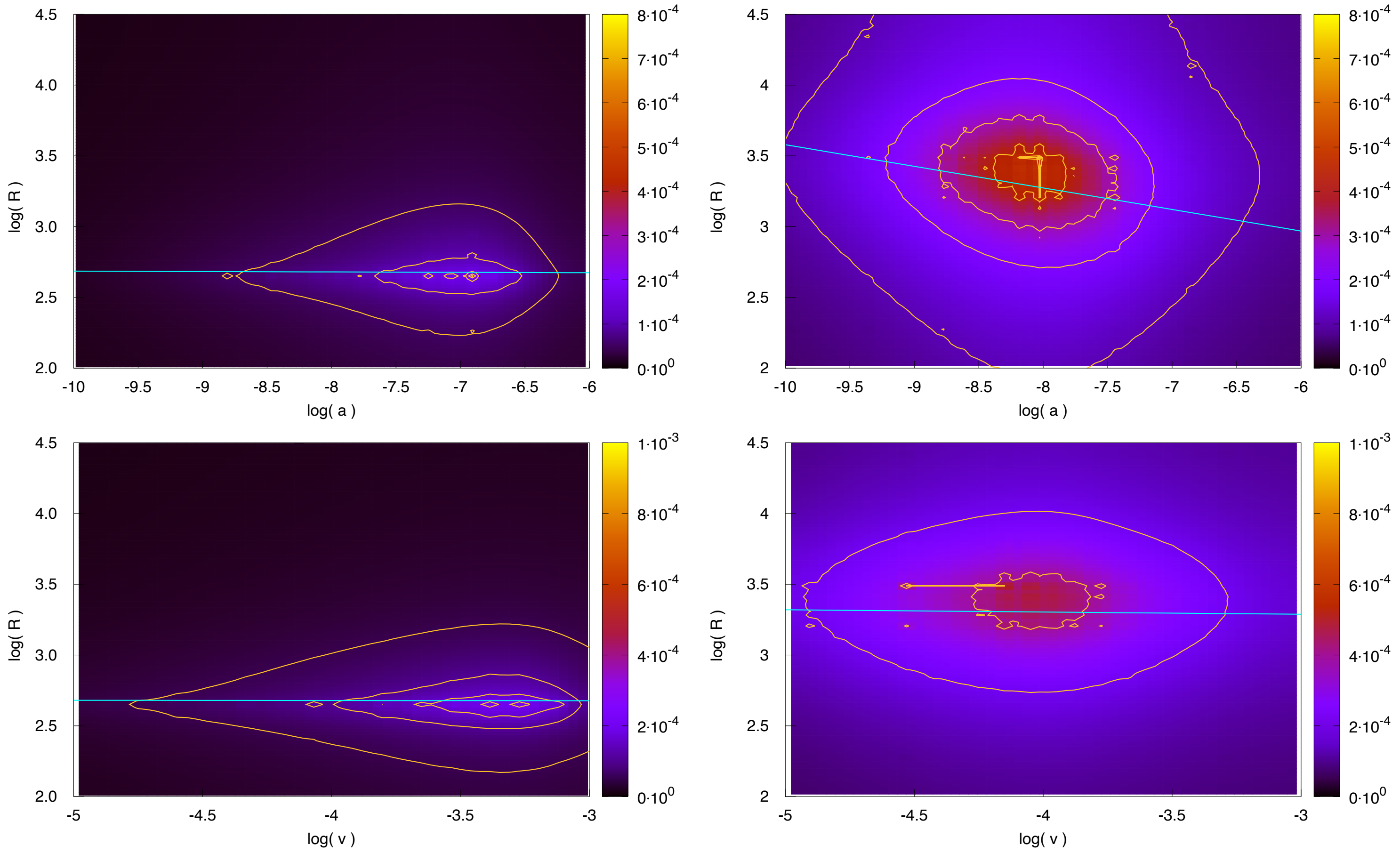
The PDF of accelerations fitted via the stretched exponential distributions:

$$P(x) = C \cdot \exp\left(-\frac{x^2}{(1+|x\beta/\sigma|^\gamma)\cdot\sigma^2}\right)$$

