Direct Lagrangian tracking simulations of droplet growth in clouds

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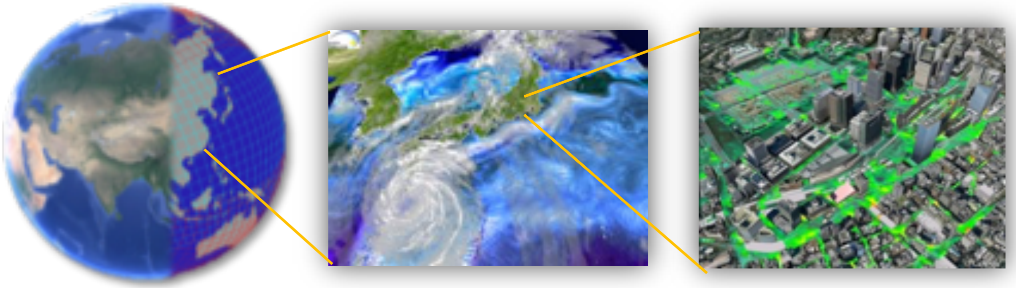
Brief introduction of ESRG activity

- We choose research themes, in Marine–Earth science, that are interesting in physics and challenging in computation.

Our research themes are often related with **turbulence**.

Atmosphere-Ocean coupled multiscale model:

Multi-Scale Simulator for the Geoenvironment (MSSG)

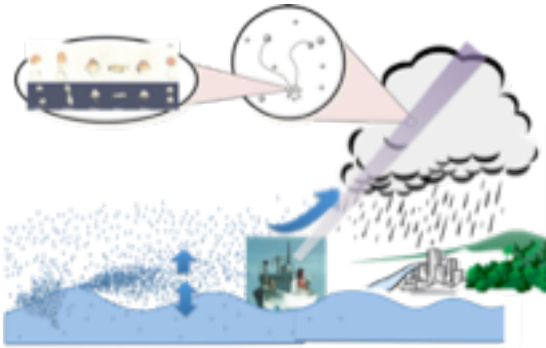


global scale	regional sale	street scale
O(1~10 km) resolution	O(100 m~1km) resolution	O(1~10 m) resolution

- ➢ Seamless simulations for global, regional and street scales
- ➢ atmosphere-ocean coupled

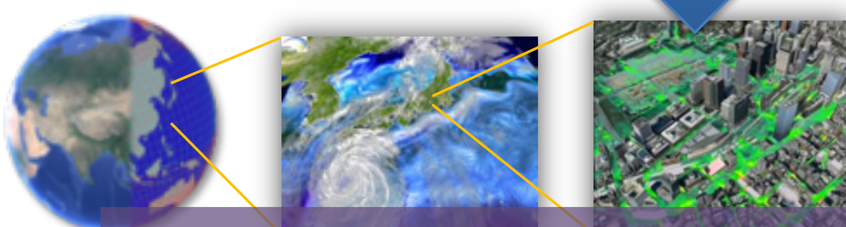
This movie is displayed at the Japan Science Museum (Miraikan) in Tokyo.

Group Mission



Research and Modeling of multiscale, multiphase and non-equilibrium turbulence processes in marine and Earth science

Apply



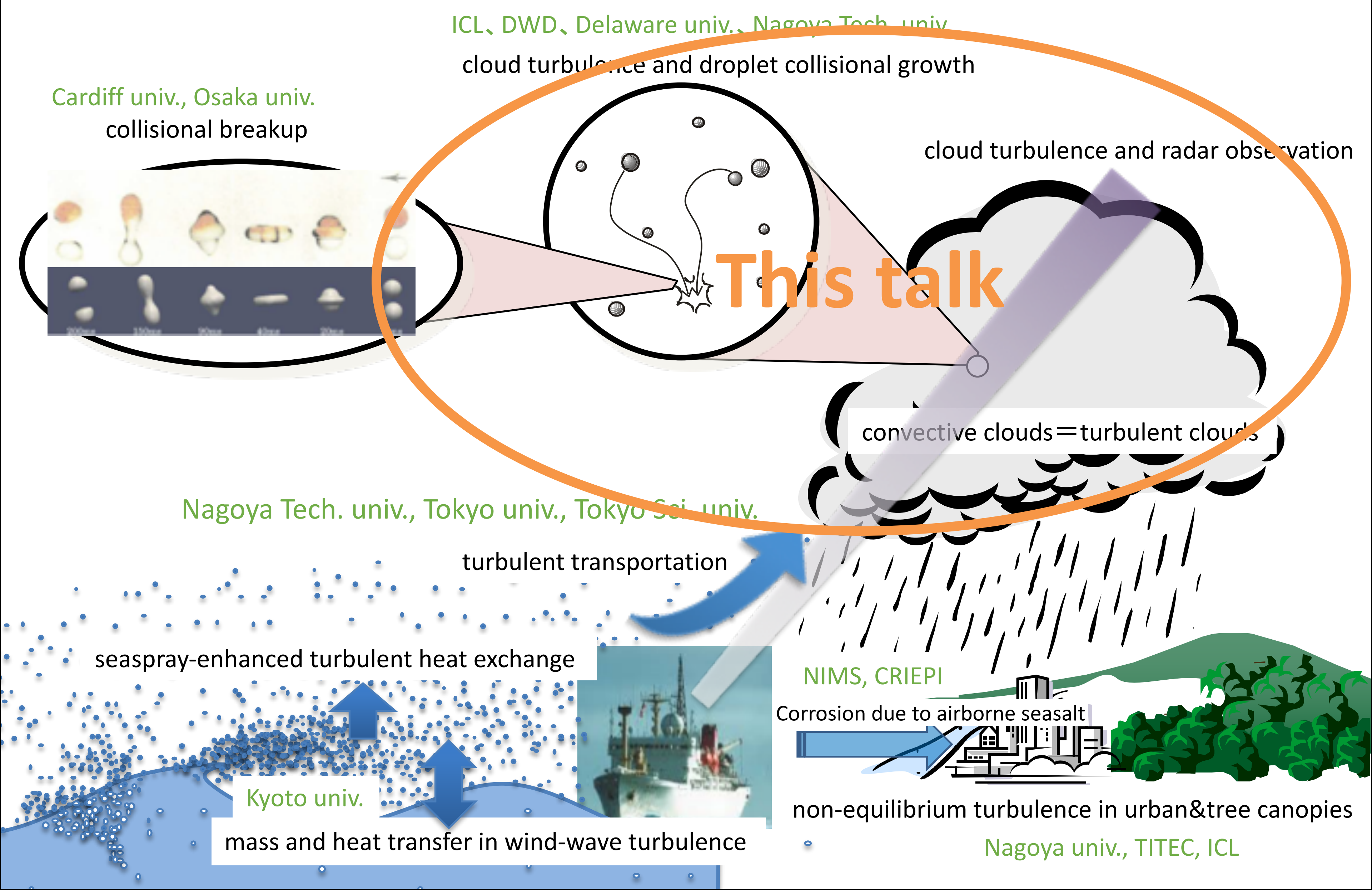
Development of Multi-scale weather/climate model : **MSSG**

+ IoT + AI

Social Implementation

Promotion of Marine and Earth informatics

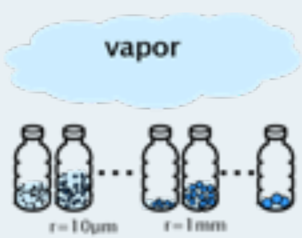
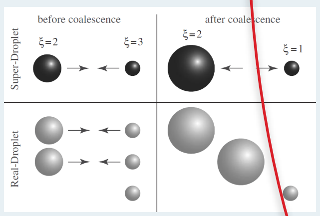
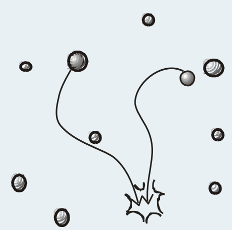
Multiscale, multiphase and non-equilibrium turbulence processes in marine and Earth Science



Contents

- Cloud microphysics simulations
  - Eulerian and Lagrangian frameworks
  - Droplet growth in clouds
- Direct Lagrangian tracking simulations
  - Turbulent collision kernels
  - Droplet collision growth in box turbulence
  - Droplet growth in a vertically-developing cloud
- Miscellaneous (on-going work)
  - Size-resolving simulation
  - Turbulence influence on Radar reflectivity

Cloud microphysics schemes

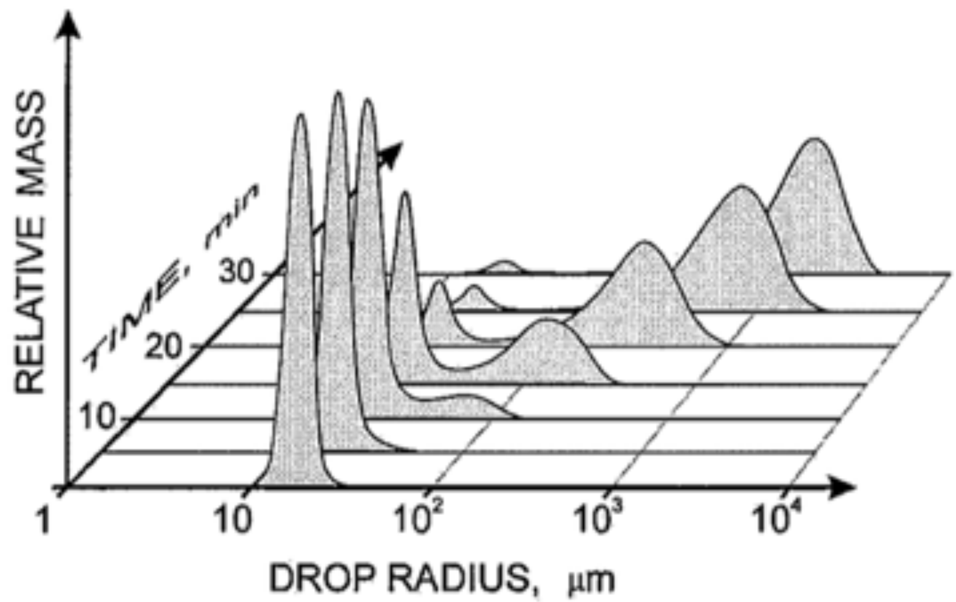
	Euler framework		**Lagrangian framework**	
Method	**Bulk**	**Bin**	**Super-Droplet**	**Direct**
Prognosed variables	Moments of size distribution $M_k^n = \int m^n f_k(m)dm$		Particle attributions $\boldsymbol{x_p}$, $\boldsymbol{u_p}$, r_p etc…	
Size distribution	Implicit	Explicit	Explicit	
Num. of Categories	<10	O(10~100)	--	
Multiplicity	--		1≦	1 (direct)
Illustration				
References	Many	Many (incl. Onishi & Takahashi(2012) JAS)	Shima et al. (2009) QJRMS	Onishi et al. (2015) JAS; Gotoh et al. (2016) NJP

Lagrangian cloud model

DIRECT Lagrangian cloud model

Droplet growth in clouds

- Activation
- Condensation/evaporation
- Collision (coagulation) →challenging in HPC
- Settling(Precipitation)

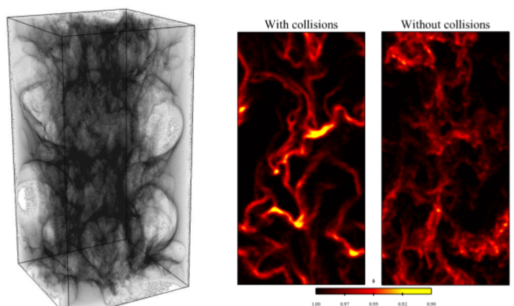


e.g., Shaw (2003) Annu. Rev. Fluid Mech.

