The dynamics of inertial particle ensembles in raindrop formation and sedimentation.

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In the early stages of raindrop formation, billions of inertial water droplets are advected by the vortices of a cloud. The inertial properties of the particles affect the rate at which they collide and consequently grow (Falkovich, Dec 2007, AMS). Particle clustering and variable sedimentation rates also govern the lifespan of plane grounding ash clouds and the distance for which river pollutants are carried. In these examples, the particles interact with one another and the surrounding fluid creating a complex and numerically costly dynamical system. We present a transfer operator, $\mathbf{W}_{ij}$, able to efficiently capture the emergent behaviour of the inertial particle ensemble in the natural world.

The trajectories of inertial particles

Dynamics of small, rigid, spherical particles can be described by the Maxey-Riley equation (*Maxey, 1983, Phys. of Fluids*). To allow the transfer operator to encapsulate the dynamics of (1) in an Eulerian sense take the following steps:

Fluid acceleration — Basset force — Buoyancy force — Stokes drag

$$\ddot{\mathbf{x}} = \left(1-\frac{3R}{2}\right)\mathbf{g} + \frac{3R}{2}\frac{D\mathbf{u}}{Dt} - \frac{R}{St}(\dot{\mathbf{x}}-\mathbf{u}(\mathbf{x},t)) - \frac{3R}{\sqrt{2\pi St}}\int_{t_0}^{t}\frac{1}{\sqrt{t-\tau}}\frac{d}{d\tau}(\dot{\mathbf{x}}-\mathbf{u}(\mathbf{x},t))\mathrm{d}\tau, \quad (1)$$

Neglect the Basset history force

$\mathbf{x}(t) = (x,y,z)$ = particle position
$\mathbf{u}(\mathbf{x},t) = (u,v,w)$ = fluid velocity

$R = 2\rho_f/(2\rho_p+\rho_f)$	$St = 2a^2\rho_f/(9\tau_n\mu)$
$St = 2a^2\rho_f/(9\tau_n\mu)$	ρ_p = particle density
ρ_f = fluid density	a = particle radius
τ_n = Kolmogorov timescale	$\mathbf{g}$ = gravity

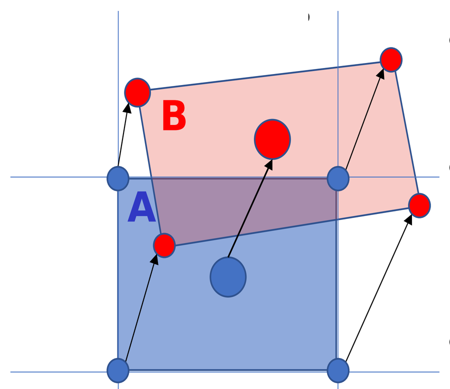
$$\dot{\mathbf{x}} = \mathbf{v}$$
$$\ddot{\mathbf{x}} = \mathbf{g} + \frac{3R}{2}\left(\frac{D\mathbf{u}(\mathbf{x},t)}{Dt} - \mathbf{g}\right) - \frac{R}{St}(\mathbf{v}-\mathbf{u}(\mathbf{x},t)). \quad (2)$$

Reduce dynamics via a series expansion in $\epsilon = St/R$ (Sapsis, 2008, Physica D)

$$\dot{\boldsymbol{x}} = \sum_{k=0}^{\infty}\epsilon^k \boldsymbol{h}_k(\boldsymbol{x},\phi) \qquad \boldsymbol{h}_1 = \left(\frac{3R}{2}-1\right)\left(\frac{D\boldsymbol{u}}{Dt}-\mathbf{g}\right) \quad (3)$$
$$\boldsymbol{h}_0 = \boldsymbol{u}(\mathbf{x},t) \qquad \boldsymbol{h}_k = -\frac{D\boldsymbol{h}_{k-1}}{Dt} - \nabla\boldsymbol{u}\cdot\boldsymbol{h}_{k-1} - \sum_{i=1}^{k-2}\nabla\boldsymbol{h}_i\cdot\boldsymbol{h}_{k-i-1},\ k\geq 2$$

Particle velocity is now uniquely defined everywhere in space, allowing $\mathbf{W}_{ij}$ to be found.

