Data Analysis of Particle Clustering in Turbulence

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

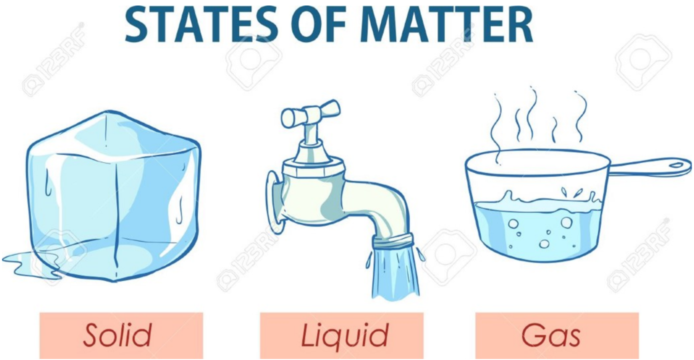
Machine Learning and Data Mining (STA 325L-001) course Fall 2019

Outline

- Turbulence
- Particle Clustering
- Clustering Analysis (or Unsupervised Learning) via Voronoï Tessellation
- Data Expedition Task

Turbulence

- Fluids, liquids and gases, have the ability to flow.
- Fluid mechanics: the study of how fluids move and the forces on them!



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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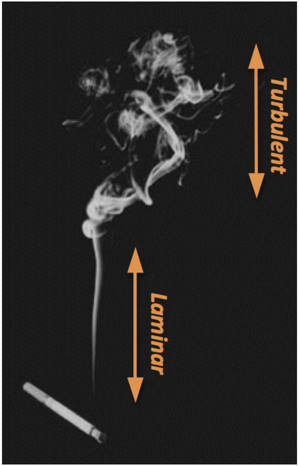
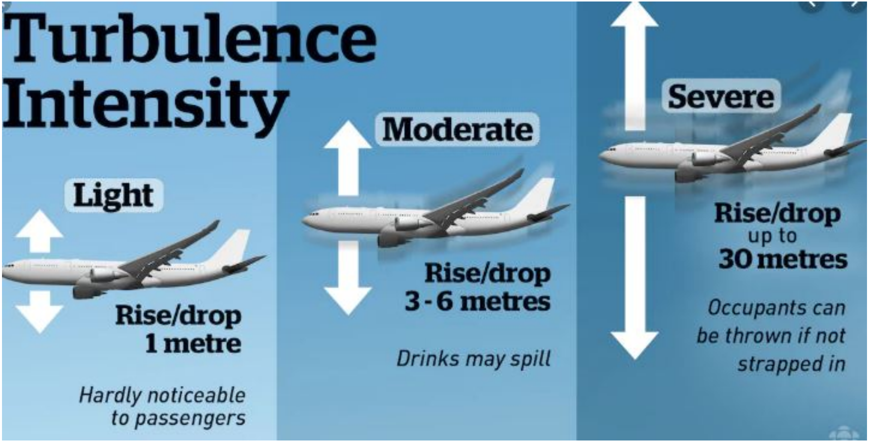


- Laminar flow is orderly, regular, predictable.
- Turbulent flow looks random, chaotic, irregular, unpredictable (depending on the intensity of turbulence).

Turbulence

Example: Airplane Turbulence.



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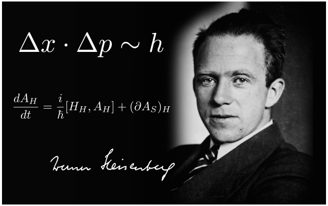

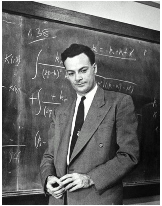

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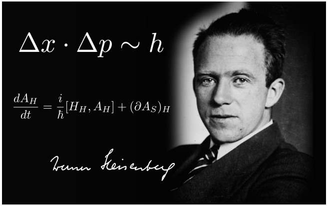
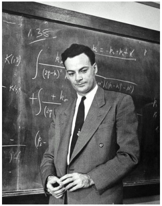
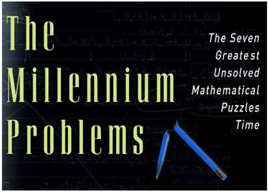
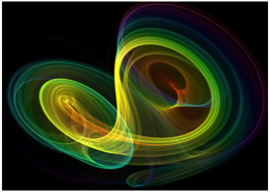




Feynman: “turbulence is the last great unsolved problem in classical physics”.

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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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.

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So there are two aspects to solving these problems: **Understanding (inference)** and **Prediction**.

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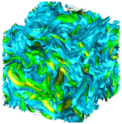
So there are two aspects to solving these problems: **Understanding (inference)** and **Prediction**.