Turbulent collisions of inertial particles

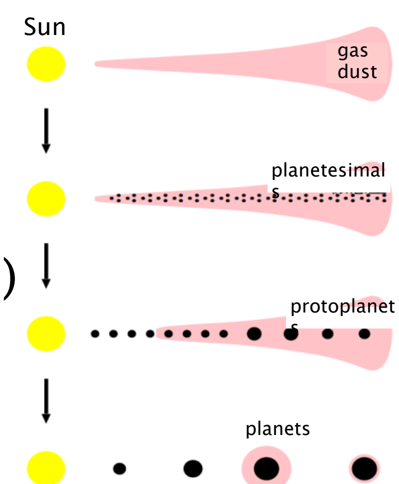
- Quick rain formation in turbulent clouds
  (refs: Shaw (2003), Grabowski & Wang (2013), etc…)

- Industrial flows
  e.g., spray combustion, pulverized coal combustion



http://www.colorado.edu/MCEN/cmes

- Dust growth in protoplanetary disks
  (refs: Pan et al. (2011), Okuzumi et al. (2012) etc…)

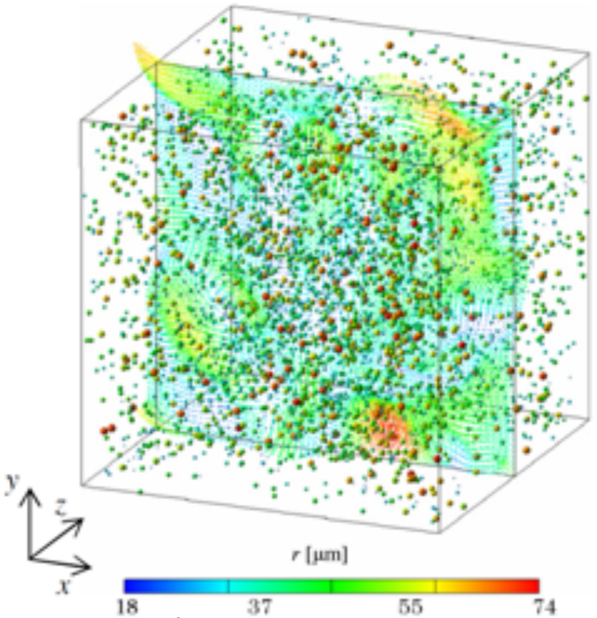


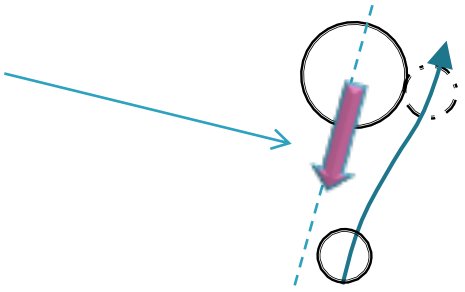
http://www-tap.scphys.kyoto-u.ac.jp/hayashi/lectures/kokubo.pdf

LCS(=Lagrangian Cloud Simulator)

(1)Onishi et al. (2011) *J. Comput. Phys.*
(2)Onishi et al. (2013) *J. Comput. Phys.*
(3)Onishi et al. (2015) *J. Atmos. Sci.*

- Flow
  - 4th-order FDM
  - 2nd-order R-K
  - RCF(1): large-scale forcing
  - 3D domain decomposition
- Particles
  - Lagrangian tracking
  - 2nd-order R-K
  - Cell-index method
  - BiSM(2) for hydrodynamic interaction
  - 3D domain decomposition



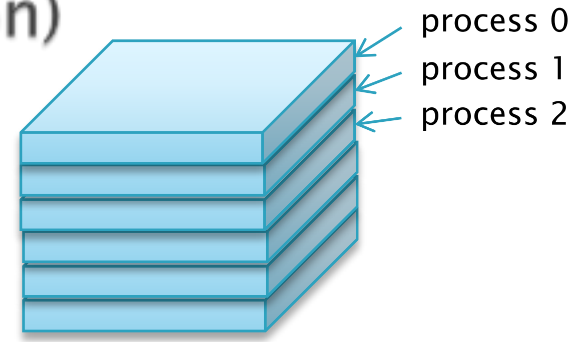


Following the so-called hybrid DNS approach
(Wang et al. 2005; Ayala et al. 2007)

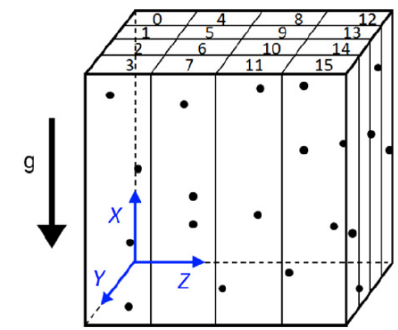
Domain Decomposition

(for distributed-memory parallelization)

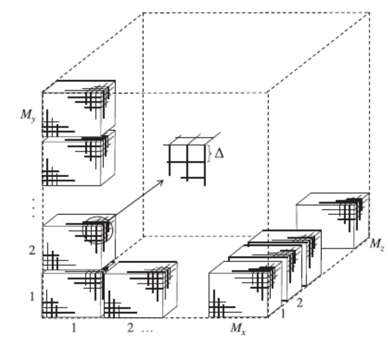
- 1D domain decomposition



- 2D domain decomposition

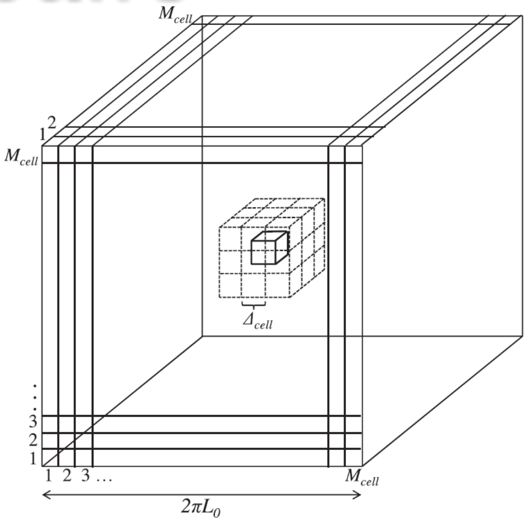


- 3D domain decomposition



2D or 3D dd is required for HPC.

Cell index method for detecting neighboring pairs



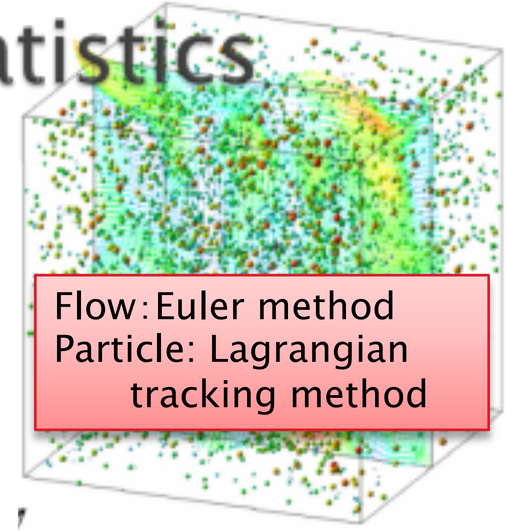
- Originally developed for MD simulation.

- (1)Divide computational domain is into cells.
- (2)Make the list that shows which particle locates in which cell.
- (3)Detect pairs in 27 cells* using the cell index.

*14 cells are enough for sequential procedure

This method can reduce the cost for detecting neighboring pairs: $O(Np^2) \rightarrow O(Np)$

DNS for Turbulent collision statistics



- Flow motion: Imcompressible N-S eq.
- Particle motion: $$\frac{d\mathbf{v}}{dt} = -\frac{1}{\tau_p}(\mathbf{v}-\mathbf{u})$$

monodisperse, no-gravity

	# of grids	$k_{max} l_\eta$	R_λ	# of particles	
	64^3	2.0	54.9	32^3	
	128^3	2.0	81.3	64^3	Onishi et al. (2009) *PoF*
	256^3	2.0	126	128^3	
ES2	512^3	2.0	207	256^3	
ES2	$1{,}000^3$	2.0	323	500^3	
ES2	$2{,}000^3$	2.0	527	1000^3 (=1 billion)	Onishi et al. (2013) *JCP*, Onishi & Vassilicos (2014) *JFM*
K	$4{,}000^3$	2.0	860	1.6 billion	
K	$6{,}000^3$	2.0	1,120	5.4 billion	Onishi & Seifert (2016) *ACP*
new ES→	$8{,}192^3$	2.0	1,390	8.2 billion	

Collision kernel, $K_c(r_1, r_2)$

- Collision frequency N_c [1/(m^{3}s)];

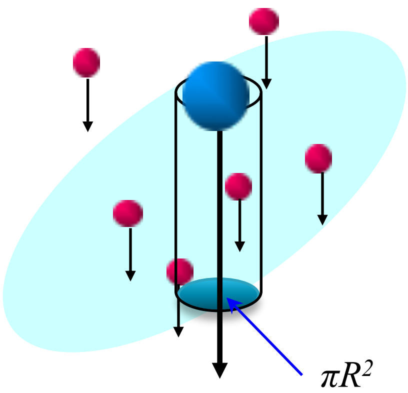
$$N_c(r_1, r_2) = n_p(r_1)\, n_p(r_2) K_c(r_1, r_2),$$

where n_p [1/m^3] is the particle number density.