Constructing the transfer operator



- Space is discretised over a regular Cartesian grid.
- Particles are advected from the corners of grid cells. After δt they define a new shape.
- The new shape is redistributed amongst its neighbours to find the between cell fluxes.
- The fluxes are encoded into $\mathbf{W}_{ij}$.
- In an unsteady flow, the remapping is repeated every fluid time step.
- In a steady flow, the dominant eigenvector of $\mathbf{W}_{ij}$ gives the long term behaviour of the system.

$\mathbf{W}_{ij}$ allows us to write $P_j^{n+1} = \mathbf{W}_{ij}P_j^n$, where P_j^n represents the number of particles in each cell of a discretised phase space. j is the cell index, and n enumerates times steps. We can now move particles in space in a probabilistic sense.

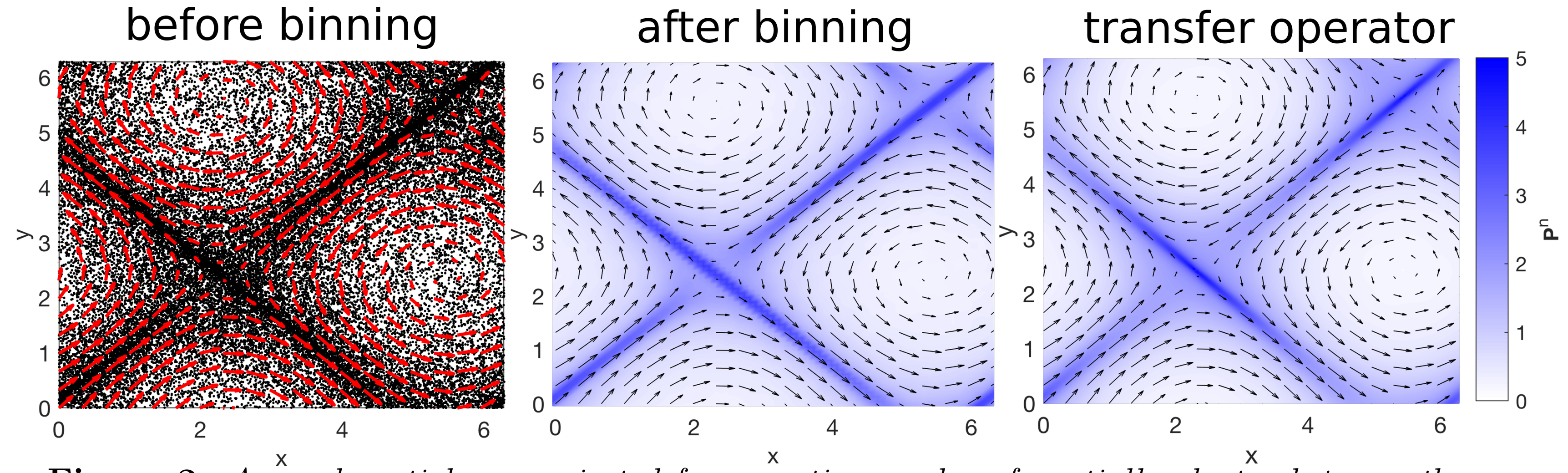
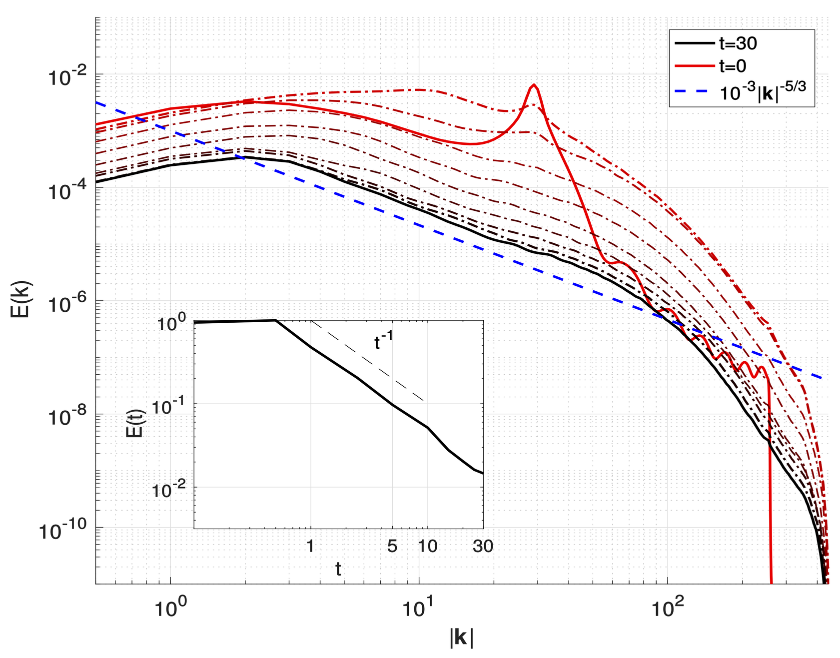