THEORY

- Phase space analysis.
- Non-equilibrium statistical physics.
- Asymptotic methods & perturbation theory.
- Dynamical systems theory.

HPC

- Direct Numerical Simulation.



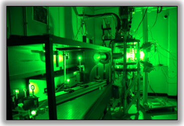
MODELING

- Simplified models that capture all scales of the problems.

GOALS

- Advance our *fundamental understanding* of the problems.
- Use this to guide the development of *simplified predictive models.*

EXPERIMENTS



Particle Clustering in Turbulent Flow

Particle-laden turbulent flows appear in a diverse range of engineering systems and natural phenomena.

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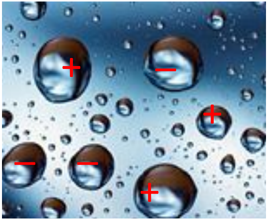

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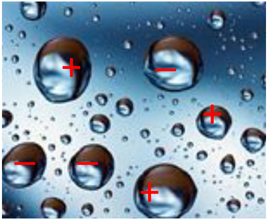

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How do the electric forces compete with the turbulent air to control the particle collisions and mixing rates?

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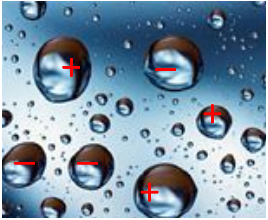

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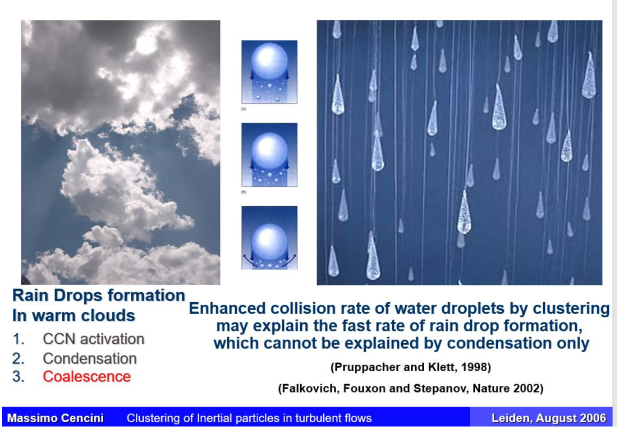
How do the electric forces compete with the turbulent air to control the particle collisions and mixing rates?

What are the implications for the electrodynamics of clouds?

Particle Clustering in Turbulent Flow

Problem of interest: rain formation



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

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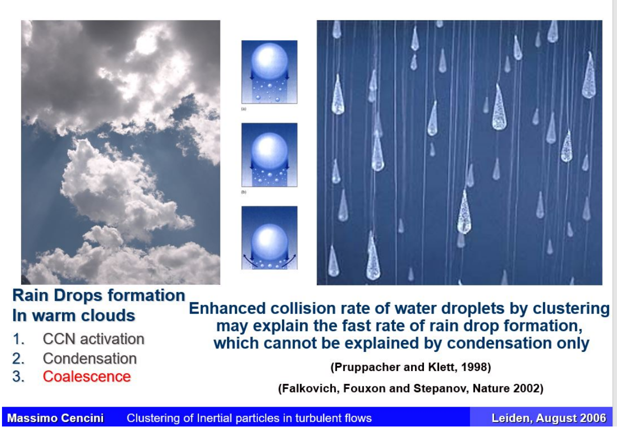

- Indeed, inertial particles are distributed non-uniformly in the turbulent flow. In addition, the presence of gravity results in finite settling velocities of inertial particles

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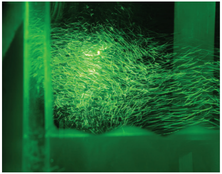
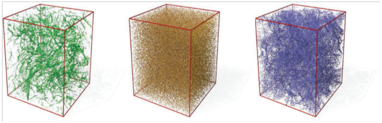
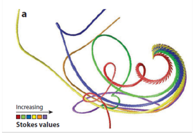


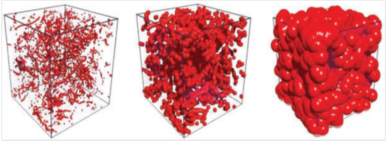
Fluid Streamlines (Polystyrene spheres 25 μm in diameter are used as **tracers** in experiments and illuminated by a laser with)



Snapshots of particle distributions in a turbulent flow field

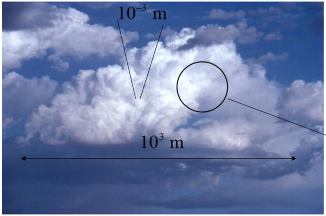


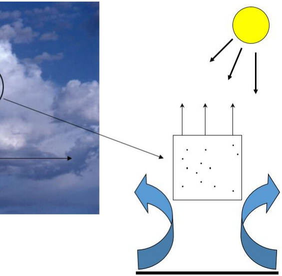
Inertial particles trajectories



- 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.