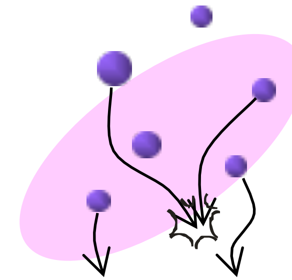
- Gravitational collision kernel

$$\boxed{K_c(r_1, r_2) = \pi R^2 \left| V_\infty(r_1) - V_\infty(r_2) \right|}$$

(R : collision radius ($=r_1+r_2$), V_∞:settling velocity)



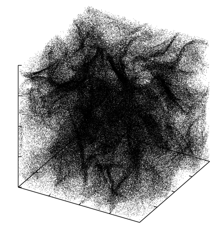
Turbulent collision kernel



<<spherical formulation (Wang et al., (2000)*JFM*)>>

$$\langle K_c(r_1,r_2)\rangle = 2\pi R^2 \langle |\, w_r(x=R)\,| \rangle g(x=R)$$

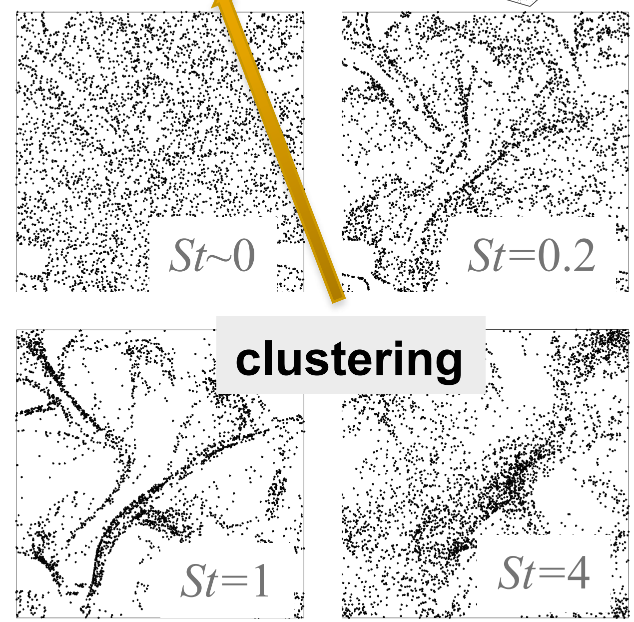
- R : collision radius (=r_1+r_2)
- $|w_r|$: radial relative velocity at contact
- $g(R)$: radial distribution function at contact (clustering effect)



$$St = {\tau_p}/{\tau_\eta} = \frac{2}{9}\frac{\rho_p}{\rho_f}\left(\frac{r}{l_\eta}\right)^2$$

- τ_p: particle relaxation time
- τ_η: Kolmogorov time

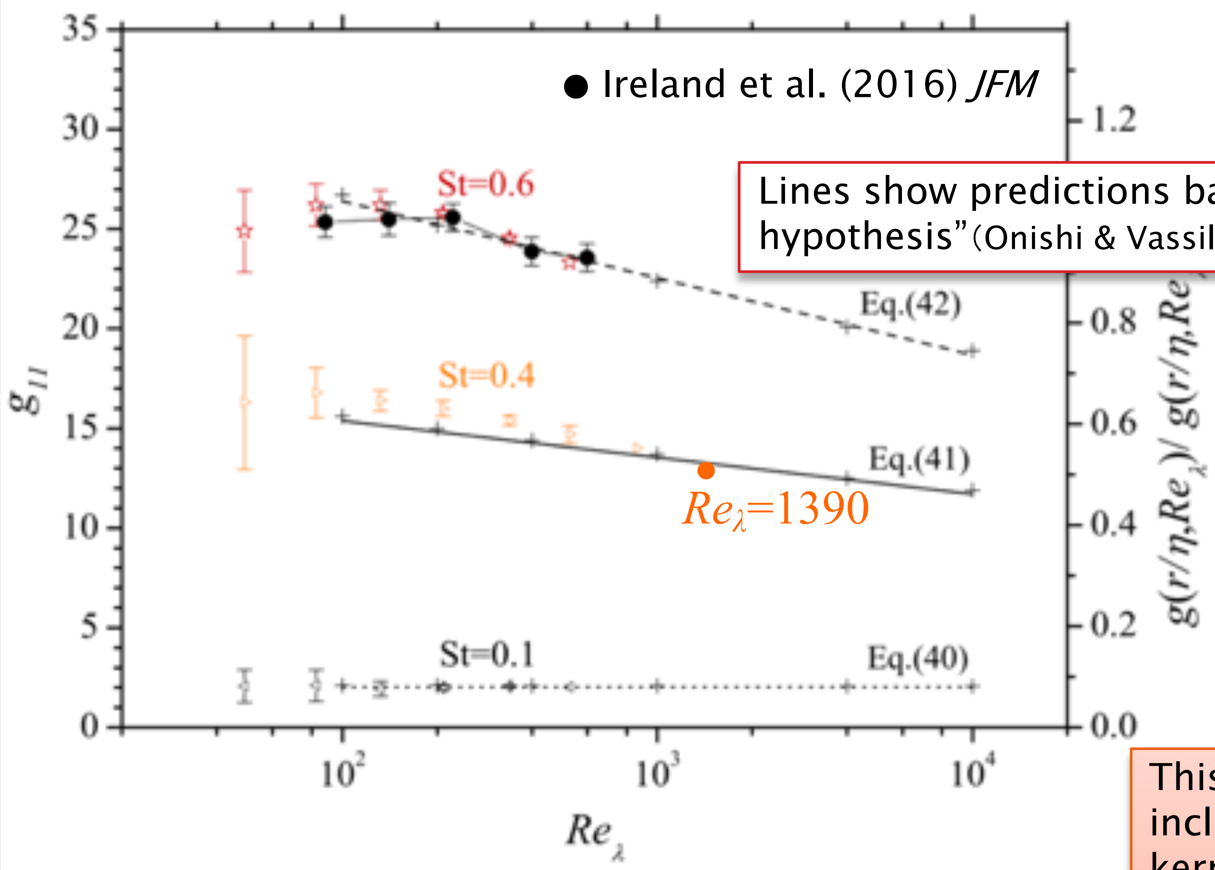
	radius[μm]	*St*
CCN	<1	<<1
Cloud droplets	10	0.01
	30	0.1
Rain drops	100	1
Large drops	1000<	10



Clustering enlarges the collision probability.

Re-dependence of $g_{11}(R)$ for St<1

Fig 2 in Onishi & Seifert (2016) ACP



Lines show predictions based on the "intermittency hypothesis"(Onishi & Vassilicos 2014 JFM)

Decreasing for increasing Re for 1/3<St<1

This Re-dependency has been included in a turbulent collision kernel model (Onishi & Seifert 2016, *ACP*) and in bulk parameterizations (Seifert & Onishi 2016, *ACP*)

Turbulent Kc modeling

- Mechanism of the Re-dependence of clustering
  - Onishi & Vassilicos (2014) JFM

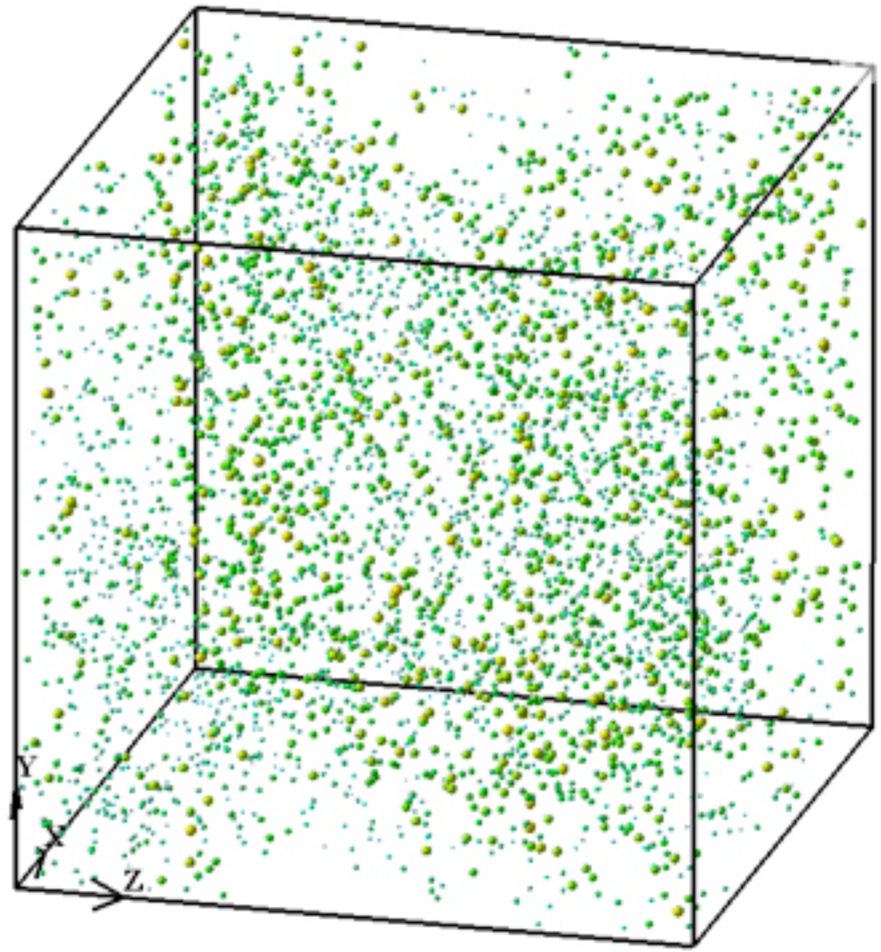
- Modeling of turbulent collision kernel
  - Onishi & Seifert (2016) ACP (where fortran code provided as a suppliment)

- Bulk parameterizations of turbulent collision growth (autoconversion and accretion)
  - Seifert & Onishi (2016) ACP

Lagrangian tracking droplet collision growth simulation

*Gravitational droplet Settling (precipitation) is considered as well.

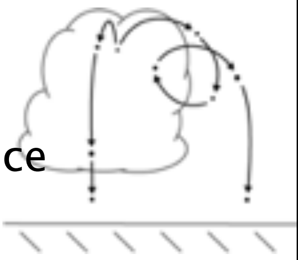
Onishi et al. (2015) JAS



courtesy of Dr. Matsuda (JAMSTEC)

Why direct Lagrangian particle tracking simulation?

- [For robust reference data]
  We can directly analyze multi-scale phenomena without separating macro- and micro-scales.
  - Recirculation of rain drops (Naumann & Seifert 2016 JAMES) or of ice particles (Yang et al. 2015 JGR Atmos.)
  - Evaporative and radiative cooling in cloud turbulent mixing layer (e.g., de Lozer & Mellado 2013JAS, Kumar et al. 2014JAS)



but several physics (particularly, **collisions**) have been skipped in literature

- [For intrinsic statistical fluctuations]
  We can obtain new kind of information regarding statistical fluctuations and can investigate individual realizations, not the ensemble-averaged statistics.

NB. [Prediction error]=[Practical error] + **[Intrinsic error]**

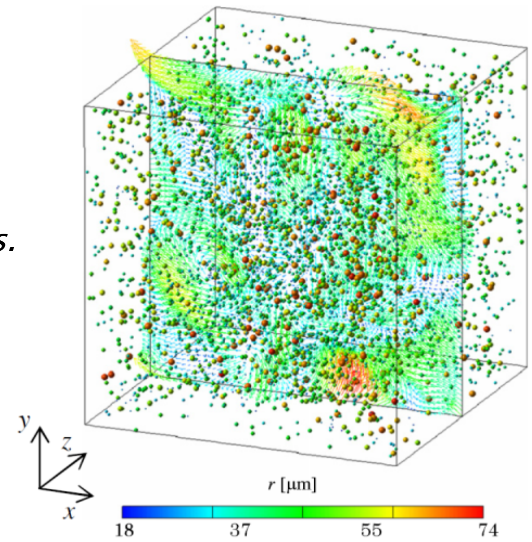
Onishi et al. (2015) J. Atmos. Sci.