Figure 2: *Aerosol particles are ejected from vortices and preferentially cluster between them. This behaviour is shown for: (left to right) a sample of 4×10^6 inertial particles; the particles after binning and one iteration of spatial smoothing; the transfer operator $\mathbf{W}_{ij}$. As the number of bins and particles are increased, the central and rightmost images converge to one another.*

The turbulent velocity field

We test $\mathbf{W}_{ij}$ in a decaying superposition of ABC flows in the presence of gravity. The flow, a good analogue for a turbulent cloud, or turbulent river, is evolved using MOBILE, a third order ILES scheme over a regular cartesian mesh.



$$\mathbf{u}(x,0) = \sum_{k_0=1}^{14}\begin{bmatrix} B\cos(2\pi k_0 z) + C\sin(2\pi k_0 y) \\ C\cos(2\pi k_0 x) + A\sin(2\pi k_0 z) \\ A\cos(2\pi k_0 y) + B\sin(2\pi k_0 x)\end{bmatrix} \quad (4)$$

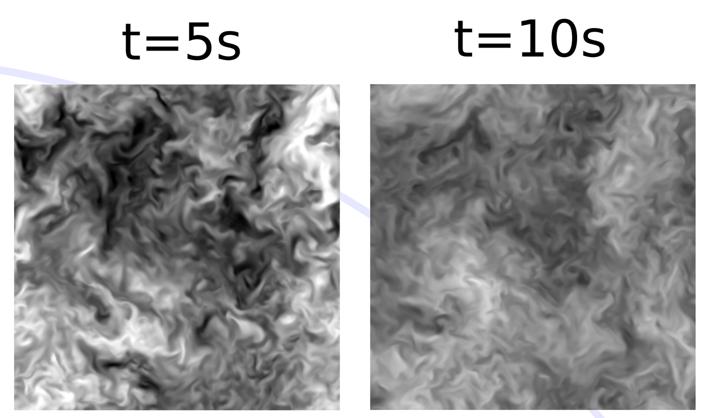
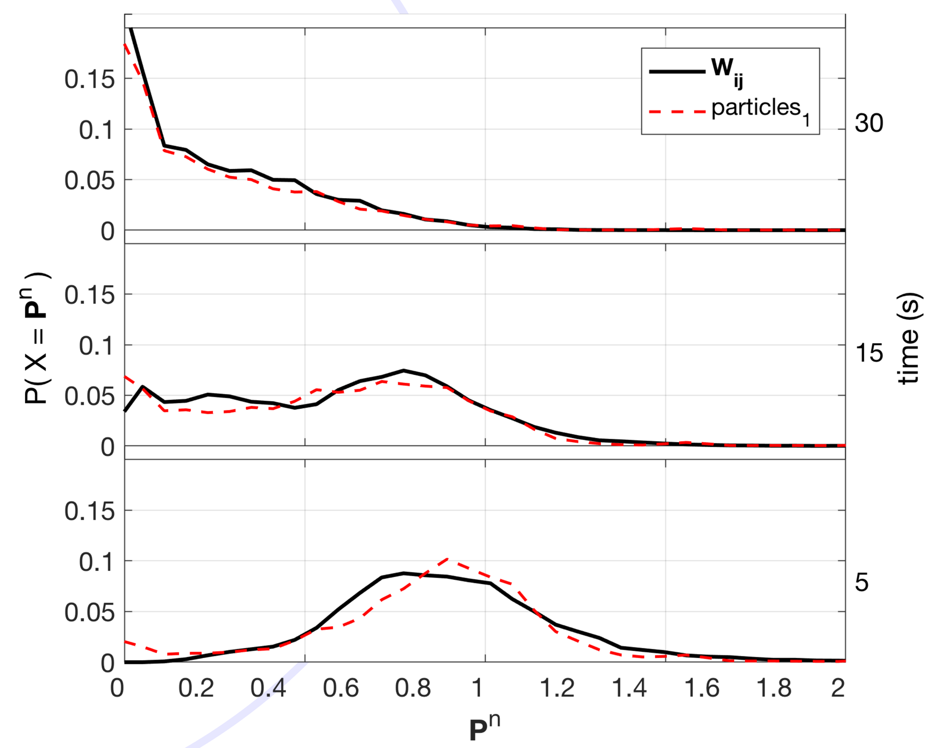