Turbulence in Clouds





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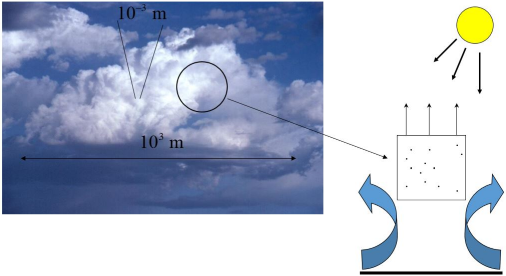

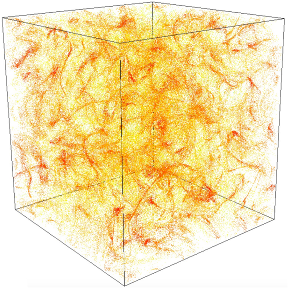

- We employ Direct Numerical Simulations (DNS) to model turbulent flow and track particles lying under an idealized turbulence in a cubic box.

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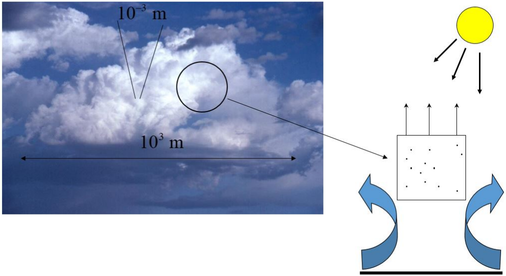

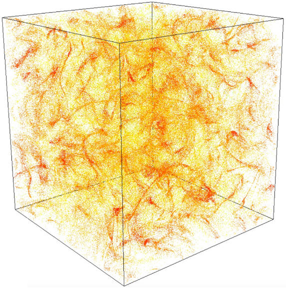

- In these simulations, three independent control parameters representing the properties of turbulent flow and particles are varied and particles' position and other dynamical properties of particles and flow fields (e.g. velocity) are stored.

Particle Clustering in Turbulent Flow

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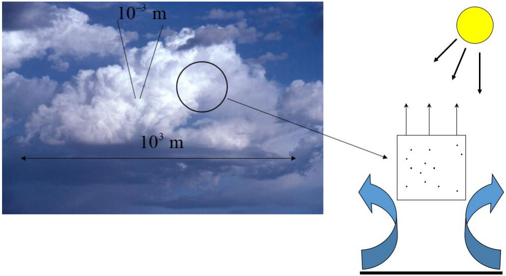
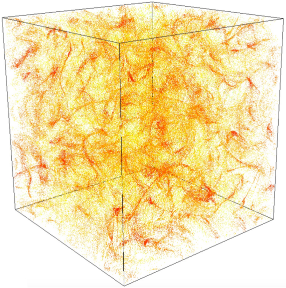
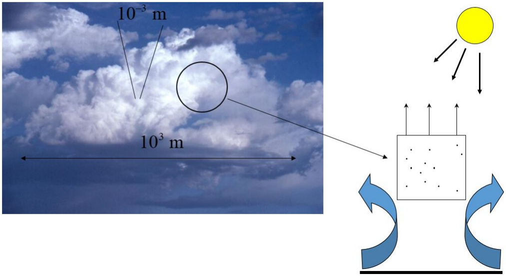


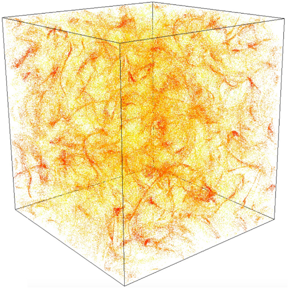


- More specifically, we want to explore how intensity of turbulence (quantified by Reynolds number or Re), gravitational acceleration (quantified by Froud number or Fr) and particles' characteristics (e.g. size, density which is quantified by Stokes number or St) affect the spatial distribution and clustering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

- High-resolution numerical simulation of the turbulent flow field can be achieved by employing direct numerical simulation (DNS) of Navier-Stokes equations (conservation of mass and momentum) which can resolve all scales of motion.

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

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- DNS is computationally prohibitive and cannot be applied to simulate flow at large Reynolds numbers.
- Reynolds Number (Re), quantifies the intensity of a turbulent flow.

