

Data Analysis of Particle Clustering in Turbulence



Reza Momenifar

Civil and Environmental Engineering (CEE), Pratt School of Engineering

Environmental Spatial Data Analysis (CEE690-02) course Fall 2019

Outline

- Turbulence
- Particle Clustering
- Clustering Analysis (or Unsupervised Learning) via Voronoï Tessellation
- Summary
- PCA analysis

Turbulence

Understanding and predicting how fluids move is of enormous importance to a vast range of problems:



Turbulence

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The difference is that in these problems the fluid motion is *turbulent*.

An extremely brief intro to turbulence: Depending upon the flow properties (velocity, boundary conditions, viscosity of fluid etc), the motion of a fluid can be either *LAMINAR* or *TURBULENT*, and these are *radically different!*

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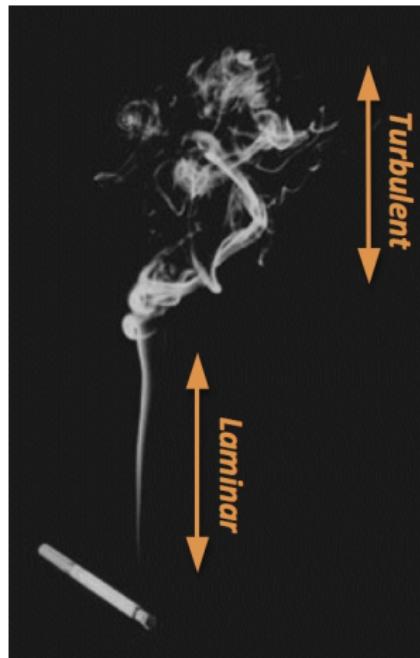
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Rising smoke illustrates the difference between laminar and turbulent flows:

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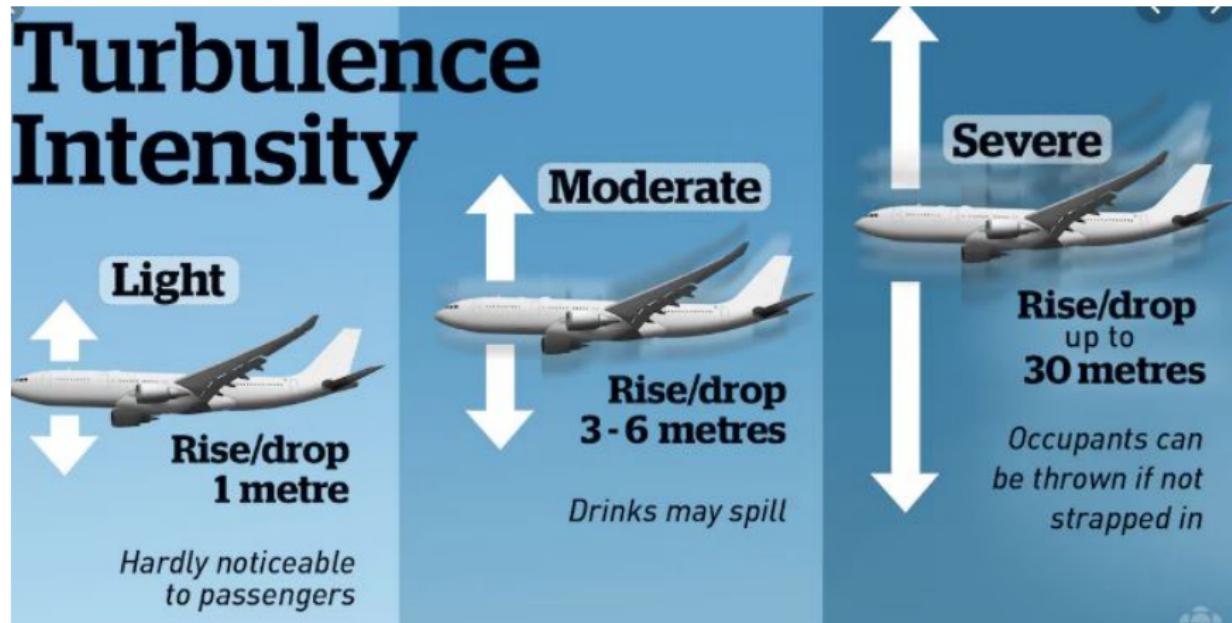
Rising smoke illustrates the difference between laminar and turbulent flows:



- Laminar flow is orderly, regular, predictable.
- Turbulent flow looks random, chaotic, irregular, unpredictable (depending on the intensity of turbulence).

Turbulence

Example: Airplane Turbulence.



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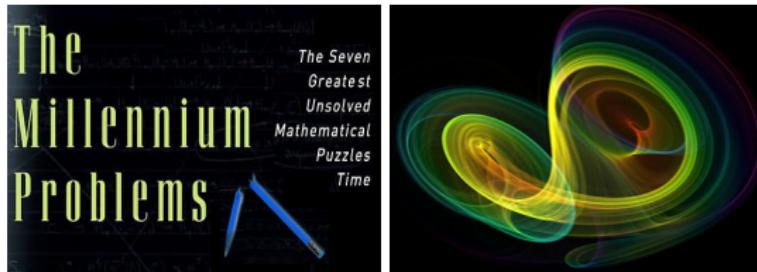
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Feynman: “turbulence is the last great unsolved problem in classical physics”. It is also connected to deep problems in pure and applied mathematics.



However, turbulence is not only a very intellectually rich and stimulating problem to work on, but it is also extremely important practically.

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This has great implications...for air pollution, combustion, chemical reactions, heat transfer...

In fact, turbulence has great implications for understanding and predicting a wide variety of problems...

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Clouds: are important not only for weather, but also for climate, and turbulence controls the thermodynamics of clouds, radiative properties, and the rate at which droplets grow to form rain.

Turbulence

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Turbulence

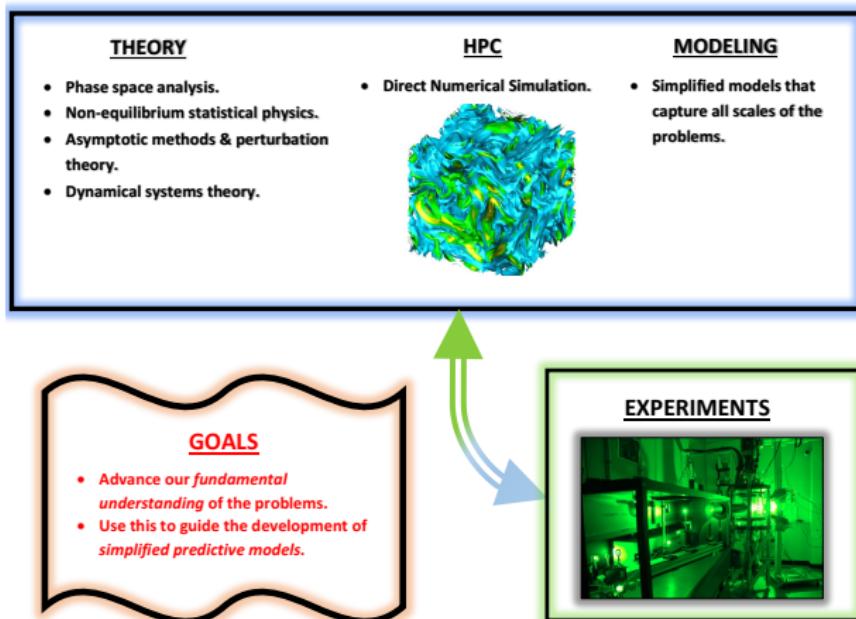
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Particle Clustering in Turbulent Flow

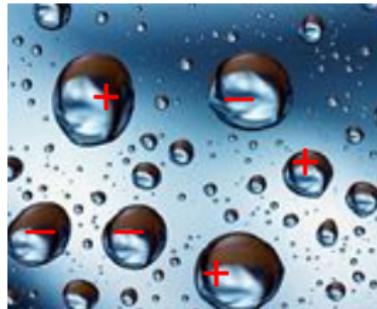
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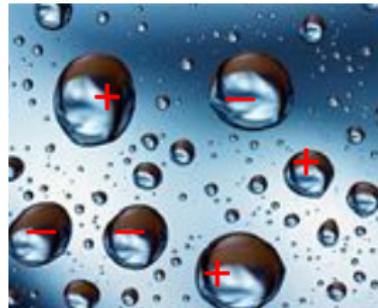


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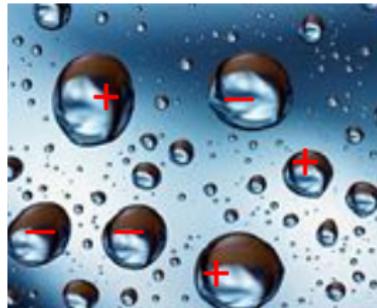
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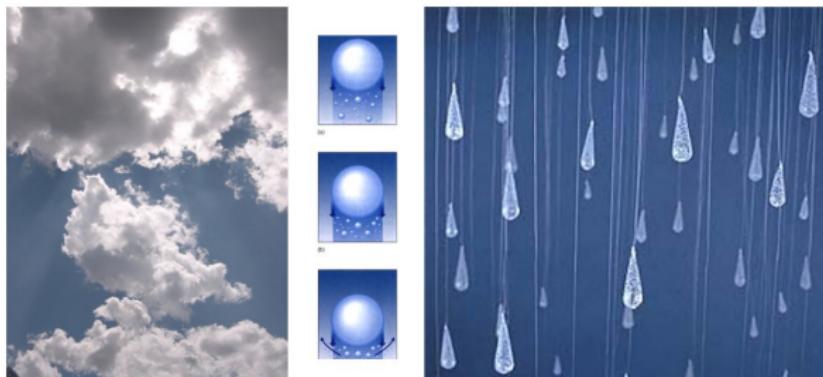
In clouds (thunderstorm and non-thunderstorm), particles (droplets or ice crystals) are often charged.