Collisional growth simulation

- Fluid and Scalars (Euler method)

Onishi et al. (2011) *J. Comput. Phys.*

$$
\begin{aligned}
\nabla \cdot \mathbf{U} &= 0 \\
\frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U}\cdot\nabla)\mathbf{U} &= -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{U} + \beta(T-T_0)\mathrm{g} + \mathbf{F}(\mathbf{x},t) \\
\frac{\partial L_v}{\partial t} + (\mathbf{U}\cdot\nabla)L_v &= \nu_v\nabla^2 L_v + S_p(\mathbf{x_p},t) \\
\frac{\partial T}{\partial t} + (\mathbf{U}\cdot\nabla)T &= \nu_T\nabla^2 T + H_p(\mathbf{x_p},t)
\end{aligned}
$$

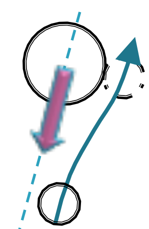


- Particles (Lagragian tracking method)

$$
\frac{d\mathbf{V}}{dt} = -\frac{f_{NL}}{\tau_p}\left(\mathbf{V} - (\mathbf{U}(\mathbf{x_p},t) + \mathbf{u}(\mathbf{x_p},t))\right) + \mathbf{F}_{impulse} + \mathbf{g}
$$

$$
\frac{dm_p}{dt} = \left(\frac{dm_p}{dt}\right)_{coll.impulse} + \left(\frac{dm_p}{dt}\right)_{cond/evap}
$$

$$
\left(\frac{dm_p}{dt}\right)_{cond/evap} = 4\pi D_v \rho_v r \sigma_v
$$



disturbance vel. due to hydrodynamic interactions.

(Onishi et al. (2013) *J. Comput. Phys.*)

Computational setting (flow)

	N^3	L_0 [m]	Re	u'/U_0	$k_{max} l_\eta / L_0$	L_f / L_0	Re_λ	ε [cm^2/s^3]
NoT	32^3	0.0127	0	0	-	-	0	0
T100	96^3	0.0180	97.4	1.00	2.04	1.64	66.1	100
T	96^3	0.0127	97.4	1.00	2.04	1.64	66.1	400
T1000	96^3	0.0101	97.4	1.00	2.04	1.64	66.1	1000
TR127	256^3	0.0338	360	0.98	2.06	1.44	127	400
TR206	512^3	0.0669	908	1.00	2.06	1.43	206	400

~Typical Cu

Computational setting (droplet)

	Flow	Hydrodynamic Interaction (HI)	initial number density n_{p0} [1/m^3]	initial number of particles, N_{p0}
NoT-NoHI	stagnant	no	1.42×10^8	7.24×10^4
NoT- HI		yes		7.24×10^4
T-NoHI	turbulent	no	1.42×10^8	7.24×10^4
T- HI		yes		7.24×10^4
T100-HI		yes		2.05×10^5
T1000-HI		yes		3.64×10^4
TR127-HI		yes		1.36×10^6
TR206-HI		yes		1.06×10^7

～Typical Cu

- Initial size dist. of the group of droplets:

$$f_0(x) = \frac{n_0}{x_m}\exp(-x/x_m),$$

where x is the particle mass, x_m (set to $m(r=15\mu m)$) is the mean particle mass.

Present SCE simulation

Stochastic Collection Equation (SCE)

$K_{coal}=E_{coal}*E_c*K_c$

$$\left(\frac{\partial n_p(m)}{\partial t}\right)_{col} = \frac{1}{2}\int_0^m \underline{K_{coal}(m-m',m')}n_p(m-m')n_p(m')dm' - \int_0^\infty \underline{K_{coal}(m,m')}n_p(m)n_p(m')dm'$$

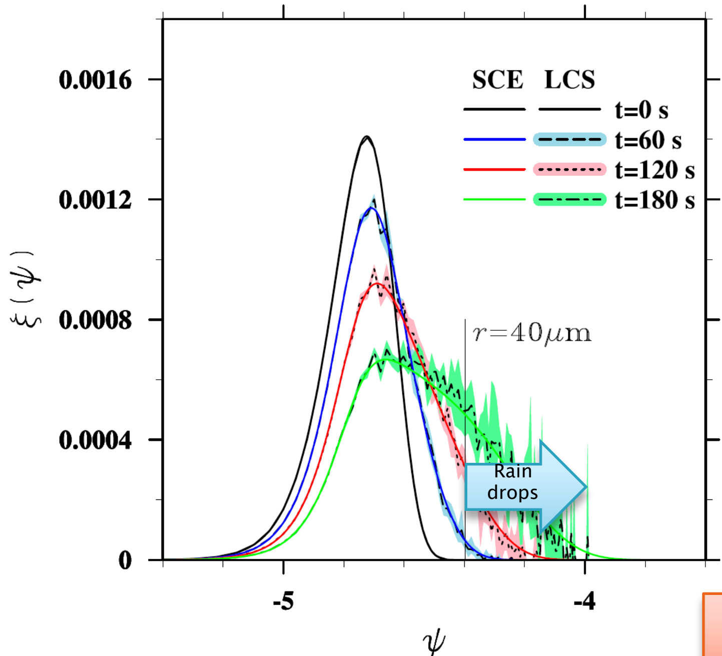
- Coalescence efficiency: $E_{coal}=1$
- Collision efficiency:
  - $E_c=1$ for NoHI
  - $E_c=E_c$(Pinsky et al., 2001) for NoT−HI
  - $E_c=E_c$(Pinsky et al., 2001)*η_E(Wang et al. 2008) for T−HI
- Collision kernel:
  - K_c[NoT]=gravitational kernel
  - K_c[T]=Onishi turbulent kernel (Onishi & Seifert 2016)

Mass density function, $\xi(\varphi)$

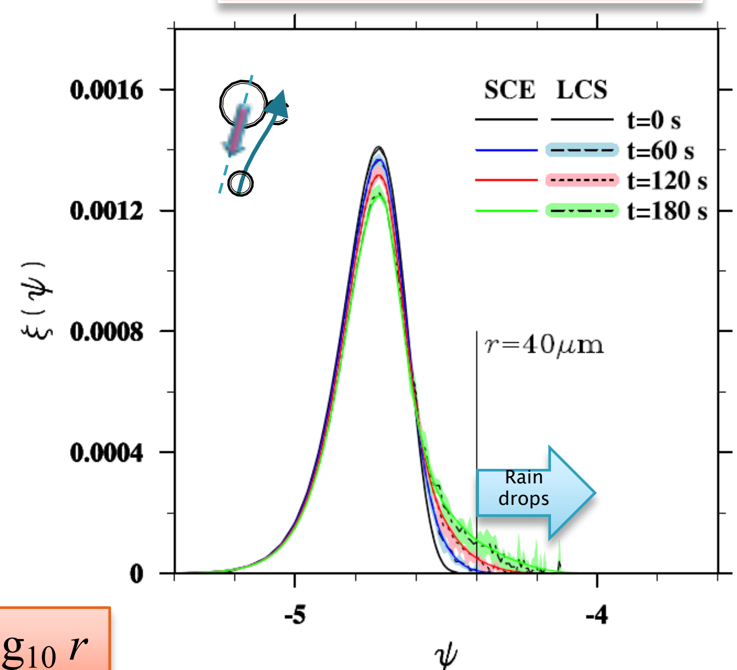
$\int \xi(\varphi)\mathrm{d}y$, where $\varphi=\log_{10} r$, obtains the liquid mixing ratio [kg/m^3].

Stagnant (NoT) case

Without HI



With HI



$\varphi=\log_{10} r$

Without HI, droplets grow unrealistically too fast.

Proof of the relevant role of HI

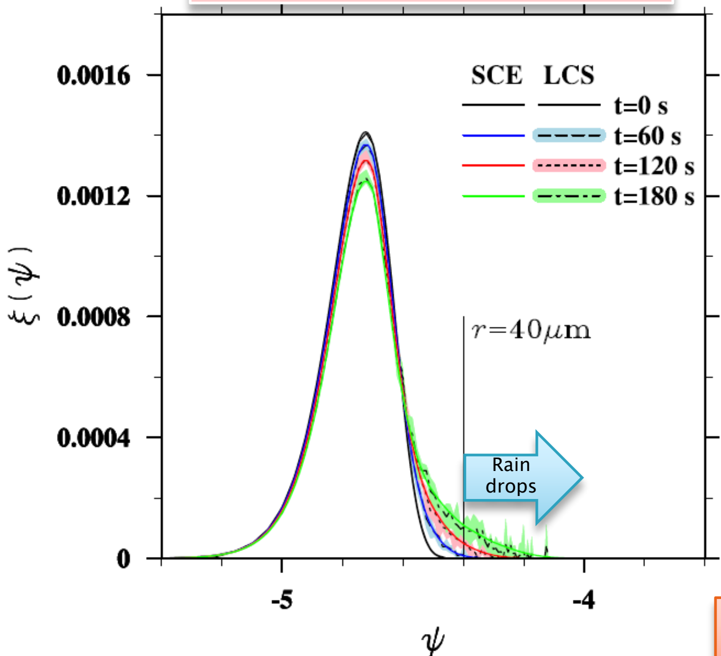
Onishi et al. (2015) J. Atmos. Sci.

Mass density function, $\xi(\varphi)$

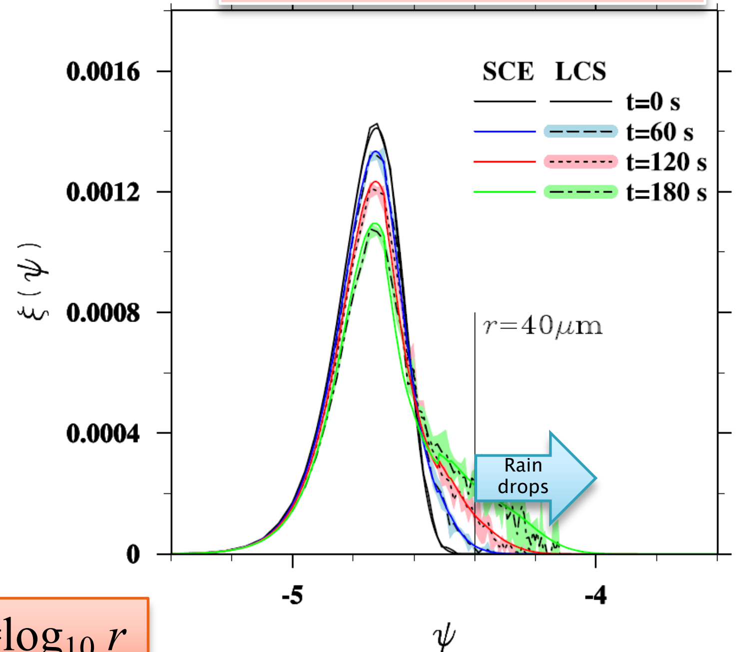
$\int \xi(\varphi)\mathrm{d}y$, where $\varphi = \log_{10} r$, obtains the liquid mixing ratio [kg/m^3].

