雲マイクロ物理過程と乱流スカラー輸送の大規模シミュレーション

名古屋大学HPC 計算科学連携研究プロジェクト成果報告シンポジウム

2013年　5月8日
名古屋大学

後藤俊幸、小崎友裕、 渡邊威、 尾形修司、小林亮
（名古屋工業大学大学院　創成シミュレーション工学専攻）

石井克哉 （名古屋大学 情報基盤センター ）

草野完也 （名古屋大学 太陽地球環境研究所 ）

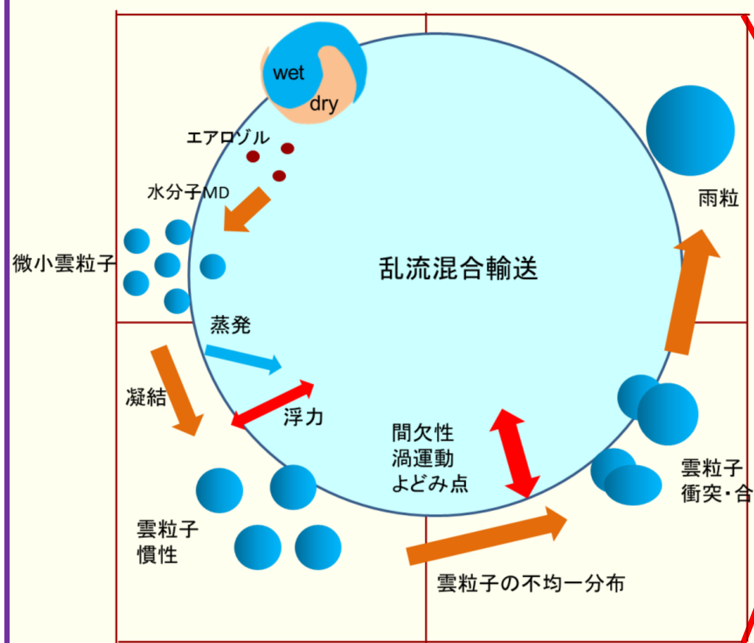
坪木和久 （名古屋大学 地球水循環研究センター ）

雲粒子はどのようにして生成され、成長し、輸送・混合され雨粒になるか？

- 雲粒子と乱流による水蒸気や温度の混合・輸送との相互作用におけるミクロからセミマクロまでのプロセスを物理の基本原理にのっとって丸ごとシミュレーションできるプログラムを開発
- 雲粒子形成のきっかけ、凝結成長、乱流による雲粒子と水蒸気の不均一な空間分布の形成、凝結と衝突による粒径分布の変化、乱流強へのフィードバックなどを調べて、雨粒形成までのプロセスを解明する

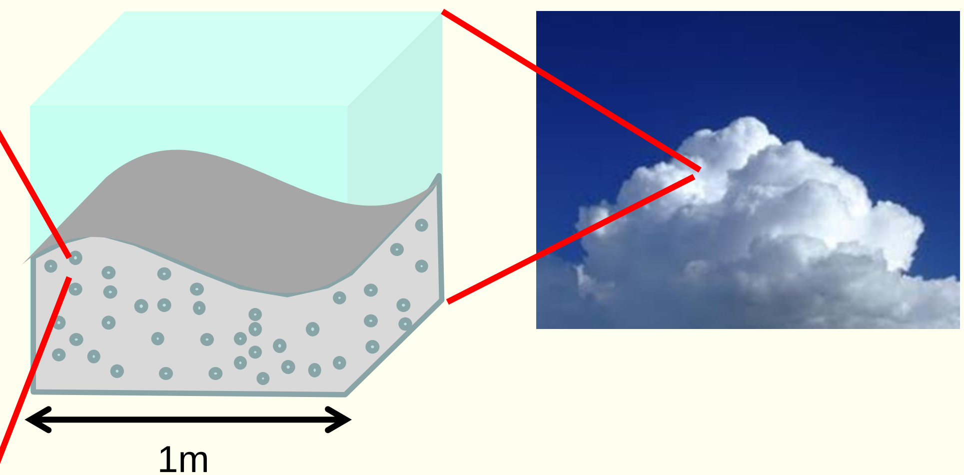
雲マイクロ物理

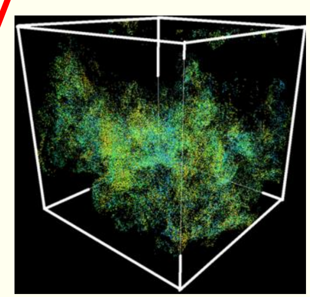
Direct Numerical Sim.　　Turbulence + Cloud droplets　　*0.5 mm < r < 1m*