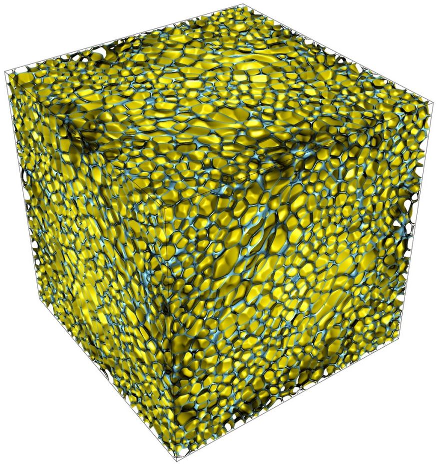


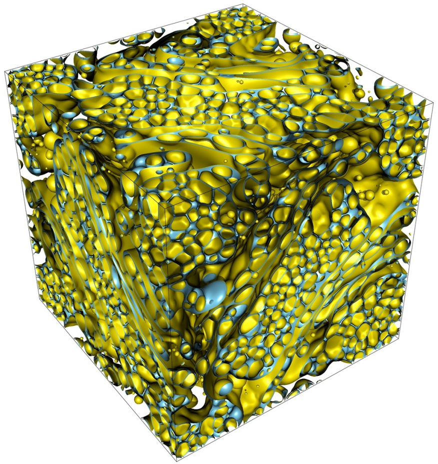
Dilute Emulsion (28%)

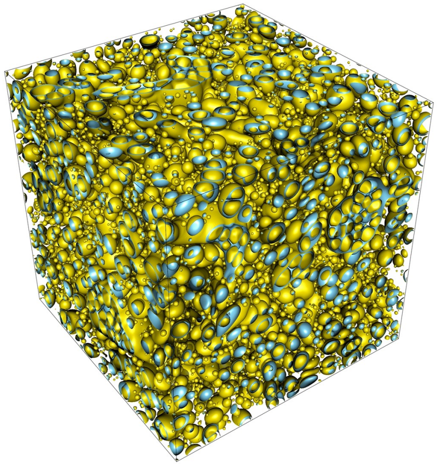
Dense Emulsion (77%)

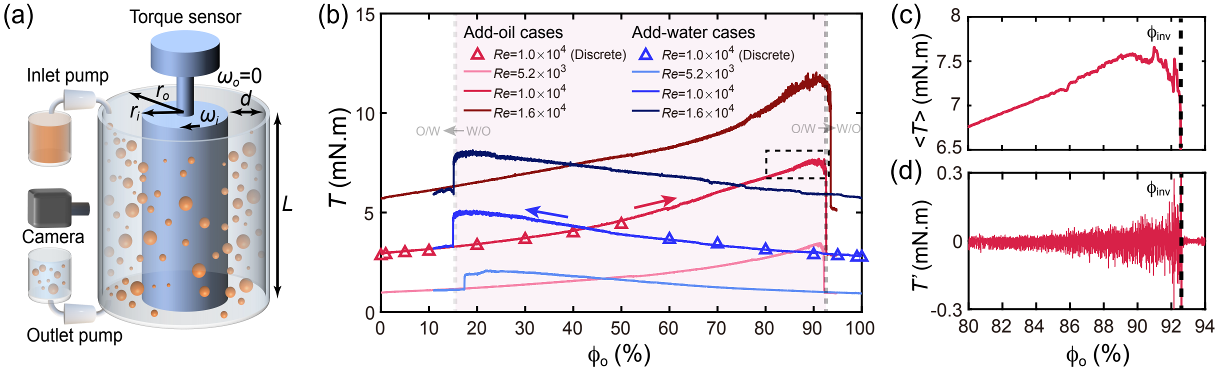


Catastrophic Phase Inversion (CPI)