HI case

Stagnant (NoT)



Turbulence (T)



$\varphi = \log_{10} r$

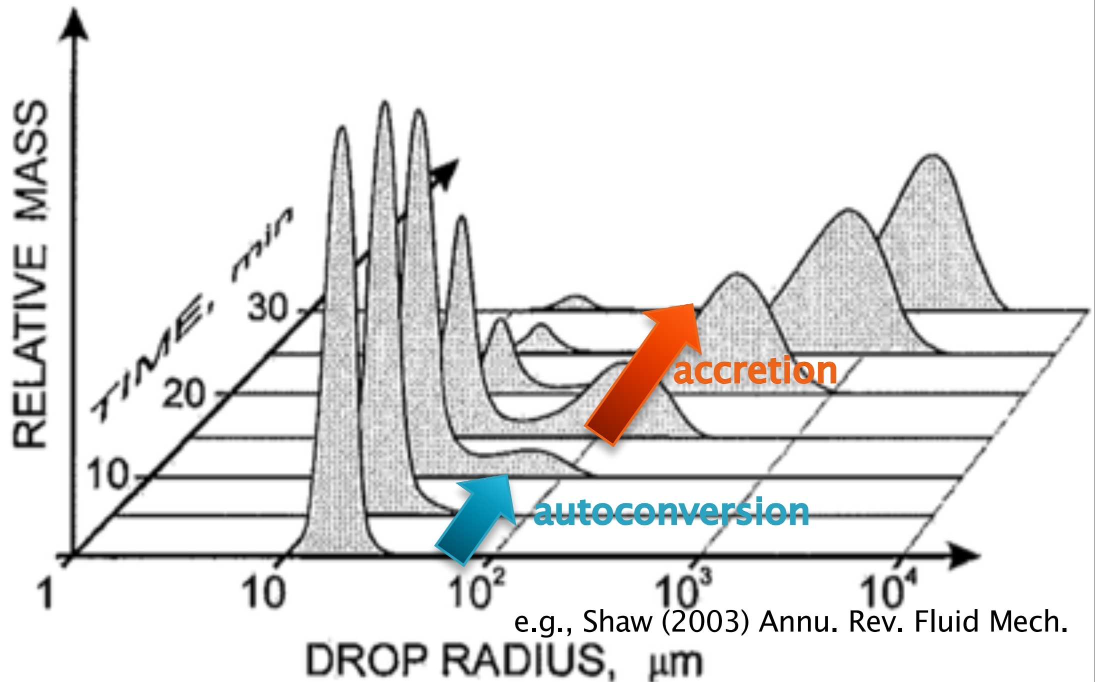
Turbulence promotes size evolutions.
Good agreement between SCE and LCS.

Warm-rain conversion parameterizations for Bulk cloud microphysics models

Liquid water is classified into CLOUD (small droplets, usually smaller than 40um in radius) and RAIN categories.

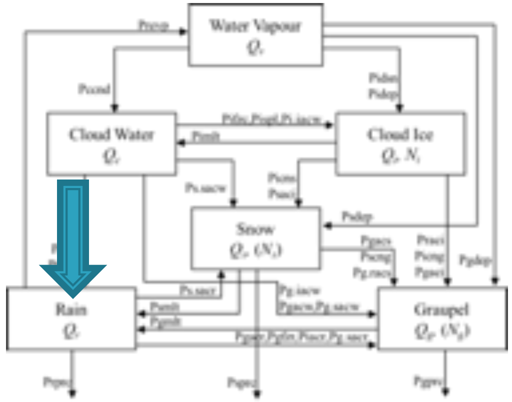
- autoconversion
  - CLOUD + CLOUD =>RAIN

    collision/coagulation
- accretion
  - CLOUD + RAIN =>RAIN
- condensation
  - vapor ⇔ CLOUD, RAIN



e.g., Shaw (2003) Annu. Rev. Fluid Mech.

Autoconversion models



- Kessler, 1969

$$P_{auto} = a\rho(q_c - q_{c,0})H(q_c - q_{c,0}),$$

Here, α is a tuning constant, $q_{c,0}$ is the threshold water mixing ratio and H is the Heaviside step function. In this study $\alpha = 10^{-3}\ \mathrm{s}^{-1}$ and $q_{c,0} = 0.5 \times 10^{-3}\ \mathrm{kgkg}^{-1}$

  - No explicit turbulence effect included.

- Seifert et al., 2010 (SNS2010)

$$P_{auto} = \frac{k_{cc}}{20m^*}\frac{(\mu+2)(\mu+4)}{(\mu+1)^2}L_c^2\overline{m_c}^2\left\{1+\frac{\Phi_{auto}(\tau)}{(1-\tau)^2}\right\},$$

$$k_{cc}(\overline{r_c},\mu,\varepsilon,Re_\lambda) = k_{cc,0}\left\{\underline{1+\varepsilon Re_\lambda^{1/4}}\left[\alpha_{cc}(\mu)\exp\left\{-\left[\frac{\overline{r_c}-r_{cc}(\mu)}{\sigma_{cc}(\mu)}\right]^2\right\}+\beta_{cc}\right]\right\}$$

  - Turbulence effect is explicitly considered in the form of

$$\boxed{P_{auto} \propto 1 + C_{SNS}\ \varepsilon\, Re_\lambda^{1/4}}$$

  - Parameterization based on the SCE results with Ayala kernel model.

Time evolutions of conversion rates

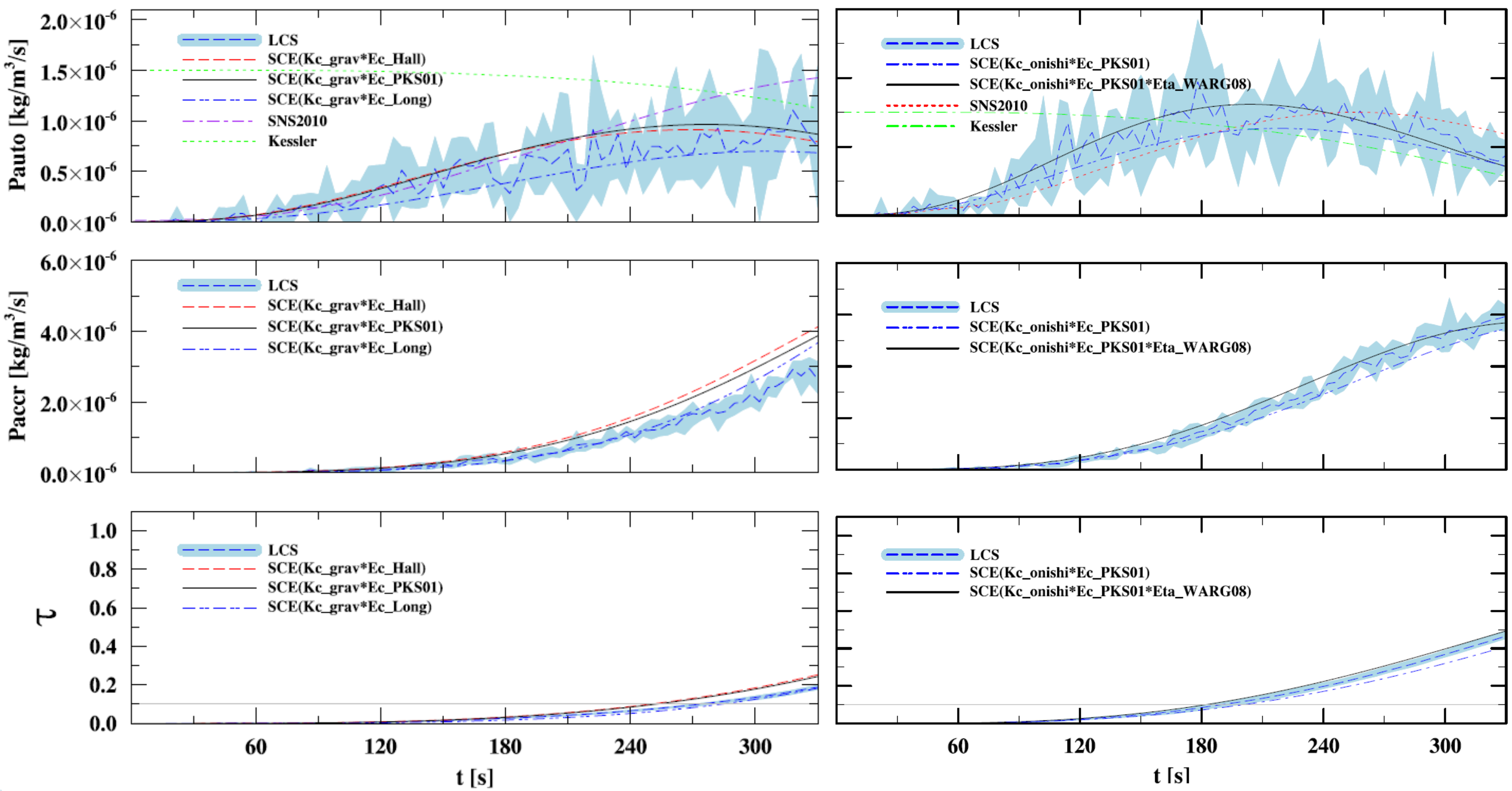
With HI

Stagnant flow case (NoT) | Turbulent flow case (T)

Autoconversion rate

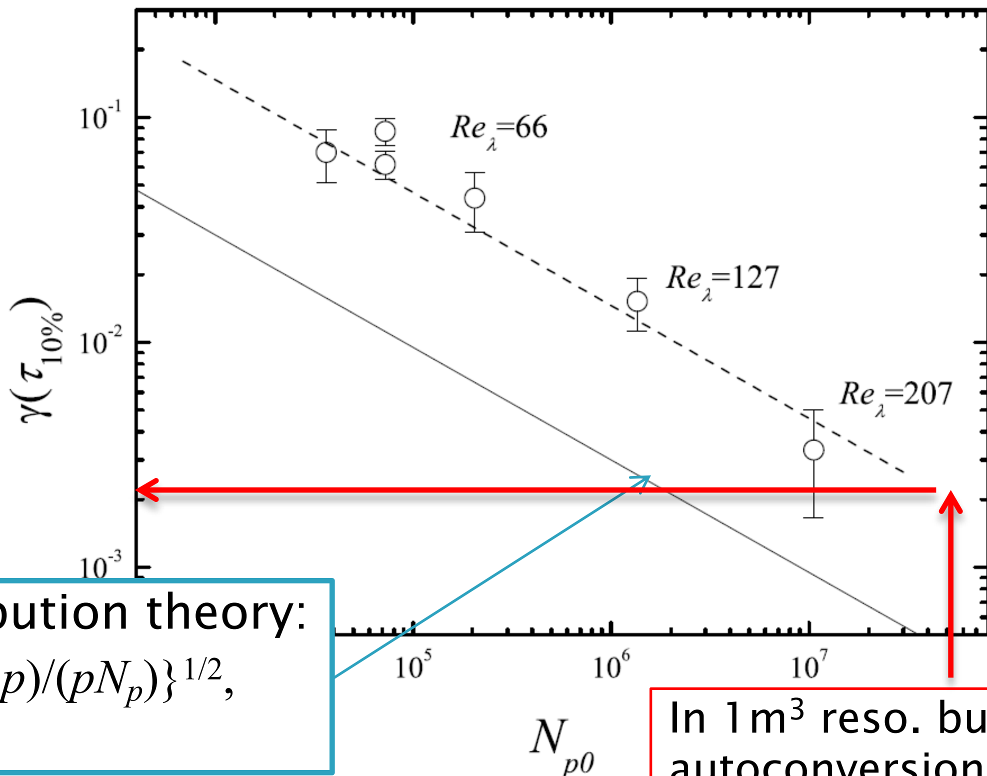
Accretion rate

Rain mass ratio



Onishi et al. (2015) J. Atmos. Sci.