Particle Clustering in Turbulent Flow

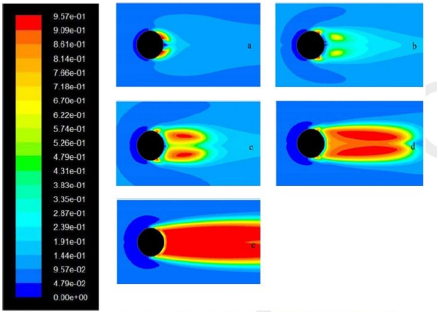
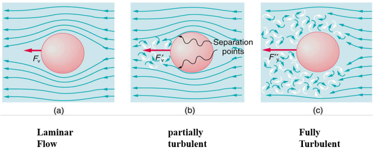


FIG. 11: Contour of void fraction around the cylinder for (a) $\mathrm{Re}_{TP} = 1{,}000$, (b) $\mathrm{Re}_{TP} = 3{,}162$, (c) $\mathrm{Re}_{TP} = 10{,}000$, (d) $\mathrm{Re}_{TP} = 31{,}623$, and (e) $\mathrm{Re}_{TP} = 100{,}000$.



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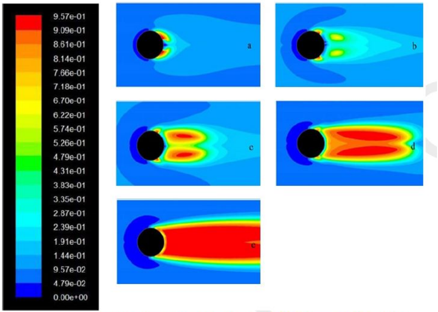

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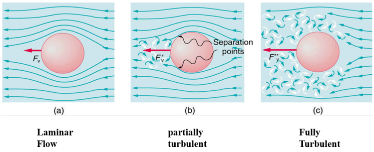
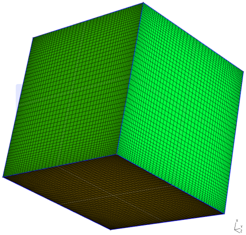


- In the real problems of interest, oceanic and atmospheric turbulent flow, the Re is very large ($O(10^7)$ or more).
- We use DNS over a range of Re to look for trends in the behavior. This can provide insight regarding the extent to which results obtained at low/moderate Re might be extrapolated the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

Particle Clustering in Turbulent Flow



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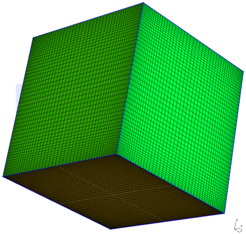

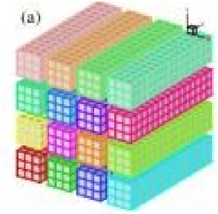

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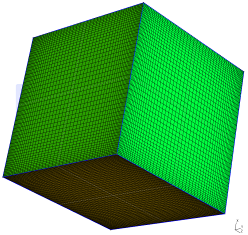
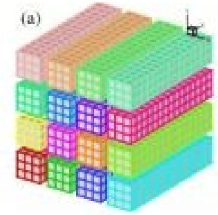
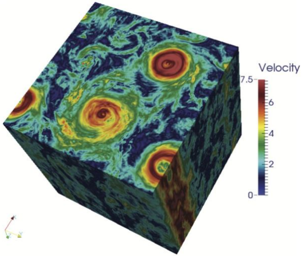
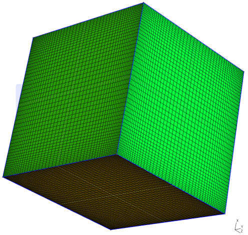


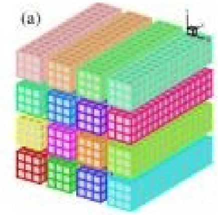


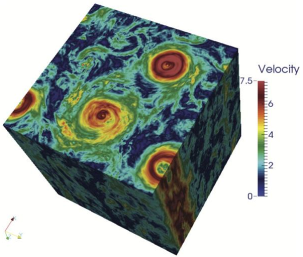


- Turbulent flow property: Our DNS study considers $R_\lambda = 90, 224, 398$, where $R_\lambda \equiv u'\lambda/\nu$.
- The higher the Re, the higher the resolution (more grid points; $N_g = 128^3$, $N_p = 16$ for $R_\lambda = 90$ versus $N_g = 1024^3$, $N_p = 1024$ for $R_\lambda = 398$; 2 days versus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

Particle Clustering in Turbulent Flow







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- particle tracking:

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

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.