How do the electric forces compete with the turbulent air to control the particle collisions and mixing rates?

What are the implications for the electrodynamics of clouds?

Particle Clustering in Turbulent Flow

Problem of interest: rain formation



**Rain Drops formation
In warm clouds**

1. CCN activation
2. Condensation
3. **Coalescence**

Enhanced collision rate of water droplets by clustering
may explain the fast rate of rain drop formation,
which cannot be explained by condensation only

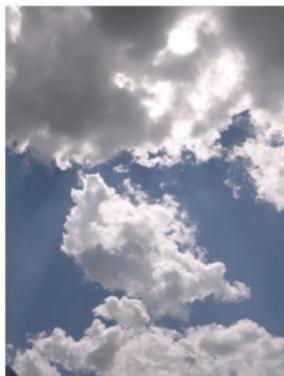
(Pruppacher and Klett, 1998)

(Falkovich, Fouxon and Stepanov, Nature 2002)

- The particle properties (particularly their inertia and fall speed) can significantly change the interaction of particles with the turbulent flow

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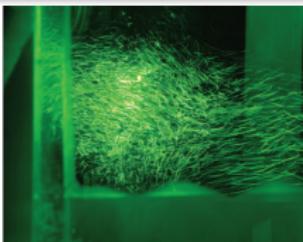
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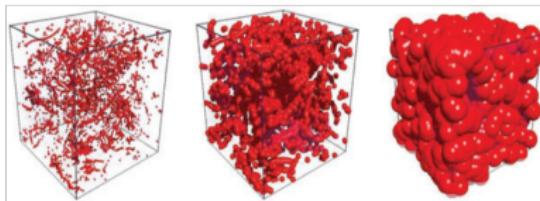
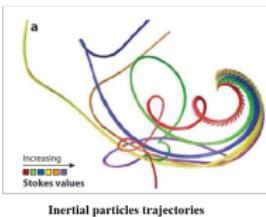
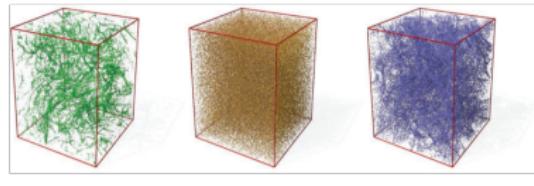
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- Indeed, inertial particles are distributed non-uniformly in the turbulent flow.
In addition, the presence of gravity results in finite settling velocities of
inertial particles

Particle Clustering in Turbulent Flow



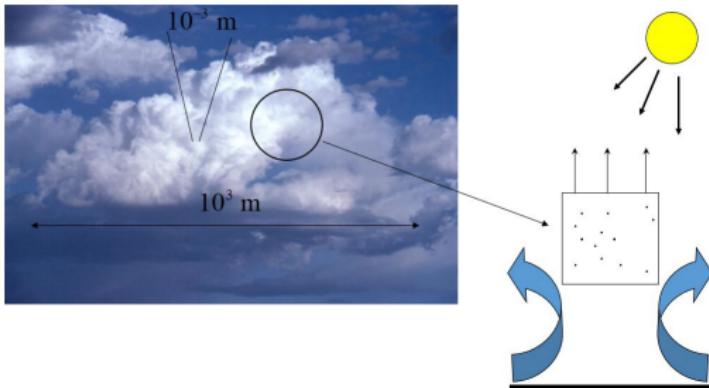
Fluid Streamlines (Polystyrene spheres 25 μm in diameter are used as tracers in experiments and illuminated by a laser with)



- The non-uniform distribution of particles can lead to the formation of clusters.
- Clusters, the group regions of highly concentrated particles, which can significantly change the structure of the turbulence and produce substantial inhomogeneities in the spatial concentration of particles.

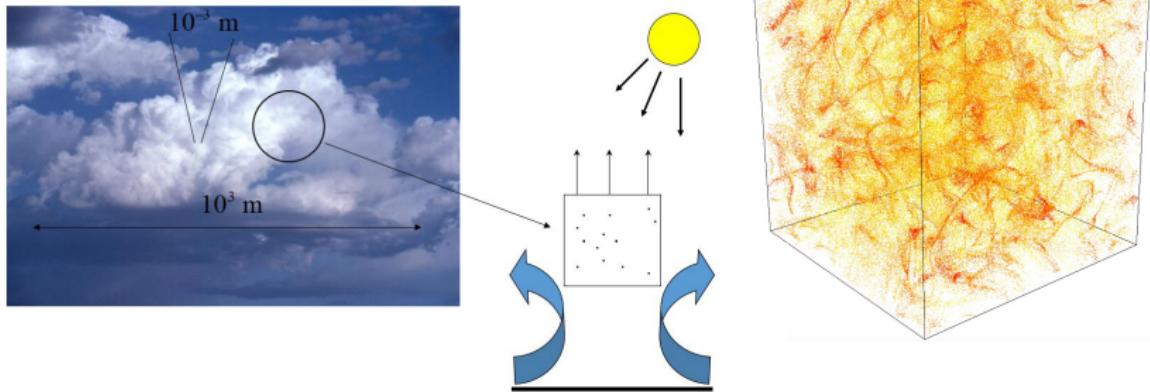
Particle Clustering in Turbulent Flow

Turbulence in Clouds



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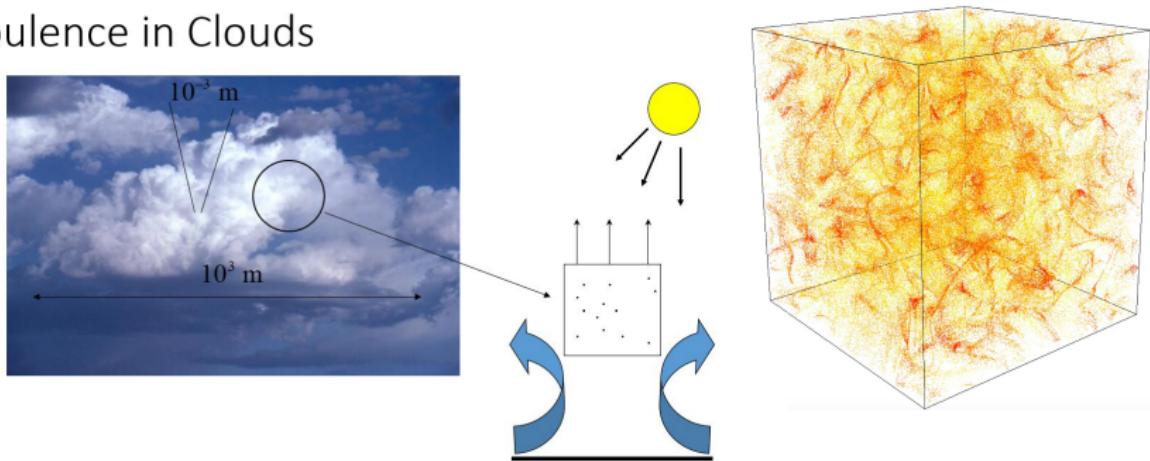
Turbulence in Clouds



- We employ Direct Numerical Simulations (DNS) to model turbulent flow and track particles lying under an idealized turbulence in a cubic box.