Statistical fluctuations (relative std.) of autoconversion timescale



binomial distribution theory:
relative std. $\gamma=\{(1-p)/(pN_p)\}^{1/2}$, where p=0.1.

In 1m^3 reso. bulk simulation, autoconversion has O($10^{-2\sim3}$) intrinsic fluctuations.

(100m)^3 reso.=>O($10^{-5\sim6}$)
(10m)^3 reso.=>O($10^{-4\sim5}$)
(1m)^3 reso.=>O($10^{-2\sim3}$) intrinsic fluctuations.

Concluding remarks

- Direct Lagrangian tracking DNS can provide
  - robust reference data regarding droplet collision growth,
  - intrinsic (due to discreteness of particle numbers) statistical fluctuations.

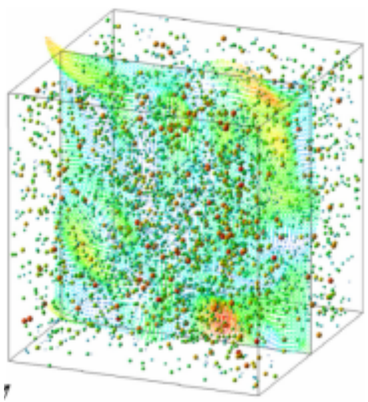
- The DNS results have shown
  - the significant impact of HI and turbulence on the droplet collision growth rate,
  - large intrinsic statistical fluctuations.

Lagrangian tracking droplet growth simulation

Includes activation, condensation, collision and precipitation

Kunishima & Onishi, Direct Lagrangian tracking simulation of droplet growth in vertically developing cloud, *Atmos. Chem. Phys. Discuss.*, https://doi.org/10.5194/acp-2018-328, under minor revision

(Quasi-) 1D simulation by LCS



(10m)^3-box simulation is feasible.

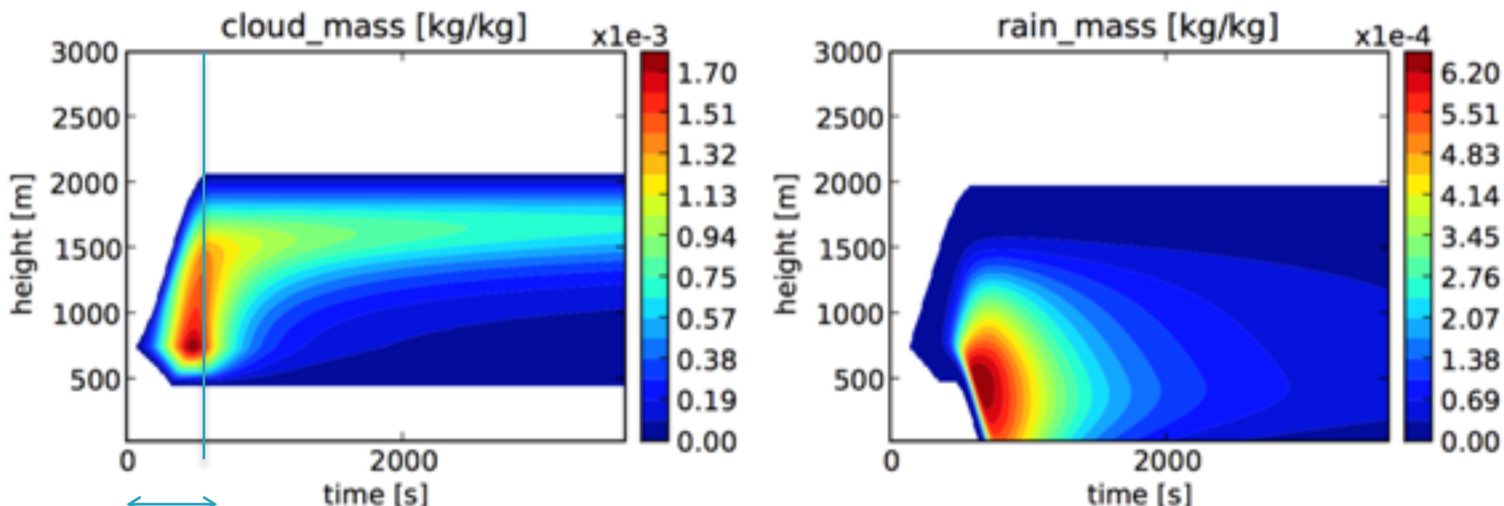
e.g., collision statistics simulations with 6,000^3 flow grids with 5.4 bil. particles (Onishi & Seifert, 2016 *ACP*) or 8,192^3 flow grids with 8.2 bil particles.

somen noodle domain!

O((1m)^2) x O(1000m) – extremely-vertically-elongated box simulation is feasible.

Kinematic (pseudo-) 1D simulation

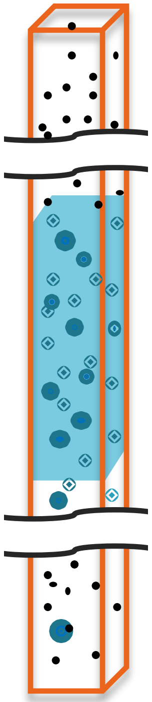
- 1D warm rain simulation (warm1) in KiD (Kinematic Driver; B. Shipway & A. Hill@UKMO)
  - cloud physics and dynamics are not coupled.
  - 3600s integration



prescribed updraft
for the first 10min

$$w(z,t) = \begin{cases} w_1 \sin(\pi t/600) & \text{for } \; t < 600\,\text{s} \\ 0.0 & \text{otherwise} \end{cases}$$, in which w_1=2m/s

LCS for KiD–warm1



- Fluid and Scalars (Euler method)

Prescribed

flow

$$\nabla \cdot \mathbf{U} = 0$$

$$\frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U}\cdot\nabla)\mathbf{U} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{U} + \beta(T - T_0)\mathbf{g} + \mathbf{F}(\mathbf{x}, t)$$

vapor

$$\frac{\partial L_v}{\partial t} + (\mathbf{U}\cdot\nabla)L_v = \nu_v\nabla^2 L_v + S_p(\mathbf{x_p}, t)$$

temp.

Prescribed

$$\frac{\partial T}{\partial t} + (\mathbf{U}\cdot\nabla)T = \nu_T\nabla^2 T + H_p(\mathbf{x_p}, t)$$

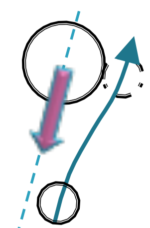
coupling

- Particles (Lagragian tracking method)

$$\frac{d\mathbf{V}}{dt} = -\frac{f_{NL}}{\tau_p}\left(\mathbf{V} - (\mathbf{U}(\mathbf{x_p}, t) + \mathbf{u}(\mathbf{x_p}, t))\right) + \mathbf{F}_{impulse} + \mathbf{g}$$

$$\frac{dm_p}{dt} = \left(\frac{dm_p}{dt}\right)_{coll.impulse} + \left(\frac{dm_p}{dt}\right)_{cond/evap}$$

+activation



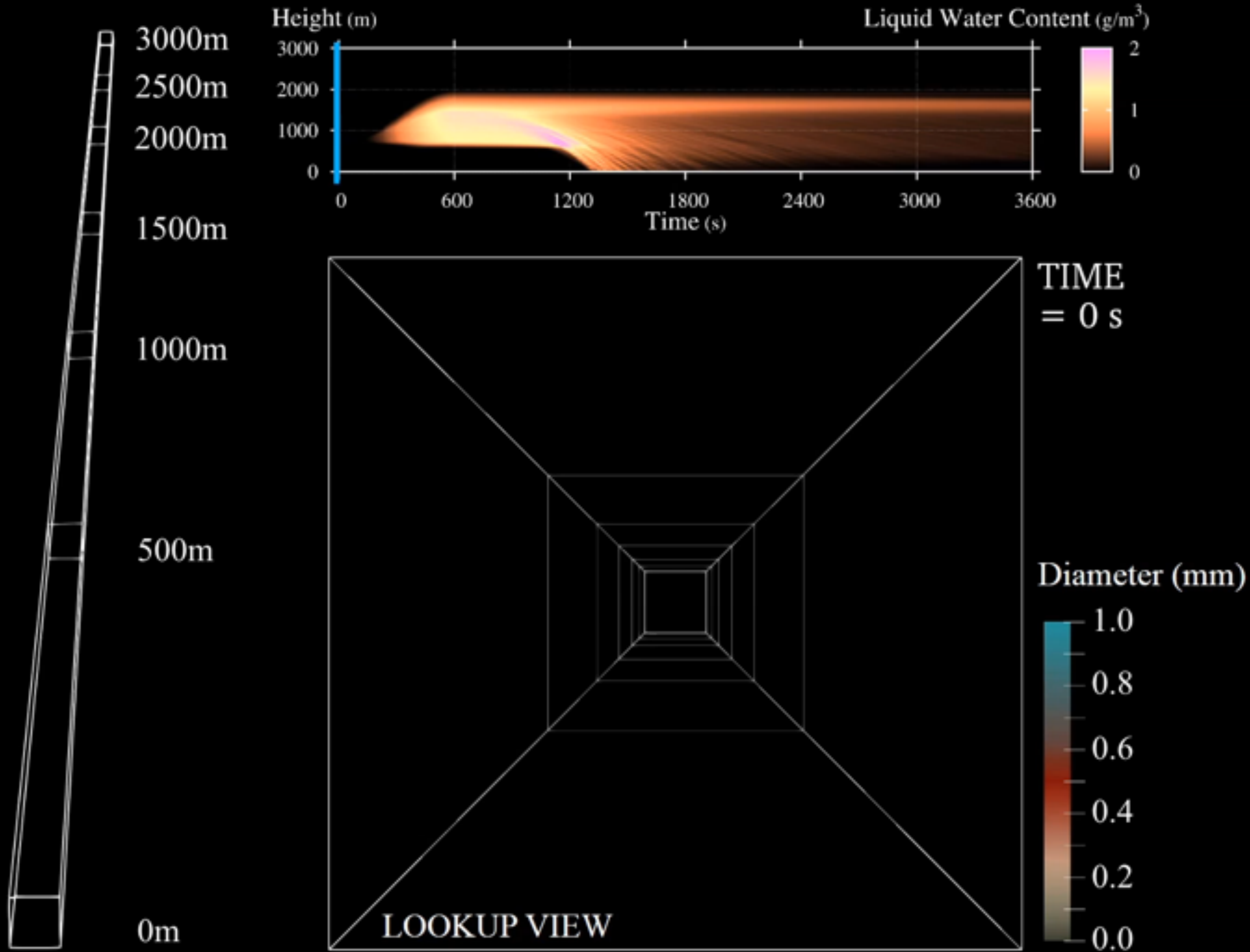
disturbance vel. due to hydrodynamic interactions.