Figure 3: *The decaying energy spectrum of the test flow (left) initialised with (4) and $A = 0.09$, $B = 0.1$, $C = 0.11$. Planar snapshot of the velocity field at two time instants (right).*

Sedimentation in a turbulent flow

To test $\mathbf{W}_{ij}$ in a sedimentation context, we compare predictions made by $\mathbf{W}_{ij}$ to actual particle distributions in the fluid velocity field described above.

Figure 4: *The distribution of particles per cell, $\mathbf{P}^n$, after 5, 15 and 30 seconds. The distribution is shown for the transfer operator (black line), and a simulation of 5×10^5 individual trajectories (red line). For the red line particle positions have undergone one iteration of spatial smoothing, allowing comparison between the continuous transfer operator and the discrete particle data. Left skewness and widening of the distribution indicates more clustering.*



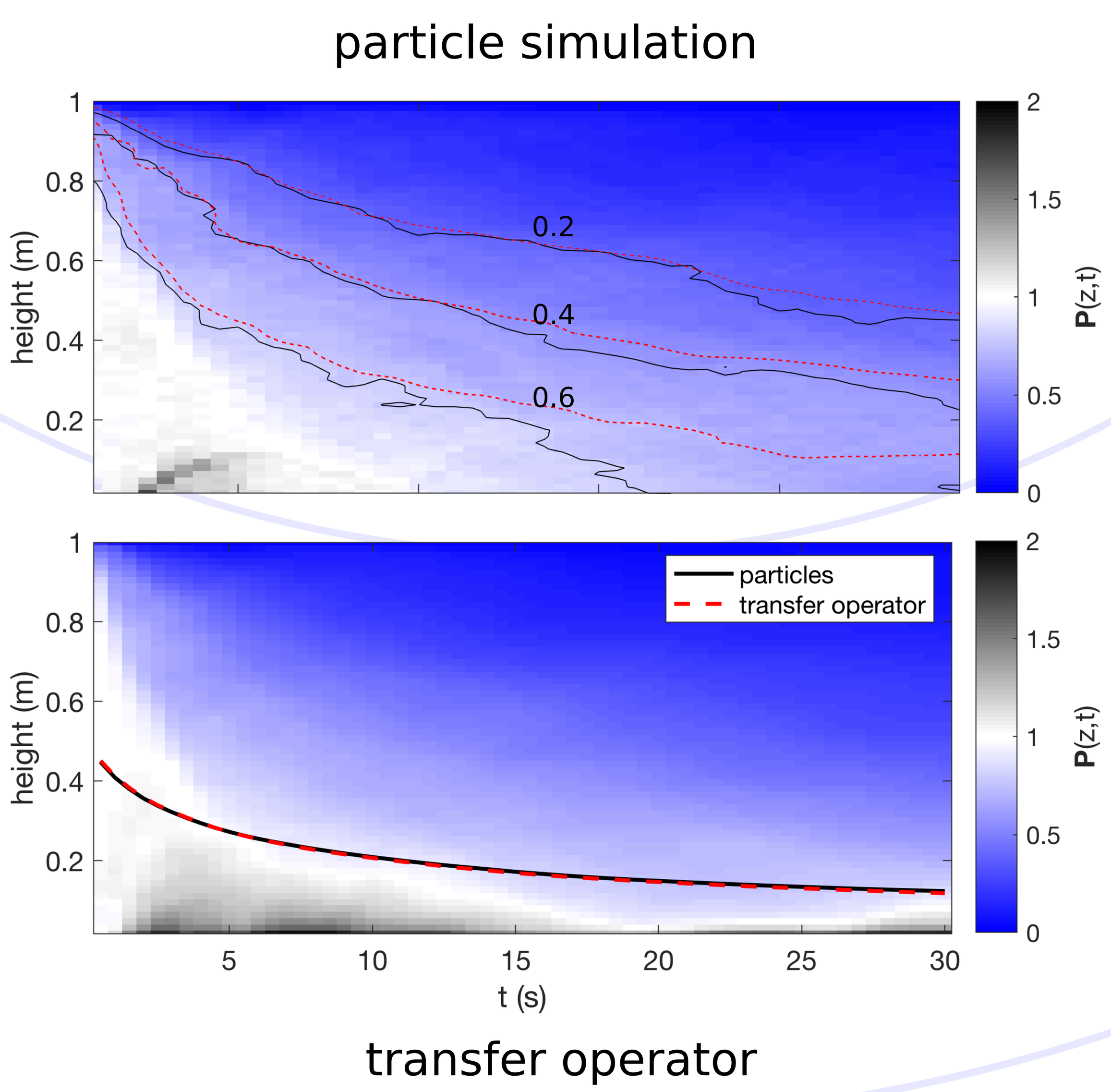
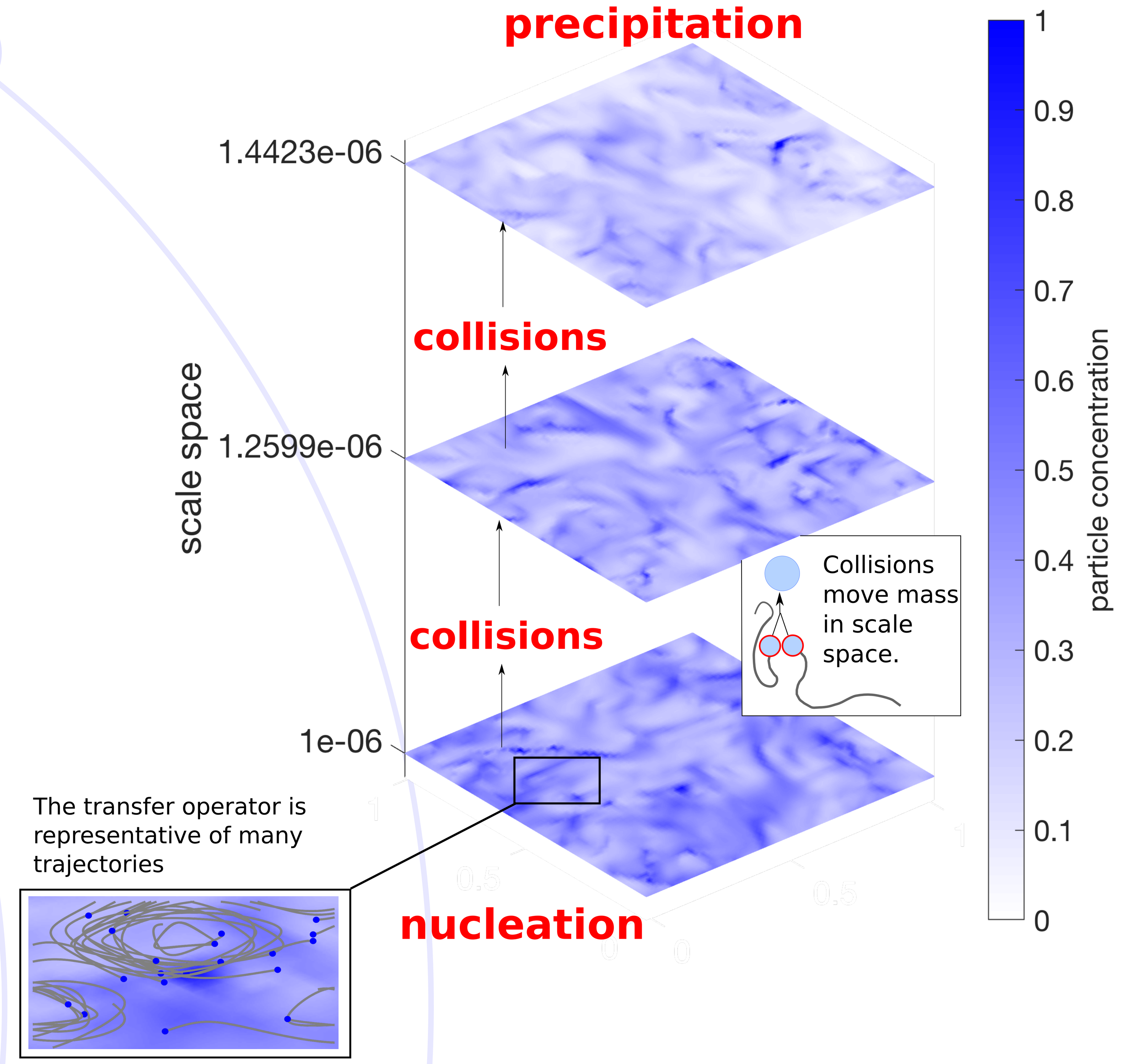