Particle Clustering in Turbulent Flow

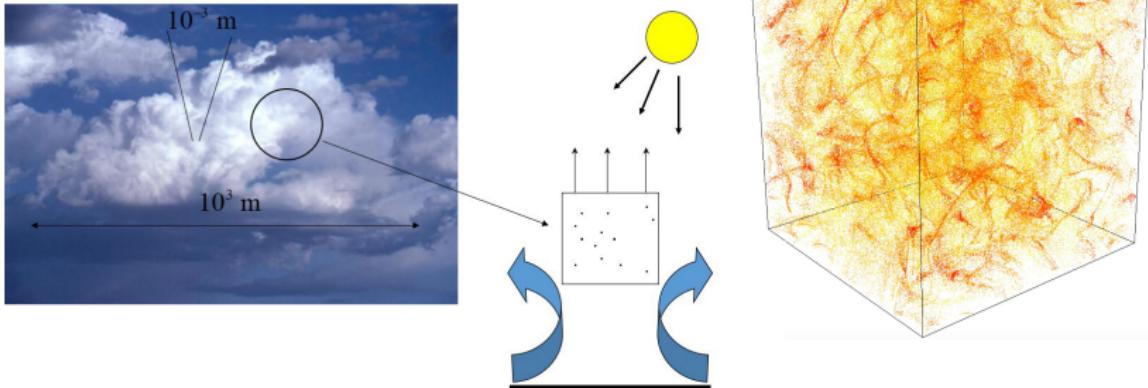
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- In these simulations, three independent control parameters representing the properties of turbulent flow and particles are varied and particles' position and other dynamical properties of particles and flow fields (e.g. velocity) are stored.

Particle Clustering in Turbulent Flow

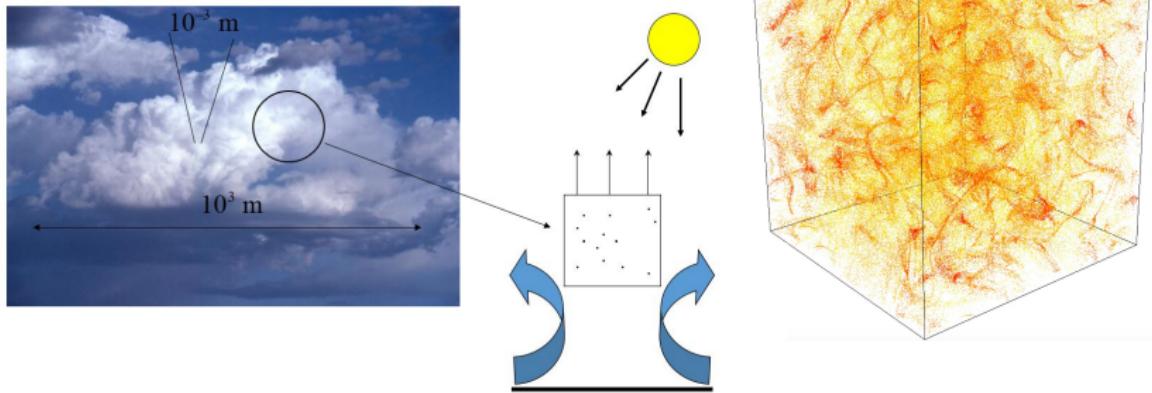
Turbulence in Clouds



- More specifically, we want to explore how intensity of turbulence (quantified by Reynolds number or Re), gravitational acceleration (quantified by Froud number or Fr) and particles' characteristics (e.g. size, density which is quantified by Stokes number or St) affect the spatial distribution and clustering of particles in an idealized turbulence (homogeneous isotropic turbulence or HIT).

Particle Clustering in Turbulent Flow

Turbulence in Clouds



- Numerical Simulation of Particle Distribution in Turbulence**video .

Particle Clustering in Turbulent Flow

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$$\partial_t \mathbf{u} + \boldsymbol{\omega} \times \mathbf{u} + \nabla \left(\frac{p}{\rho_f} + \frac{\|\mathbf{u}\|^2}{2} \right) = \nu \nabla^2 \mathbf{u} + \mathbf{f}, \quad \nabla \cdot \mathbf{u} = 0$$

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- Reynolds Number (Re), quantifies the intensity of a turbulent flow.

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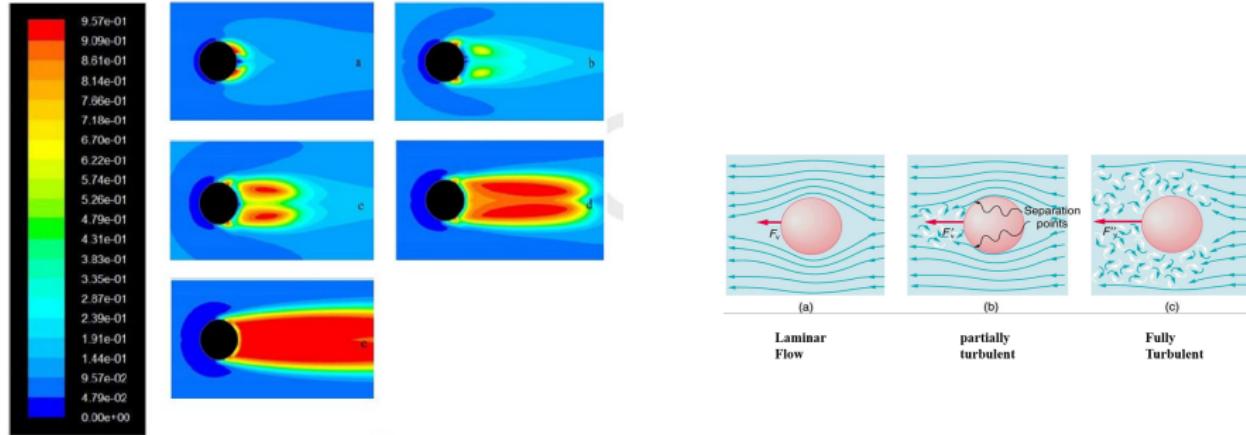


FIG. 11: Contour of void fraction around the cylinder for (a) $Re_{TP} = 1,000$, (b) $Re_{TP} = 3,162$, (c) $Re_{TP} = 10,000$, (d) $Re_{TP} = 31,623$, and (e) $Re_{TP} = 100,000$.

- In the real problems of interest, oceanic and atmospheric turbulent flow, the Re is very large ($O(10^7)$ or more).

Particle Clustering in Turbulent Flow

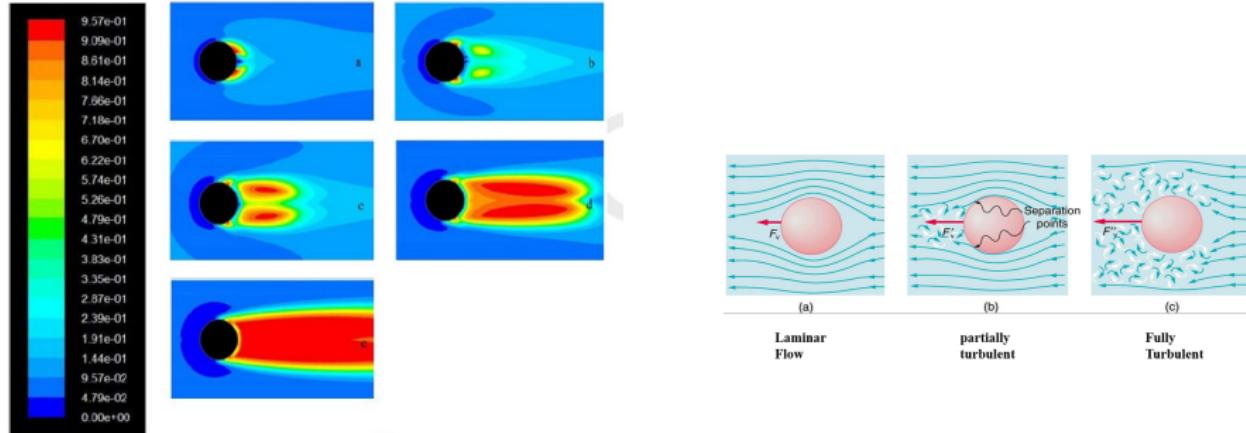
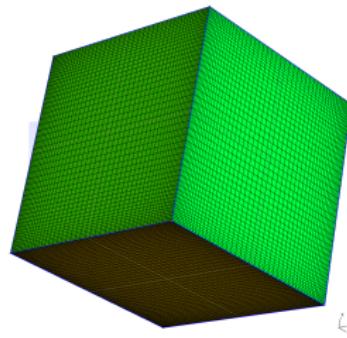


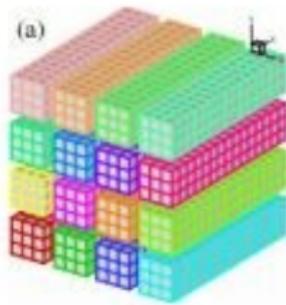
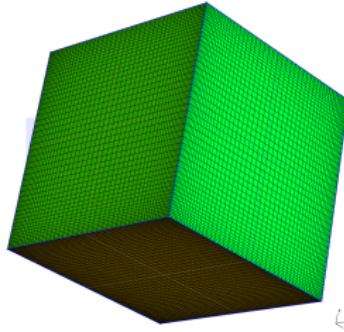
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- In the real problems of interest, oceanic and atmospheric turbulent flow, the Re is very large ($O(10^7)$ or more).
- We use DNS over a range of Re to look for trends in the behavior. This can provide insight regarding the extent to which results obtained at low/moderate Re might be extrapolated to the real problems of interest.