computational setups

	domain [m^3]	number of particles	initial N_{aero} [m^{-3}]	number of time steps
SMALL	0.01x0.01 x 3000	1.50×10^7	5.0×10^7	2.88×10^6
LARGE	0.03x0.03 x 3000	1.35×10^8	5.0×10^7	2.88×10^6
VERY LARGE	0.1 x0.1 x 3000	1.50×10^9	5.0×10^7	

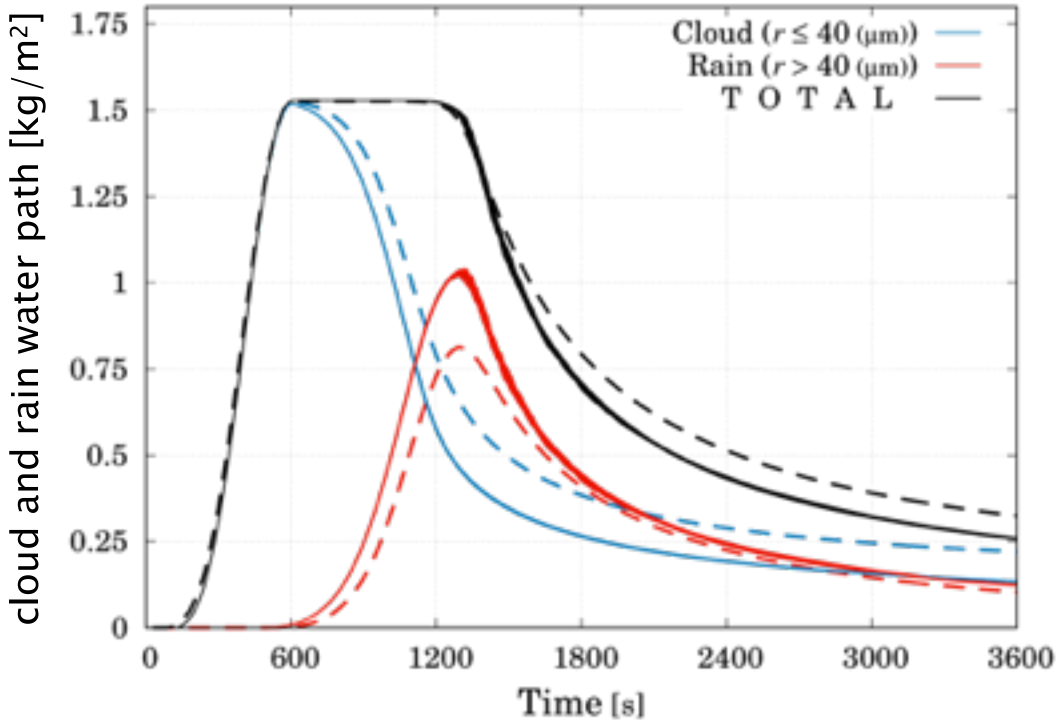
- Many (30) runs for SMALL.
- 2 runs for LARGE so far.
- VERY LARGE is feasible but painful (i.e., not yet done).

Present talk is based on SMALL setup.



3000m
2500m
2000m
1500m
1000m
500m
0m
Height (m)
Liquid Water Content (g/m³)
3000
2000
1000
0
0
600
1200
1800
2400
3000
3600
Time (s)
2
1
0
TIME
= 0 s
LOOKUP VIEW
Diameter (mm)
1.0
0.8
0.6
0.4
0.2
0.0

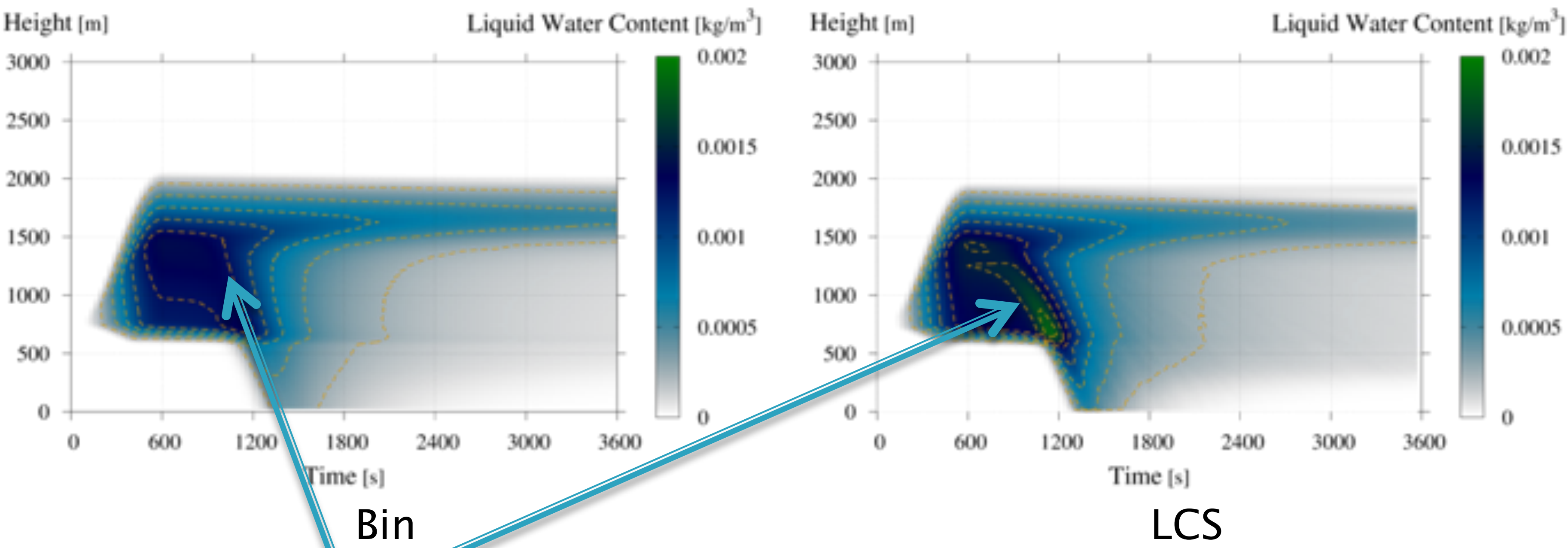
Bulk statistics – water path



- LCS results agree with Bin results with 528 classes [1].
  [NB] $N_{aerosol}$ is kept constant in Bin, while it changes in LCS.

[1] Onishi, Takahashi. *J. Atmos. Sci.* **69** (2012)

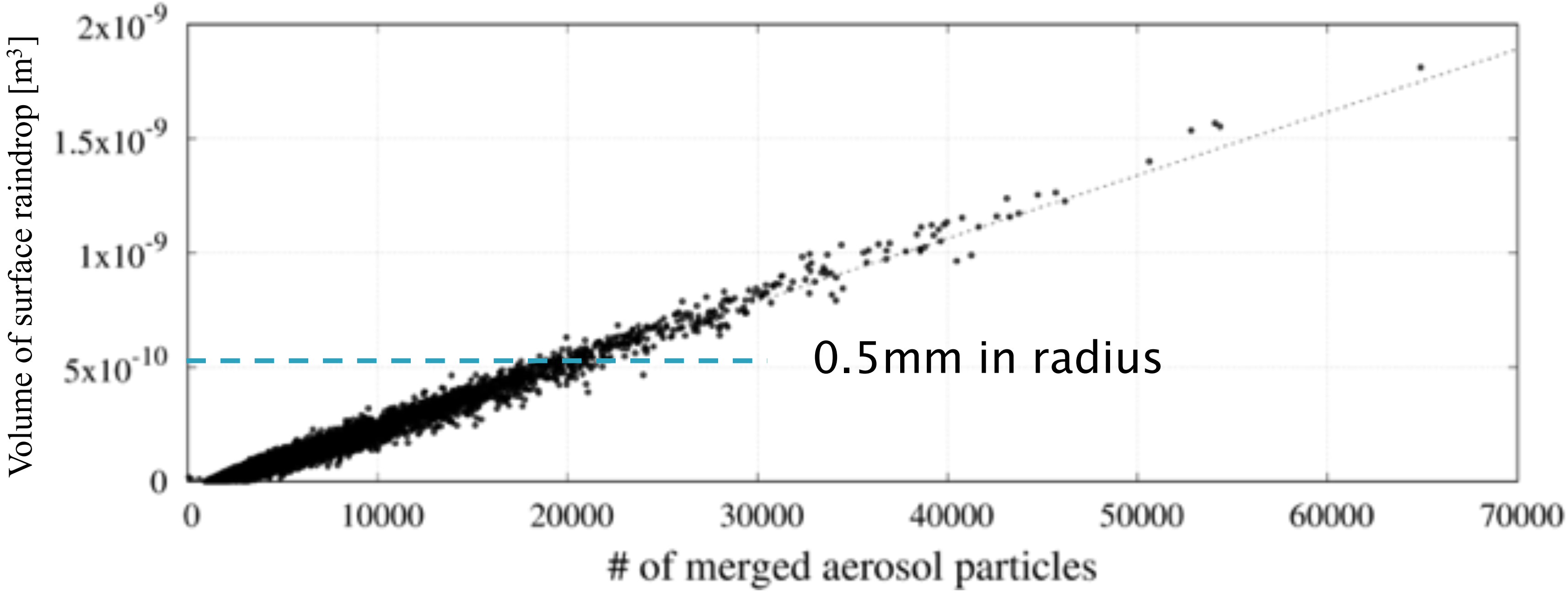
Bulk statistics –Liquid Water Content



- Bin simulation [1] suffers from numerical diffusion, while LCS does not.