Particle Clustering in Turbulent Flow

- 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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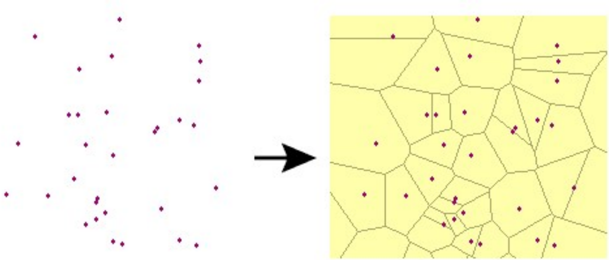
Clustering Analysis via Voronoï Tessellation

- Voronoi diagrams are used to understand patterns over an area of interest.



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

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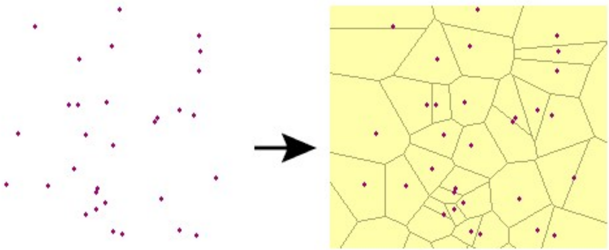

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- After collecting data points and recording their location, the plane can be divided into sections, or Voronoi cells, that are representative of each data point.

- 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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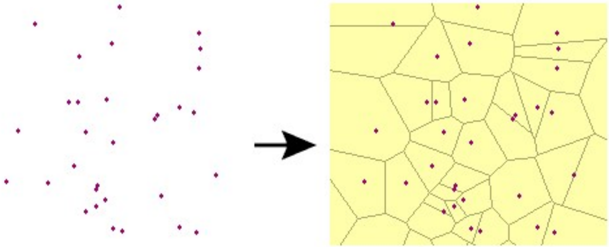

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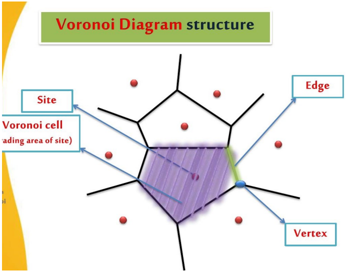
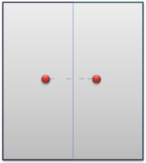


Clustering Analysis via Voronoï Tessellation

- 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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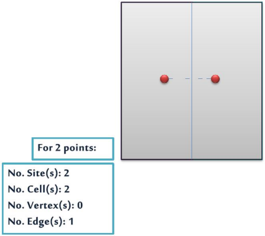

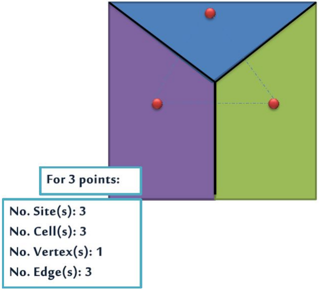

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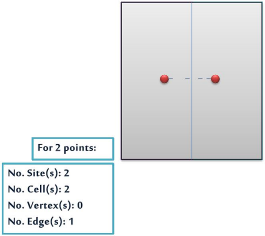

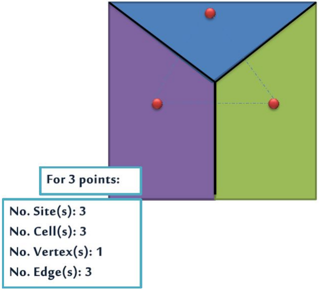

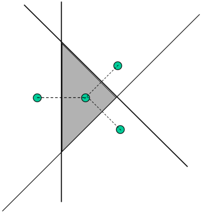

Clustering Analysis via Voronoï Tessellation

- 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 .

Clustering Analysis via Voronoï Tessellation

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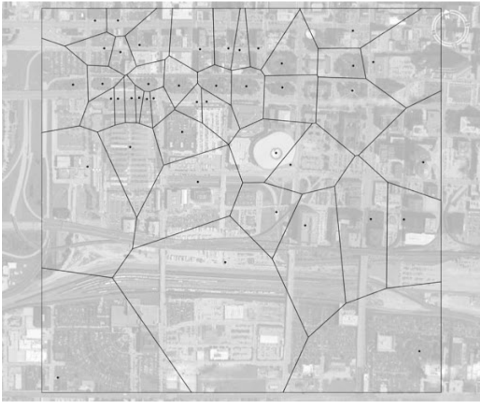
  City Planning: one can easily determine where is the nearest shop or hospital, and urban planners can study if certain area need a new hospital