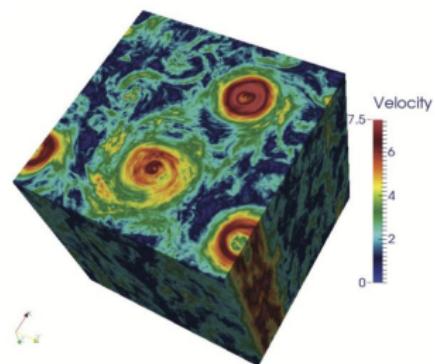
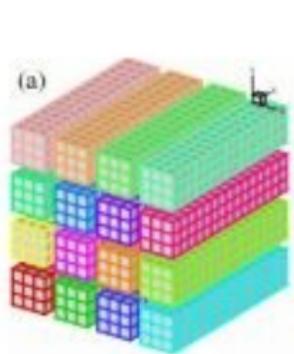
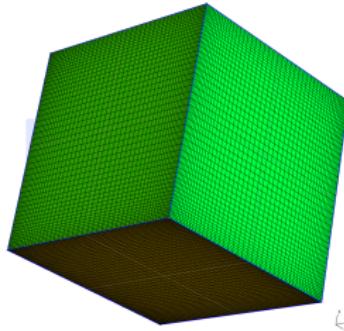
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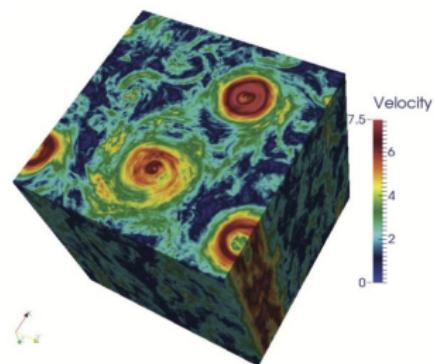
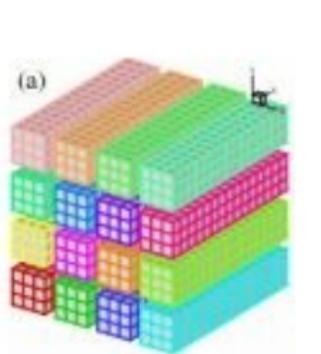
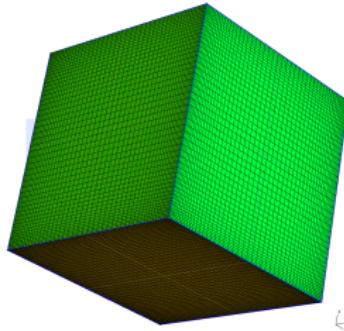


Particle Clustering in Turbulent Flow



- Turbulent flow property: Our DNS study considers $R_\lambda = 90, 224, 398$, where $R_\lambda \equiv u' \lambda / \nu$.
- The higher the Re , the higher the resolution (more grid points; $N_g = 128^3$, $N_p = 16$ for $R_\lambda = 90$ versus $N_g = 1024^3$, $N_p = 1024$ for $R_\lambda = 398$; **2 days versus 4 months!**)

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- particle tracking:

$$\frac{d^2}{dt^2} \boldsymbol{x}^p(t) = \frac{d}{dt} \boldsymbol{v}^p(t) = \frac{\boldsymbol{u}(\boldsymbol{x}^p(t), t) - \boldsymbol{v}^p(t)}{\tau_p} + \boldsymbol{g}$$

Particle Clustering in Turbulent Flow



cumulus clouds: low-level clouds, generally less than 2 km (6,600 ft)



Cumulonimbus clouds: high-level clouds, up to 12 km (40,000 ft)

- Particle property (effect of gravity or fall speed): $Fr = \infty$, 0.3 (cumulonimbus clouds), 0.052 (cumulus clouds). The stronger gravity, the larger the domain.
- Particle property (effect of inertia; e.g. size, density): fifteen St in the range of $0 \leq St \leq 3$. The larger the St , the more difficult to solve the particle's equation.

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- To obtain local insight into the clustering of particles, the Voronoi diagrams (tessellation) approach is employed as the data processing technique to identify regions of high (clusters) and low (voids) concentration of particles.

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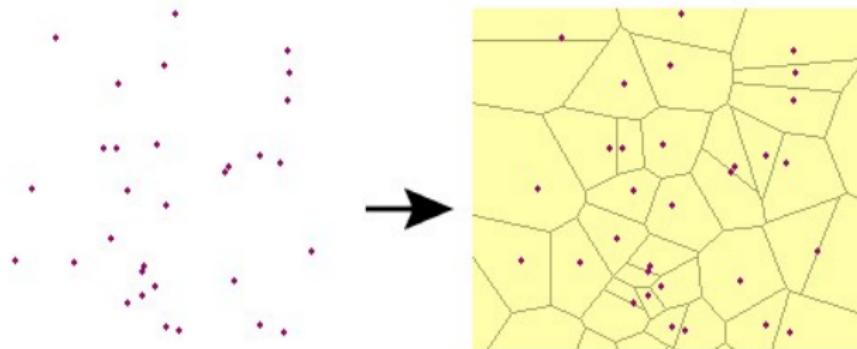
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- The appearance of clustering and its strength is diagnosed by exploring the distribution of Voronoi volumes over a significant range of the three parameter space $Fr = \infty, 0.3, 0.052$, $R_\lambda = 90, 224, 398$ and $0 \leq St \leq 3$ which are varied independently.

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Clustering Analysis via Voronoï Tessellation

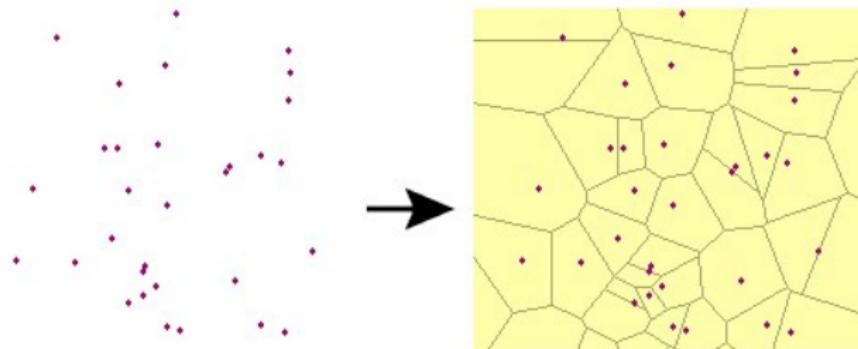
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(<https://www.safe.com/transformers/voronoi-diagrammer/>)

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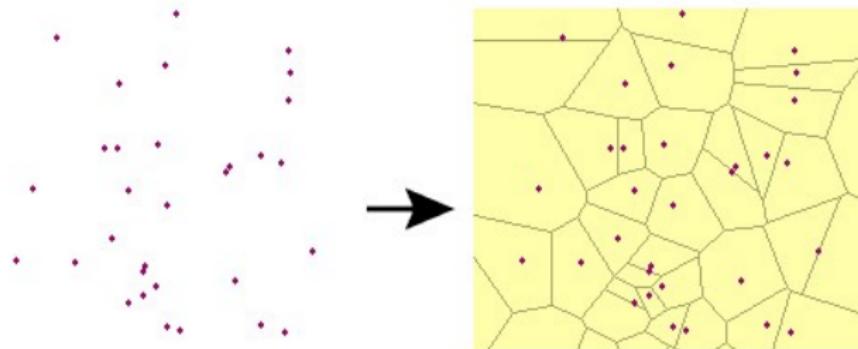


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- After collecting data points and recording their location, the plane can be divided into sections, or Voronoi cells, that are representative of each data point.
- A Voronoi diagram describes the spatial relationship between points that are near each other, or their nearest neighbours. It is a set of connection polygons derived from points or locations.

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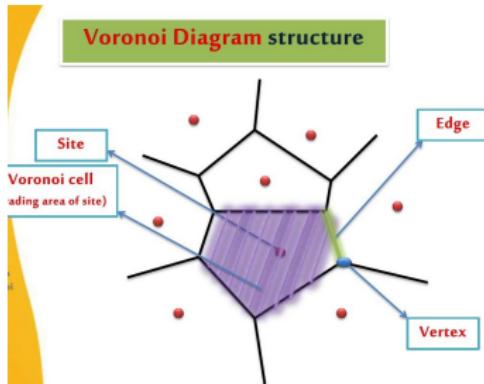
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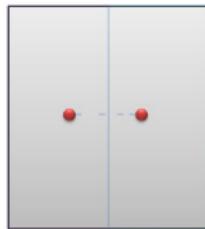
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Clustering Analysis via Voronoï Tessellation

- First step is to draw a line connecting adjacent points.
- Second step is to draw a perpendicular line to the one you just drew in the midpoint of it.
- Last step is to connect lines, drawn in the second step, in to an network.