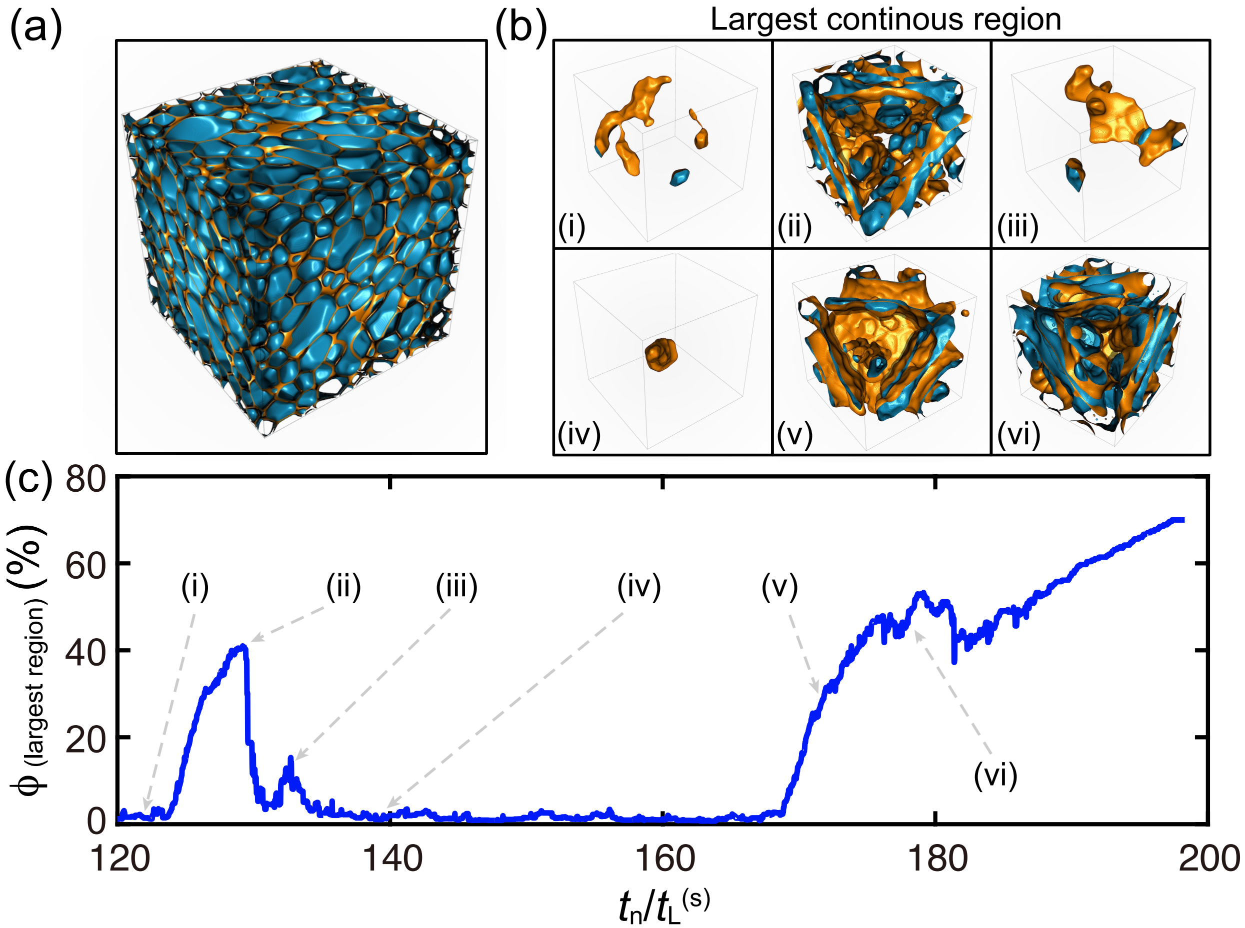






Yi, Lei and Girotto, Ivan and Toschi, Federico and Sun, Chao,
Divergence of Critical Fluctuations on Approaching Catastrophic Phase Inversion in Turbulent Emulsions, Phys. Rev. Lett. 2024

CPI: Simulations




Dense/Stable ϑ = 41%
$N_D'(y)$
$X(y)$
$U_{rms}(y2)$
t_0 + #LB steps (millions)
Packed/Metastable ϑ = 62%
$N_D'(y)$
$X(y)$
$U_{rms}(y2)$
Packed/Unstable ϑ = 77%
$N_D'(y)$
$X(y)$
U_{rms} (y2)
t_0 + #LB steps (millions)
Preliminarly Results

Contributions to this work:

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(UniFE/INFN)

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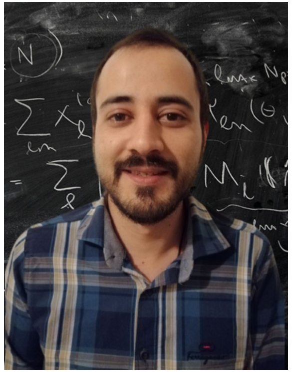
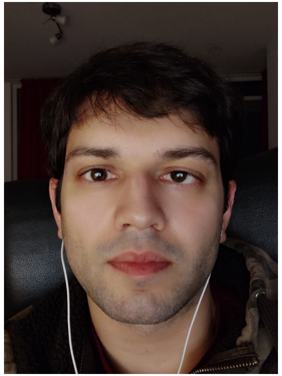
(TU/e)



Saied Aliei (ICTP)



Karun Datadien (TU/e)

Jean-Paul van Woensel
(TU/e)

Dr. Prasad Perlekar
(Tata Institute of Fundamental Research)

Acknowledgements:

PRACE

ICTP
The Abdus Salam
International Centre
for Theoretical Physics

TU/e
Technische Universiteit
Eindhoven
University of Technology

CINECA

INFN
Istituto Nazionale di Fisica Nucleare

BSC
Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación

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