Clustering Analysis via Voronoï Tessellation

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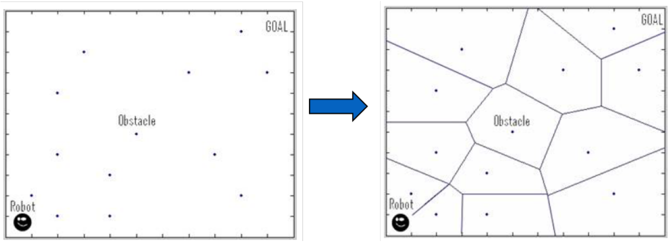
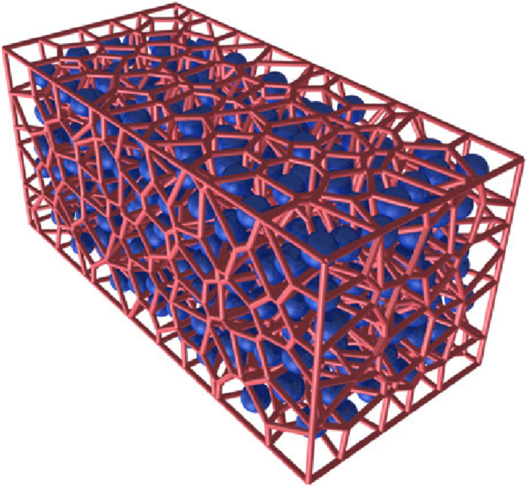
  Robot Path Planning: restricting a robot to traverse the edges created by the voronoi diagram



Clustering Analysis via Voronoï Tessellation

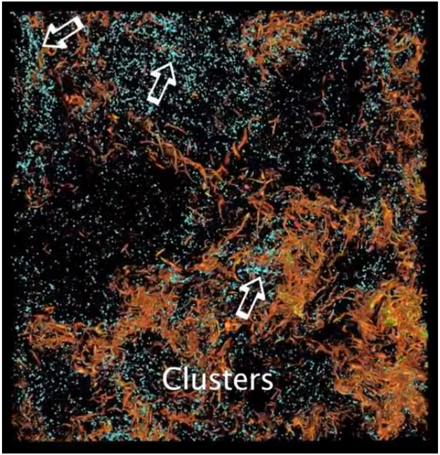
- A voronoi diagram records information about the distances between sets of points in any dimensional space.

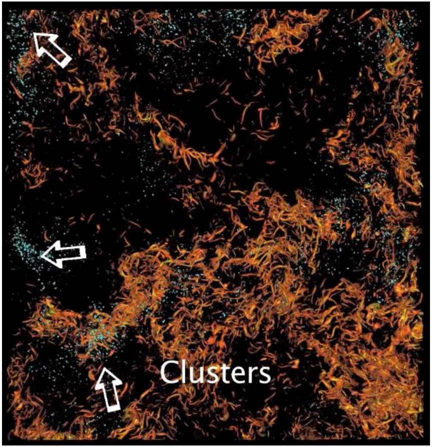
- Higher Dimensions Voronoi Diagrams: Cells are convex polytopes



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.

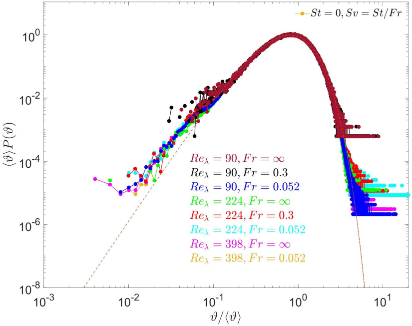




Clustering Analysis via Voronoï Tessellation

- 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).

- 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.



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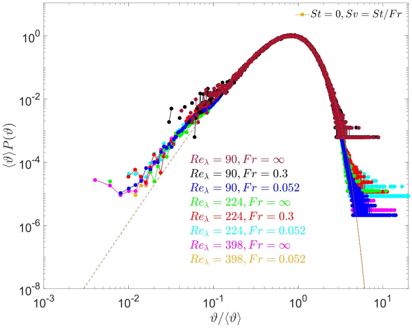
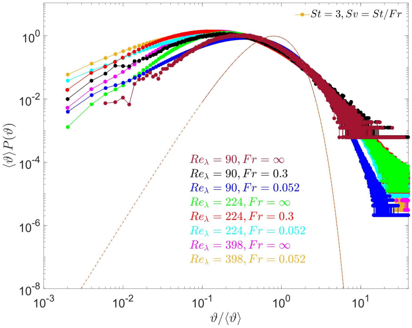
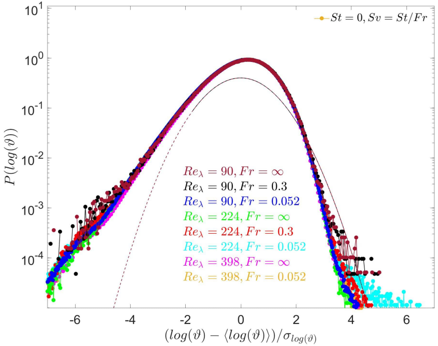