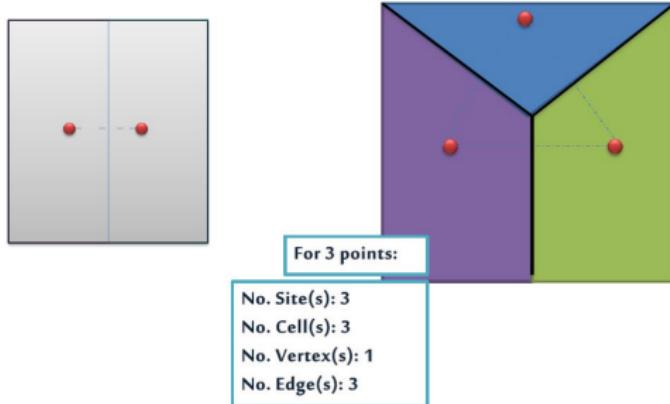


For 2 points:

No. Site(s): 2
No. Cell(s): 2
No. Vertex(s): 0
No. Edge(s): 1

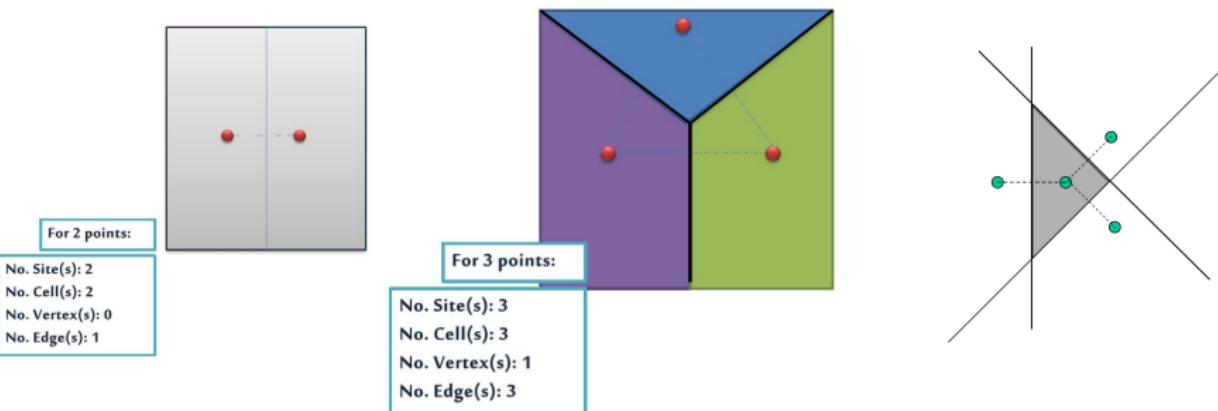
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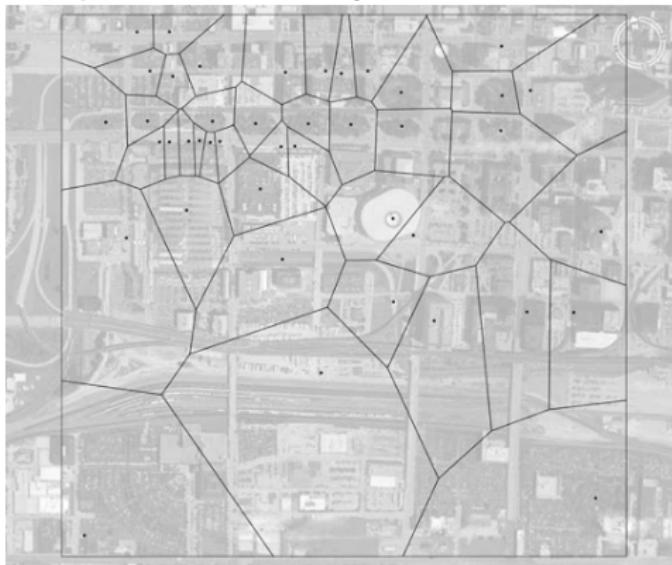
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- Application: They find widespread applications in areas such as nearest neighbor queries for data structure problems in computational geometry, business applications such as determining where to locate a store so it is no closer to any existing store of its kind, epidemiology, geophysics, and meteorology .

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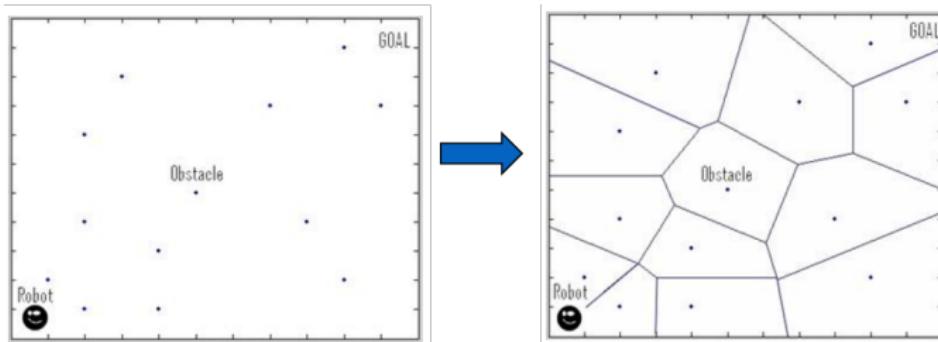
City Planning: one can easily determine where is the nearest shop or hospital, and urban planners can study if certain area need a new hospital



Clustering Analysis via Voronoï Tessellation

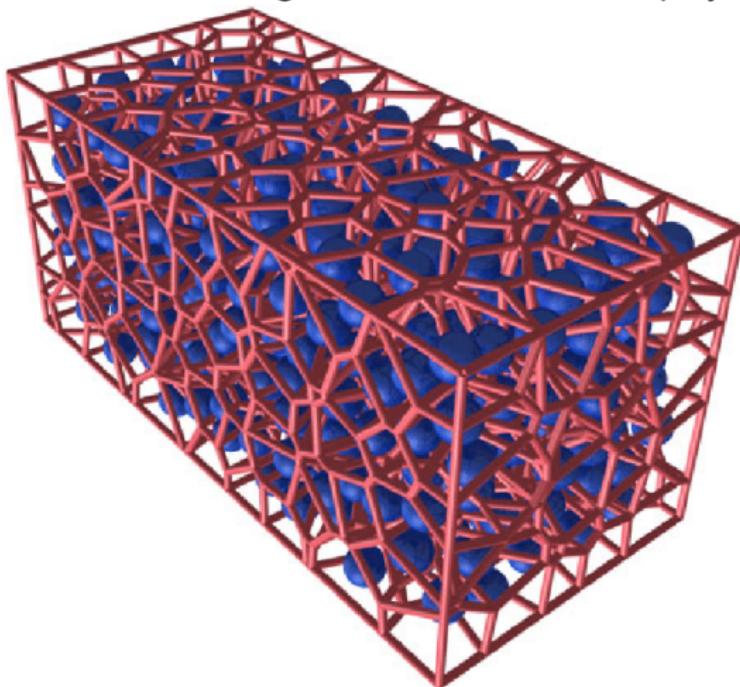
- Application: They find widespread applications in areas such as nearest neighbor queries for data structure problems in computational geometry, business applications such as determining where to locate a store so it is no closer to any existing store of its kind, epidemiology, geophysics, and meteorology .

Robot Path Planning: restricting a robot to traverse the edges created by the voronoi diagram