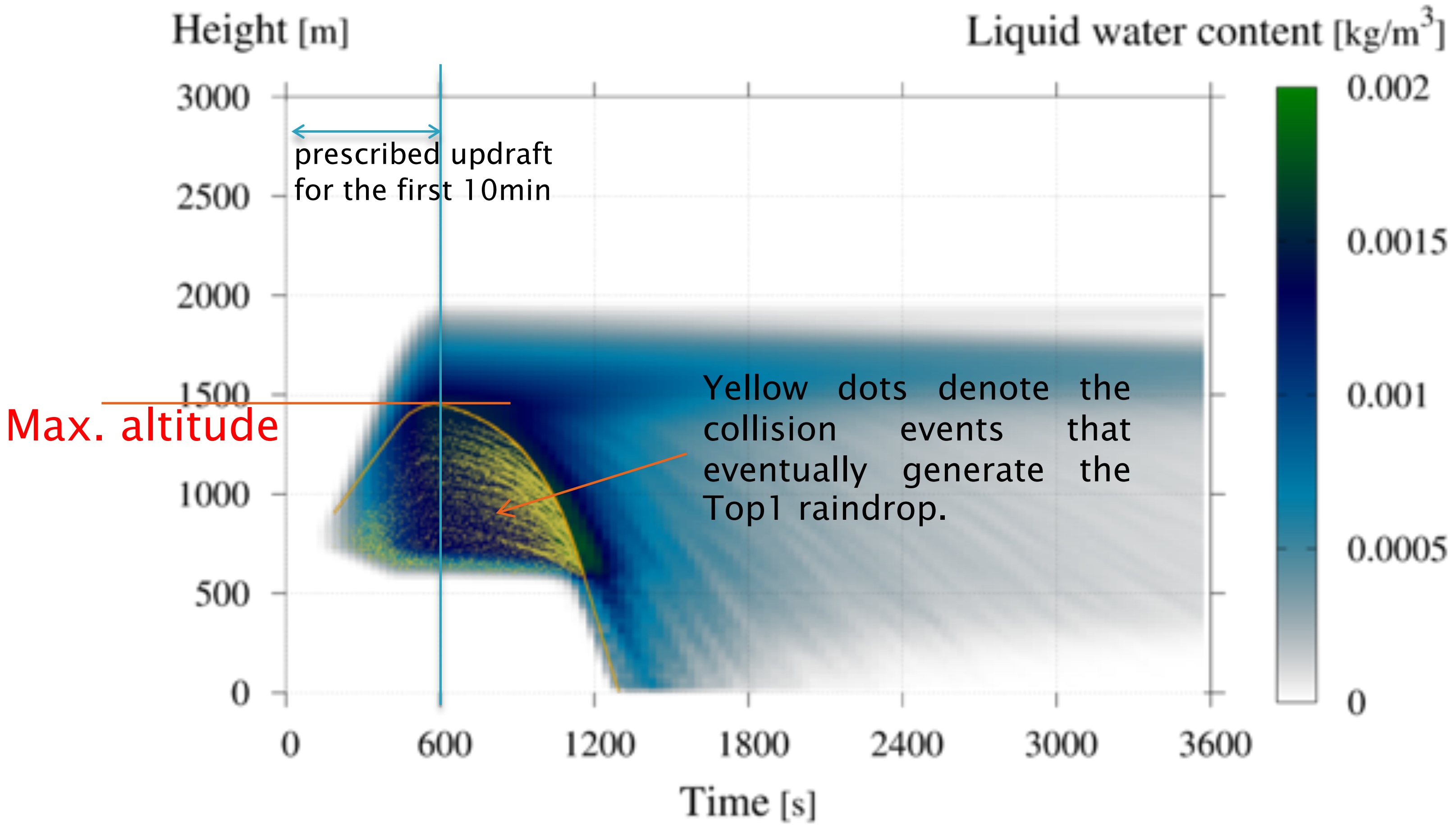
[1] Onishi, Takahashi. *J. Atmos. Sci.* **69** (2012)

Lagrangian statistics – no. of collisions



- Each rain drop consists of $O(10^4)$ particles.
- i.e., Each rain drop collects droplets with 17.8 um in radius on average.

Back trajectory of a surface raindrop

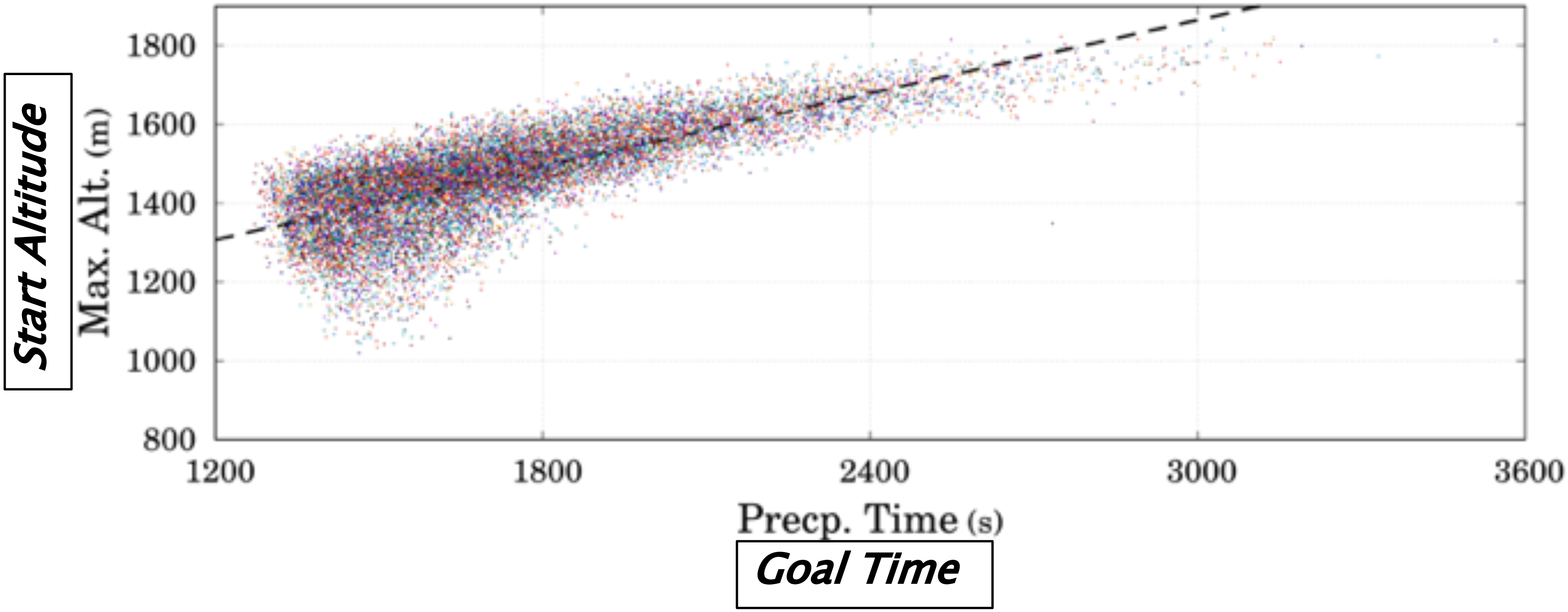


- Max. altitude is attained at t~600s, when the updraft is halted.

Down-sky Race to the ground!

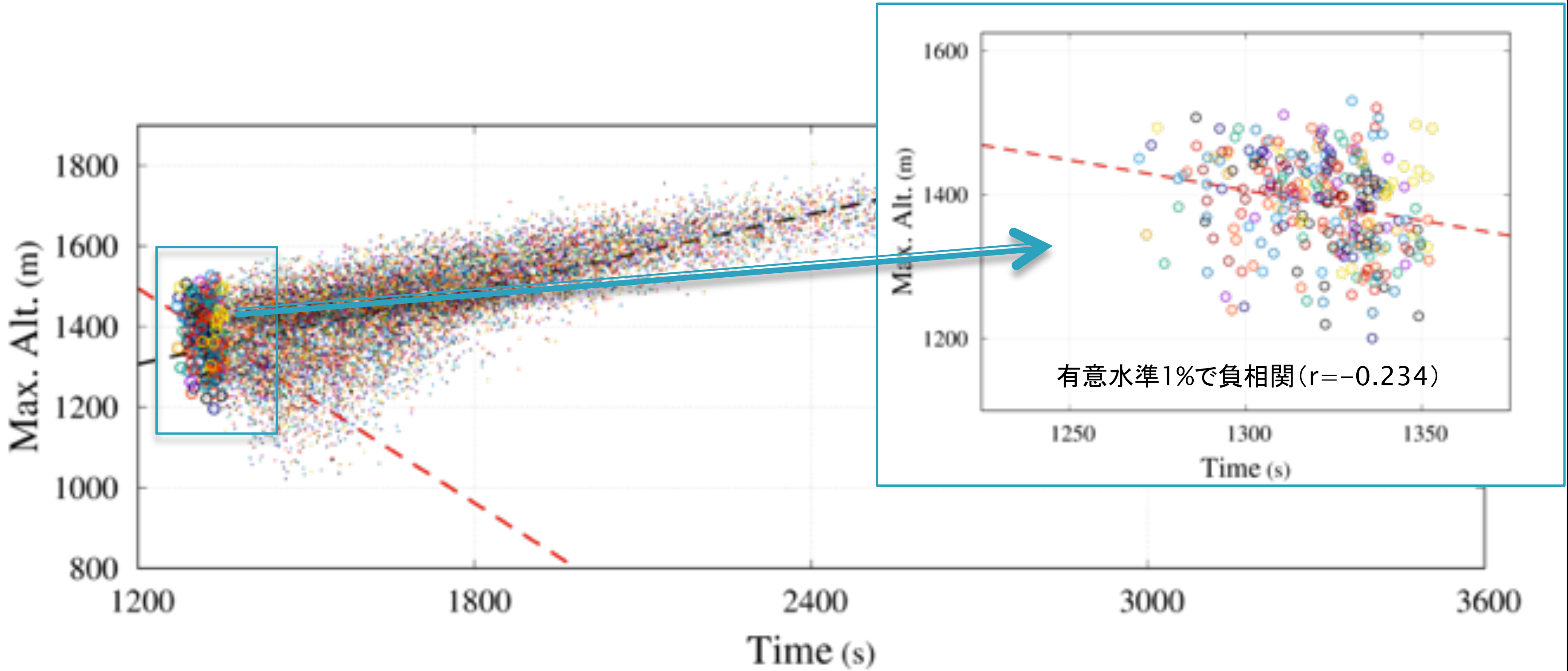
- Start ‘Bang’ at t=600s. The goal is the ground.
- “Top1” drop reaches the ground around t=1280s (fluctuates race to race).

Lagrangian statistics –Max. altitude agaist T_{surf}



- Total nominated surface raindrops (*participants*): 15,221 for 30 races
- Positive correlation

Lagrangian statistics –Max. altitude against T_{surf} for *Top10* particles



Goal Time

- If limited to Top10 particles, negative correlation.

Concluding remarks

- Lagrangian Cloud Simulator (LCS)
  - Powerful meteorological tool –to fill the gap between microscale (microphysics) and large scale (cloud development).
  - Unique tool to investigate the intrinsic statistical fluctuations in cloud microphysics.

- LCS for quasi-1D domain with KiD-warm1 condition succeeded in investigating Lagrangian statistics (Back-trajectory analysis) of droplet growth.

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