Clustering Analysis via Voronoï Tessellation

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



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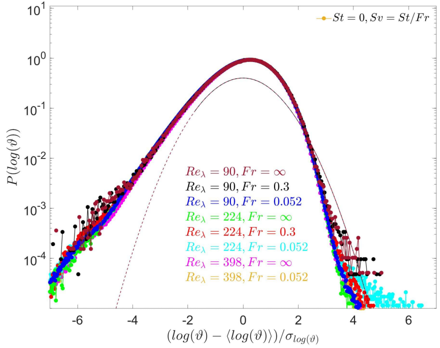
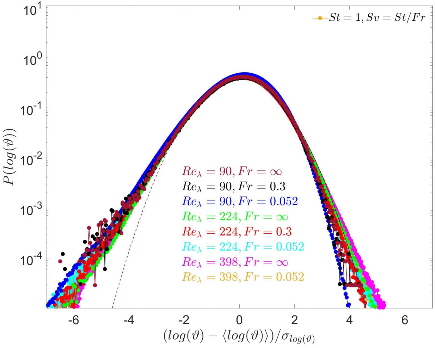
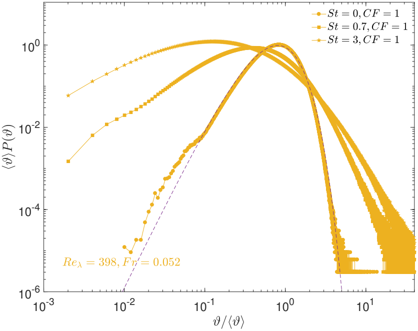


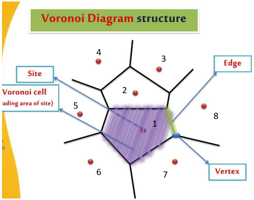


Clustering Analysis via Voronoï Tessellation

- 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.

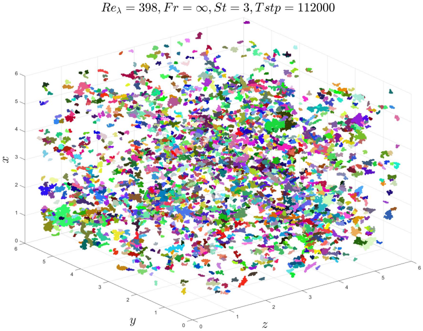


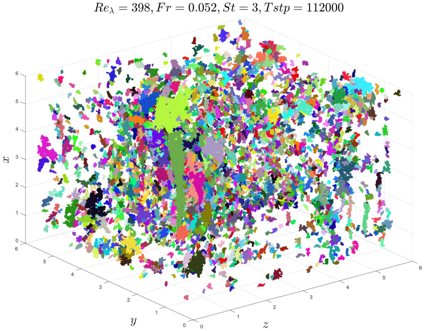
Clustering Analysis via Voronoï Tessellation



- 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!

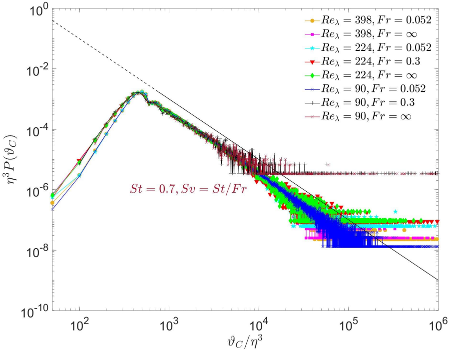
Clustering Analysis via Voronoï Tessellation

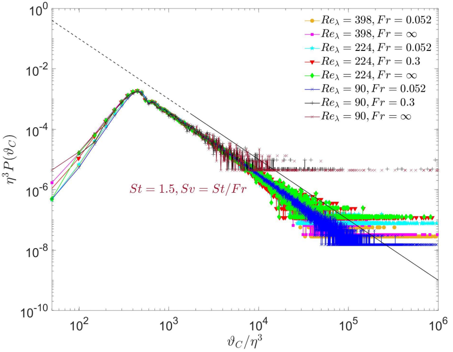




Clustering Analysis via Voronoï Tessellation

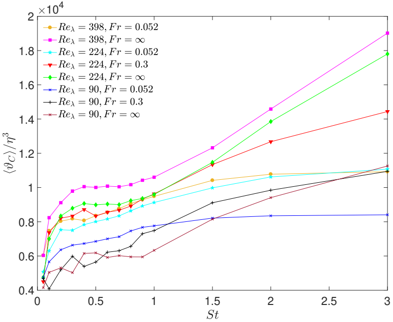
- Volume of each cluster is sum of the Voronoï volumes of its constituent particles. Let's see how the PDF of cluster volumes behaves:





Clustering Analysis via Voronoï Tessellation

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



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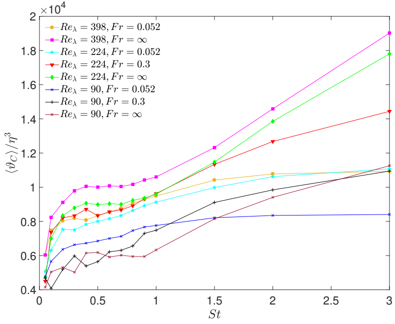
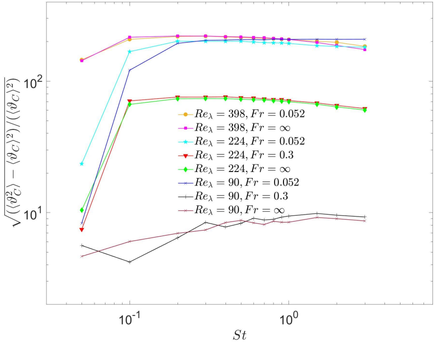




Data Expedition task

- Given the first four moments of cluster volumes for 112 tuple of (Re, Fr, st), build a supervised machine learning model that take a tuple and outputs the first four moments.

	A	B	C	D	E	F	G	H	I	J
1	St	Re	Fr	Sv	eta	u_eta	R_moment_1	R_moment_2	R_moment_3	R_moment_4
2	0	398	0	1	0	0.09	0.00022182	0.0010347	0.011354	0.12509
3	0	398	0	2	0	0.09	0.00027479	0.0032549	0.058006	1.0344
4	0	398	0	4	0	0.09	0.0002954	0.0041561	0.079922	1.5377
5	0	398	0	6	0	0.09	0.00030066	0.0043488	0.083446	1.6023
6	0	398	0	8	0	0.09	0.00029691	0.0041375	0.076124	1.4014
7	1	398	0	10	0	0.09	0.00030716	0.0043494	0.080143	1.477
8	1	398	0	12	0	0.09	0.00031431	0.0044672	0.08206	1.5077


Thank You

Backup slides: DNS table

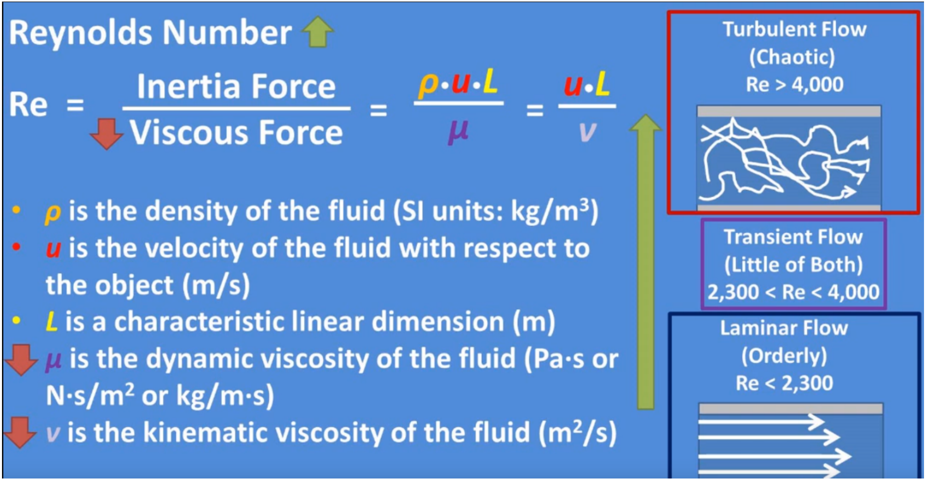
Parameter	DNS 1	DNS 2	DNS 3	DNS 4
N	128	128	1024	512
R_λ	93	94	90	224
Fr	∞	0.3	0.052	∞
$\mathscr{L}$	2π	2π	16π	2π
ν	0.005	0.005	0.005	0.0008289
ϵ	0.324	0.332	0.257	0.253
l	1.48	1.49	1.47	1.40
l/η	59.6	60.4	55.6	204
u'	0.984	0.996	0.912	0.915
u'/u_η	4.91	4.92	4.82	7.60
T_L	1.51	1.50	1.61	1.53
T_L/τ_η	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
$\mathscr{L}$	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 1 621

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
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
$k_{max}\eta$	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
$N_{tracked}$	32 768	32 768	262 144	2 097 152	16 777 216
N_{proc}	16	16	64	1024	16 384

TABLE 1. 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.

Backup slides: Re number



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.