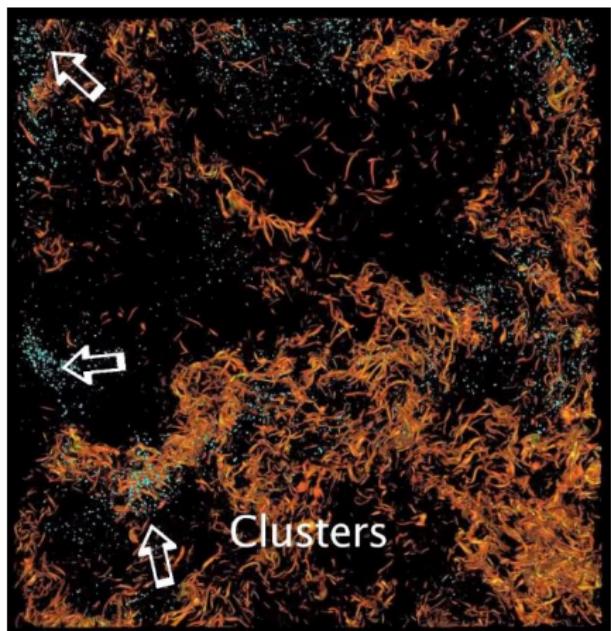
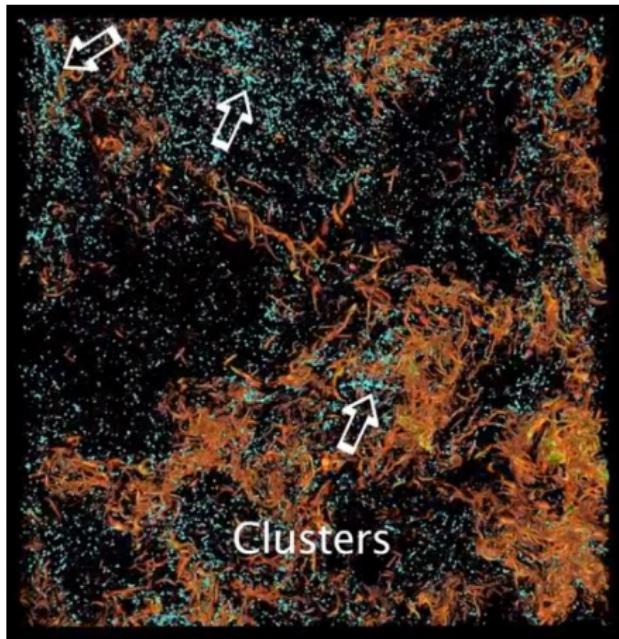
Clustering Analysis via Voronoï Tessellation

- A voronoi diagram records information about the distances between sets of points in any dimensional space.
- Higher Dimensions Voronoi Diagrams: Cells are convex polytopes



Clustering Analysis via Voronoï Tessellation

- Now that we are familiar with Voronoï Tessellation concept and particle clustering in turbulence, we are ready to analyze clusters.

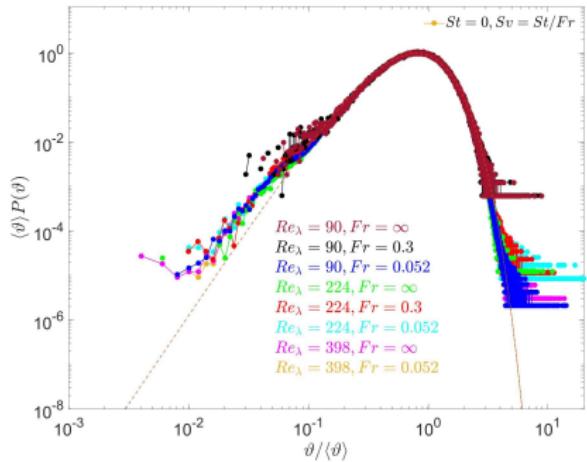


Clustering Analysis via Voronoï Tessellation

- Recall that for each simulation we write out the particles' position and this data serve as input for the 3D Voronoï analysis.
- We employ the 3D Voronoï diagrams on DNS simulations over a wide range of three control parameters R_λ , Fr and St . For each tuple (Re, Fr, St) , we analyze multiple (~ 25) snapshots (time step) of simulations to collect sufficient data for statistical convergence.
- Given the particles' position and box volume, an id (index) is assigned to each particle. The output of 3D Voronoï analysis is the cell volume as well as neighbors list for each particle.
- Considering the Voronoï volume as a random variable, we compute its probability distribution function (PDF) for different combinations of (Re, Fr, St) .

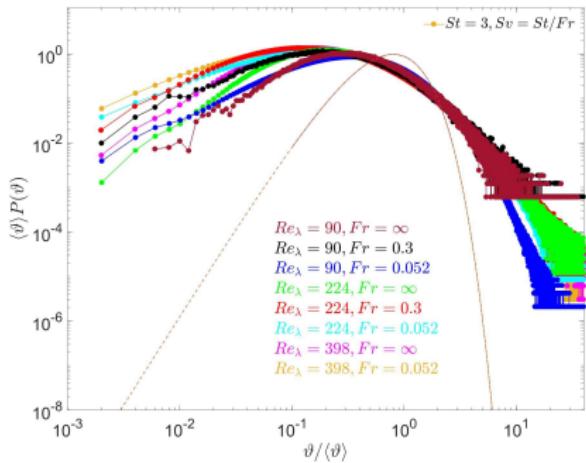
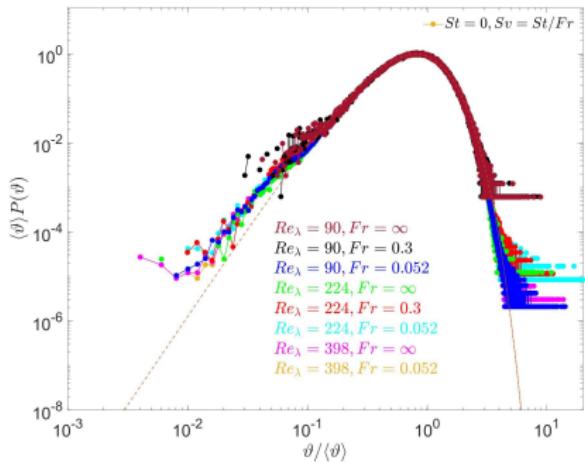
Clustering Analysis via Voronoï Tessellation

- Indeed, the local particle concentration field is represented by the inverse of the volume of Voronoï cells. The small/large Voronoï volumes represent the high/low concentration regions of the flow.



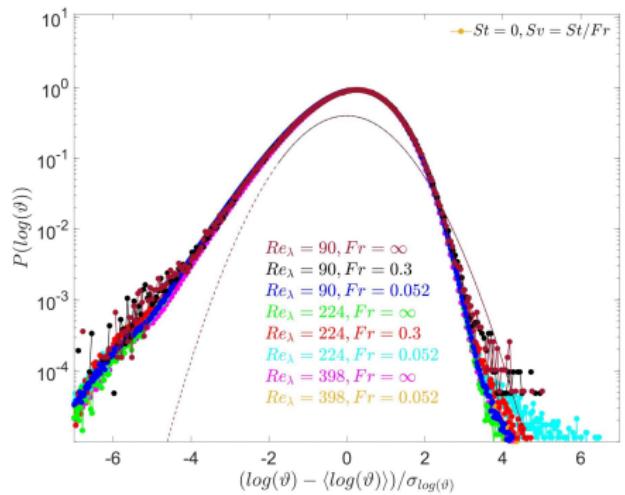
Clustering Analysis via Voronoï Tessellation

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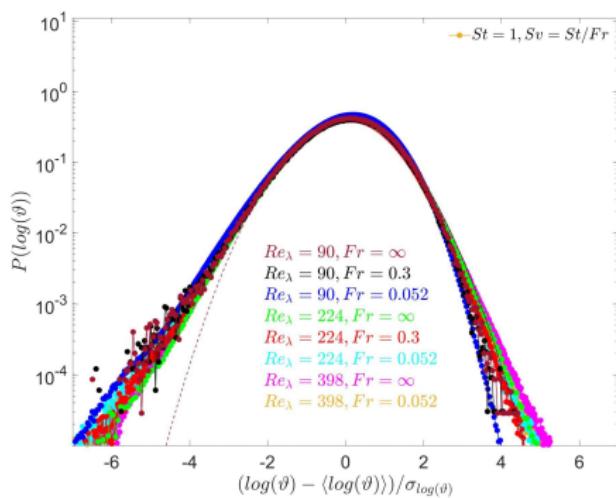
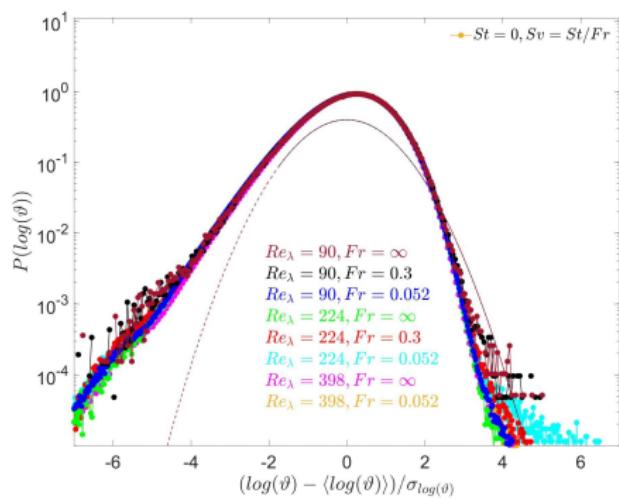
Clustering Analysis via Voronoï Tessellation

- In certain regimes, the PDF of Voronoï volumes follows a log-normal distribution!