Figure 5: *The vertical distribution of particles $\mathbf{P}(z,t)$ produced by $\mathbf{W}_{ij}$ (top), and a simulation of 5×10^5 particles (bottom). The particle radius was $5\times10^{-6}(m)$. Early in the simulation, the transfer operator produces a sedimentation rate close to that of the particle simulation. As the number of particles in the simulation reduces, the two simulations begin to diverge. This behaviour is related to the loss of statistical convergence in the particle simulation.*

Where next? Building a statistical model of raindrop formation.



A key motivation for our approach is that it can be extended to model more complicated and interesting processes. As an example we present the steps for creation of a statistical model of raindrop formation (a work in progress).

- 1 Particles behave differently at different diameters: their scale space is discretised.
- 2 The transfer operator redistributes particles in each level of scale space.
- 3 We assume particles are normally distributed at the subgrid scale.
- 4 Collision rates are approximated probabilistically based on the local particle concentration.
- 5 Assuming coalescence, collisions move particles in scale space.
- 6 The rate of mass flux, through the scales, governs the rate at which a cloud produces rain.

Summary

- We have developed a method for tracking an ensemble of inertial particles in an Eulerian sense.
- Particle dynamics are reduced to an inertial manifold to allow a linearisation of the Perron-Frobenius-Ruelle or transfer operator to be constructed.
- The transfer operator makes good predictions about sedimentation rates and degree of preferential concentration of particles.
- The method is readily augmented to statistically model complicated processes such as particle collisions in raindrop formation and density forcing on the fluid phase. In both cases this work is ongoing.

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