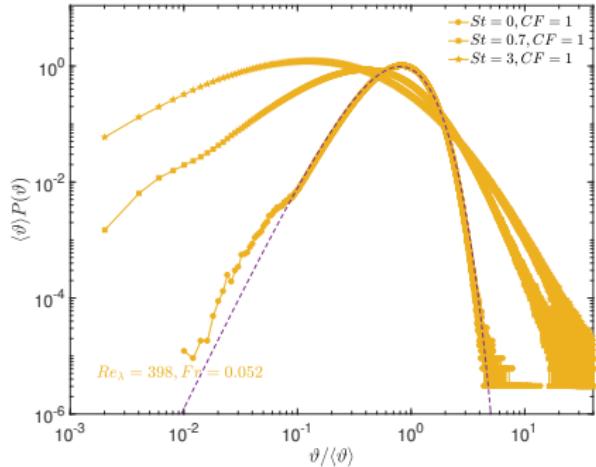
Clustering Analysis via Voronoï Tessellation

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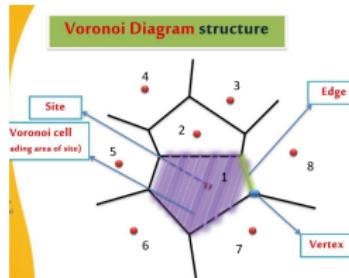


Clustering Analysis via Voronoï Tessellation

- The PDF of inertial particles intersect the RPP at two points, one is smaller and the other one is greater than the mode of RPP, which are denoted by ϑ_C and ϑ_v , respectively. These points serve as thresholds to detect clusters and voids.



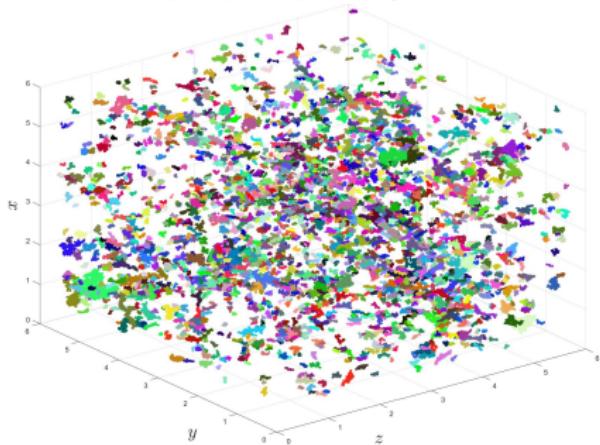
Clustering Analysis via Voronoï Tessellation



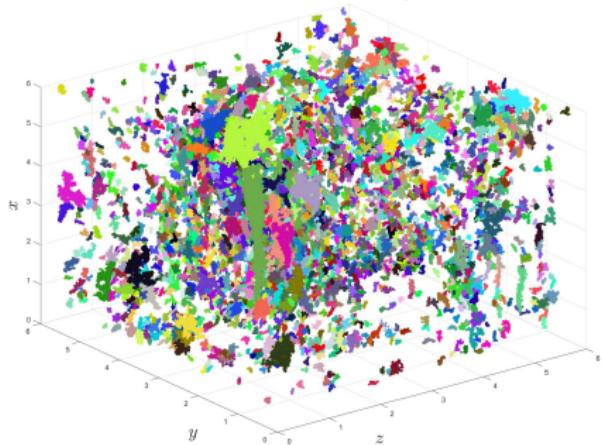
- We then consider the properties of particles in clusters, which are regions of connected Voronoï cells whose volume is less than a certain threshold.
- To detect the clusters in each simulation of (Re, Fr, St) , we first choose the particle ids that their cell volumes is smaller than the threshold (ϑ_C). These particles may form a cluster, if they are connected together.
- Then we run a searching algorithm to go through the neighbors of those particles and pick neighbors that also their cell volumes are smaller than the threshold.
- We continue this procedure recursively for the neighbors of neighbors of neighbors of ... until we find all the connected cells of clusters. For some cases it may take 12 days to find all the clusters of one snapshot of flow!

Clustering Analysis via Voronoï Tessellation

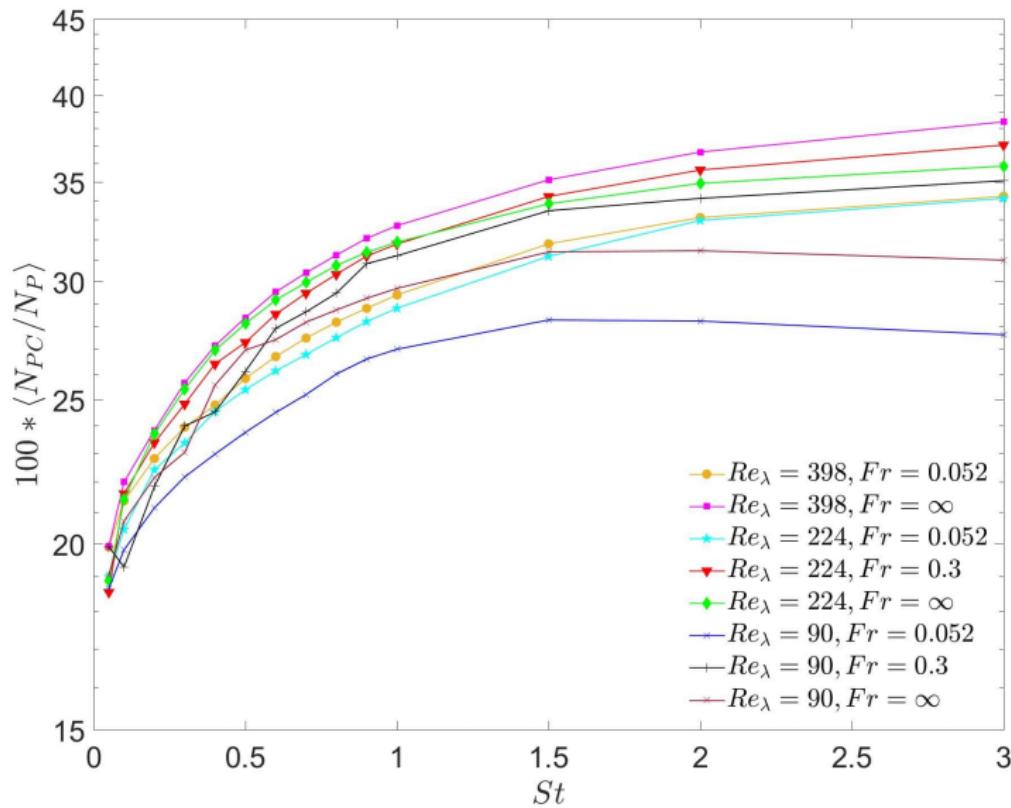
$Re_\lambda = 398, Fr = \infty, St = 3, Tstp = 112000$



$Re_\lambda = 398, Fr = 0.052, St = 3, Tstp = 112000$

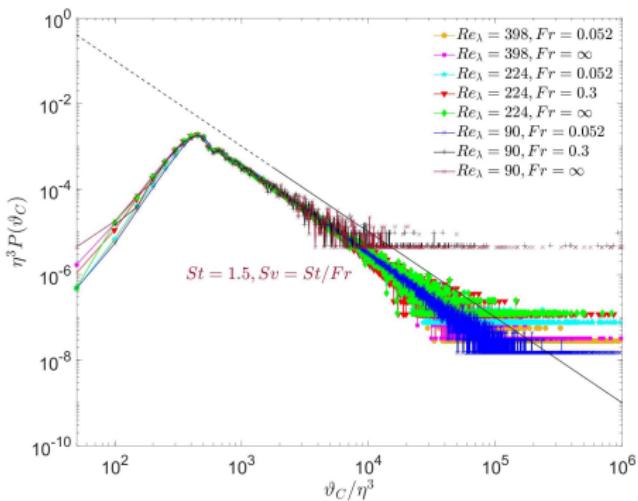
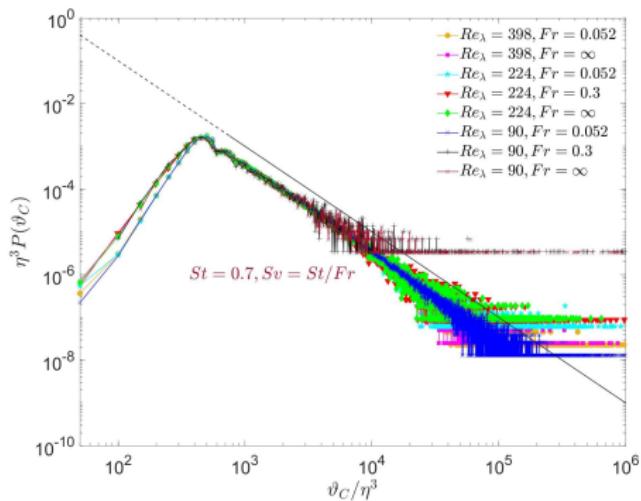


Clustering Analysis via Voronoï Tessellation



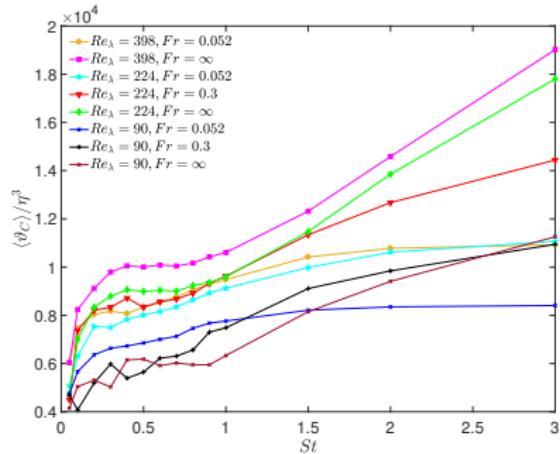
Clustering Analysis via Voronoï Tessellation

- Volume of each cluster is sum of the Voronoï volumes of its constituent particles. Let's see how the PDF of cluster volumes behaves:



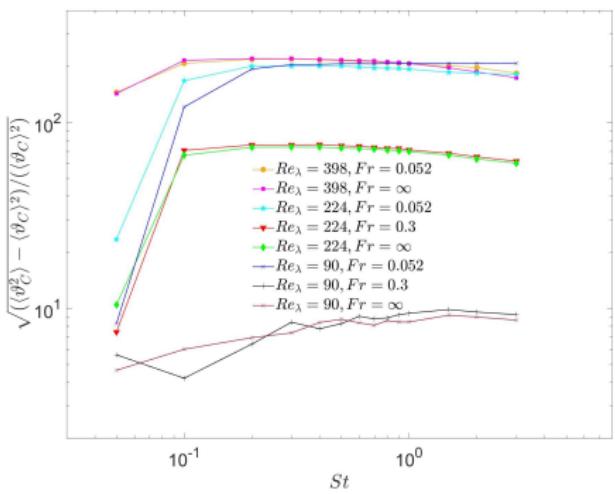
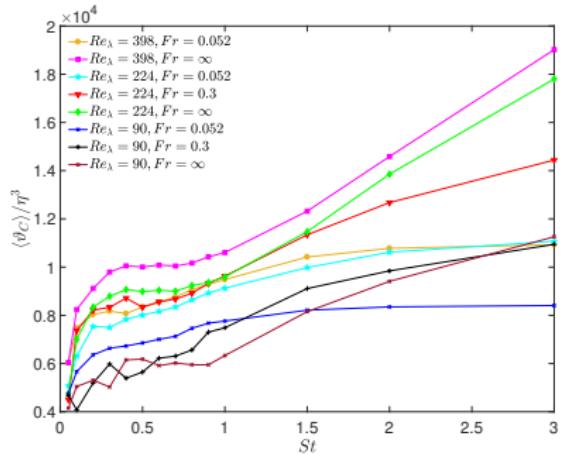
Clustering Analysis via Voronoï Tessellation

- How about the average (first moment) size and the standard deviation (second moment) of clusters?



Clustering Analysis via Voronoï Tessellation

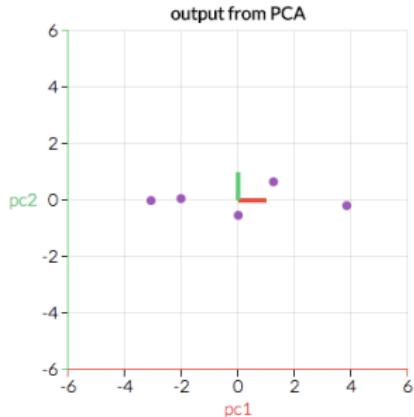
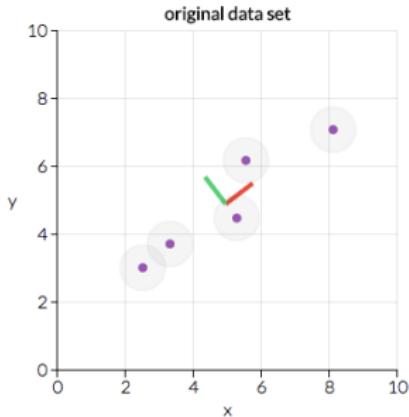
- How about the average (first moment) size and the standard deviation (second moment) of clusters?



Summary

- Particle-laden flows have a wide variety of applications both in nature and industry.
- The goal of DNS is to understand the underlying physics rather than direct numerical prediction in real-world turbulence.
- Voronoï tessellation is a powerful tool to obtain local information on the spatial data.
- Different properties of particles and turbulent flow have a unique effect on the topology of clusters.

PCA (Principal Component Analysis)



- A new representation of the dataset in a way that the new features are statistically uncorrelated. Indeed, each of the “new” variables after PCA are all independent of one another.
- The algorithm proceeds by finding the main directions in the dataset (directions of maximum variance).
- The correlation matrix of the transformed dataset is zero except for the diagonal.

Thank You

Backup slides: DNS table

Parameter	DNS 1	DNS 2	DNS 3	DNS 4
N	128	128	1024	512
R_λ	93	94	90	224
Fr	∞	0.3	0.052	∞
\mathcal{L}	2π	2π	16π	2π
ν	0.005	0.005	0.005	0.0008289
ϵ	0.324	0.332	0.257	0.253
l	1.48	1.49	1.47	1.40
l/η	59.6	60.4	55.6	204
u'	0.984	0.996	0.912	0.915
u'/u_η	4.91	4.92	4.82	7.60
T_L	1.51	1.50	1.61	1.53
T_L/τ_η	12.14	12.24	11.52	26.8
$\kappa_{\max}\eta$	1.5	1.48	1.61	1.66
N_p	262,144	262,144	16,777,216	2,097,152

Parameter	DNS 5	DNS 6	DNS 7	DNS 8
N	512	1024	1024	1024
R_λ	237	230	398	398
Fr	0.3	0.052	∞	0.052
\mathcal{L}	2π	4π	2π	2π
ν	0.0008289	0.0008289	0.0003	0.0003
ϵ	0.2842	0.239	0.223	0.223
l	1.43	1.49	1.45	1.45
l/η	214	213	436	436
u'	0.966	0.914	0.915	0.915
u'/u_η	7.82	7.7	10.1	10.1
T_L	1.48	1.63	1.58	1.58
T_L/τ_η	27.36	27.66	43.0	43.0
$\kappa_{\max}\eta$	1.62	1.68	1.60	1.60
N_p	2,097,152	16,777,216	2,097,152	2,097,152

Reynolds-number effects on inertial particle dynamics. Part I

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	Simulation	I	II	III	IV	V
R_λ	88	140	224	398	597	
ν	0.005	0.002	0.0008289	0.0003	0.00013	
ϵ	0.270	0.267	0.253	0.223	0.228	
\mathcal{L}	1.46	1.41	1.40	1.45	1.43	
l/η	55.8	107	204	436	812	
u'	0.914	0.914	0.915	0.915	0.915	
u'/u_η	4.77	6.01	7.60	10.1	12.4	
T_L	1.60	1.54	1.53	1.58	1.57	
T_L/τ_η	11.7	17.7	26.8	43.0	65.4	
T/T_L	15.0	10.4	11.4	11.1	5.75	
$\kappa_{\max}\eta$	1.59	1.59	1.66	1.60	1.70	
N	128	256	512	1024	2048	
N_p	262,144	262,144	2,097,152	16,777,216	134,217,728	
N_{tracked}	32768	32768	262,144	2,097,152	16,777,216	
N_{proc}	16	16	64	1024	16,384	

TABLE I. Flow parameters for the DNS study. All dimensional parameters are in arbitrary units and all statistics are averaged over time T . All quantities are defined in the text in §§ 2.1 and 2.2.

Reynolds Number

$$Re = \frac{\text{Inertia Force}}{\text{Viscous Force}} = \frac{\rho \cdot u \cdot L}{\mu} = \frac{u \cdot L}{v}$$

- ρ is the density of the fluid (SI units: kg/m^3)
- u is the velocity of the fluid with respect to the object (m/s)
- L is a characteristic linear dimension (m)
- ↓ μ is the dynamic viscosity of the fluid ($\text{Pa}\cdot\text{s}$ or $\text{N}\cdot\text{s}/\text{m}^2$ or $\text{kg}/\text{m}\cdot\text{s}$)
- ↓ v is the kinematic viscosity of the fluid (m^2/s)

Turbulent Flow
(Chaotic)
 $Re > 4,000$



Transient Flow
(Little of Both)
 $2,300 < Re < 4,000$

Laminar Flow
(Orderly)
 $Re < 2,300$



Clustering Analysis via Voronoï Tessellation

- Given the Voronoï volumes, the clustering of inertial particles is explored by comparing the PDF of inertial particles ($St > 0$) with the fluid particles ($St = 0$).
- The fluid particles always follow the streamlines, have a uniform random distribution and their Voronoï tessellation PDF is unique (Random Poisson process or RPP).
- We then consider the properties of particles in clusters, which are regions of connected Voronoï cells whose volume is less than a certain threshold.