$$2\Delta x \approx \eta \approx 1\text{mm}$$

η :　Kolmogorov 長さ





スペクトルコード＋雲粒子動力学コード

乱流場（非圧縮流体）　スペクトル法（+結合コンパクト）
格子点数　N_g=2048^3
雲粒子　粒子追跡＋PIC法　粒子数　N_p=10^9

水分子MDコード

角運動量時間反転対称性保存型 FT法
水分子ポテンシャル　TIP4P

Motivation 1

Turbulence Cloud interaction

Turbulence: transport and mixing of momentum, heat and mass
many scales of motion
Eulerian representation

Interaction buoyancy (heat, water vapor), momentum

small scales or all scales, time scale

Cloud: water droplets, radius, mass, heat
particle interaction (collision)
Lagrangian representation

Motivation 2

Development of high performance code of turbulence + particles

Many nodes + Many cores

Eulerian code for continuum

Incompressible fluid
Poisson equation : non-local in space $N^3 \log_2 N$
Scalar equation : local in space

Needs for Accuracy and Less communication

Hybrid scheme

spectral + combined compact difference) for scalar solver
acceleration 30%(Sc=1), 400% (Sc>50)

Lagrangian code for particle

Particle tracking random access to the memory
Relabeling
interpolation

Direct Numerical Simulation of Turbulence and Cloud Droplets

Andfrejczuk et al JAP. 2004
Kumar, Schumacher, Shaw, TCFD 2012

Included
- stratocumulus cloud at about 1500m
- turbulence + buoyancy
- temperature
- water vapor mixing ratio
- water droplets of radius 10μm～20μm
- condensation, evaporation
- Stokes drag + radius dependent relaxation time + gravity
- Collision

Not included
- Collision of droplets, coagulation
- Nucleation of water droplets
- Rain, ice

Goal

Cloud droplets

- How fast do the droplets grow in mean and distribution ?
- What are key processes ?
- What is the spatial distribution of cloud droplets?

Turbulence

- What is role of turbulence in cloud evolution?
- To what extent is turbulence modified or driven?
- What is intermittency of velocity and scalar in turbulence?

Basic Equations

Turbulence (Eulerian) **Boussinesq approximation**

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla p + \nu \nabla^2 u + e_z B + f, \qquad \nabla \cdot u = 0$$

buoyancy external force

$$\frac{\partial T}{\partial t} + u \cdot \nabla T = \kappa \nabla^2 T + \frac{L}{c_p} C_d$$

$$\frac{\partial q_v}{\partial t} + u \cdot \nabla q_v = \kappa \nabla^2 q_v - C_d$$

condensation, evaporation

$$B = g \left(\frac{T - T_0}{T_0} + \epsilon (q_v - q_{v0}) - q_l \right)$$

High Reynolds number turbulence : Spectral method

Scalar transport : Spectral (or hybrid method)

Andfrejczuk et al JAP. 2004
Kumar, Schumacher, Shaw, TCFD 2012

Cloud droplets (Lagrangian)

$$\frac{dX_j}{dt} = V_j(t)$$

$$\frac{dV_j}{dt} = \frac{1}{\tau_j(t)}\left(u(X_j(t),t) - V_j(t)\right) + ge_3$$

Stokes approximation

$$R_j(t)\frac{dR_j(t)}{dt} = KS(X_j(t),t)), \qquad R_j = \text{droplet radius}$$

Diffusion process

$$C_d(x,t) \equiv \frac{1}{m_{air}}\frac{dm_l(x,t)}{dt} = \frac{4\pi r_l K}{\rho_0(\Delta x)^3}\sum_{k=1}^{N_\Delta} R_j(t)S(X_j(t),t)$$

Condensation rate

$$S = \frac{q_v}{q_{vs}(T)} - 1, \qquad \text{supersaturation rate}$$

$$K^{-1} = \frac{\rho_l R_v T}{D_v e_{sat}(T)} + \frac{\rho_l L}{\kappa_a T}\left(\frac{L}{R_v T} - 1\right)$$

PIC

Interpolation of velocity and scalar fields at particle position

Redistribution of cloud properties onto grid points

Simulation of cloud evolution

Domain : $(25.6\ \mathrm{cm})^3$ ⇒ $(102.4\ \mathrm{cm})^3$

Water droplets : sphere (initially 10〜20μm)

Turbulence : homogeneous isotropic steady

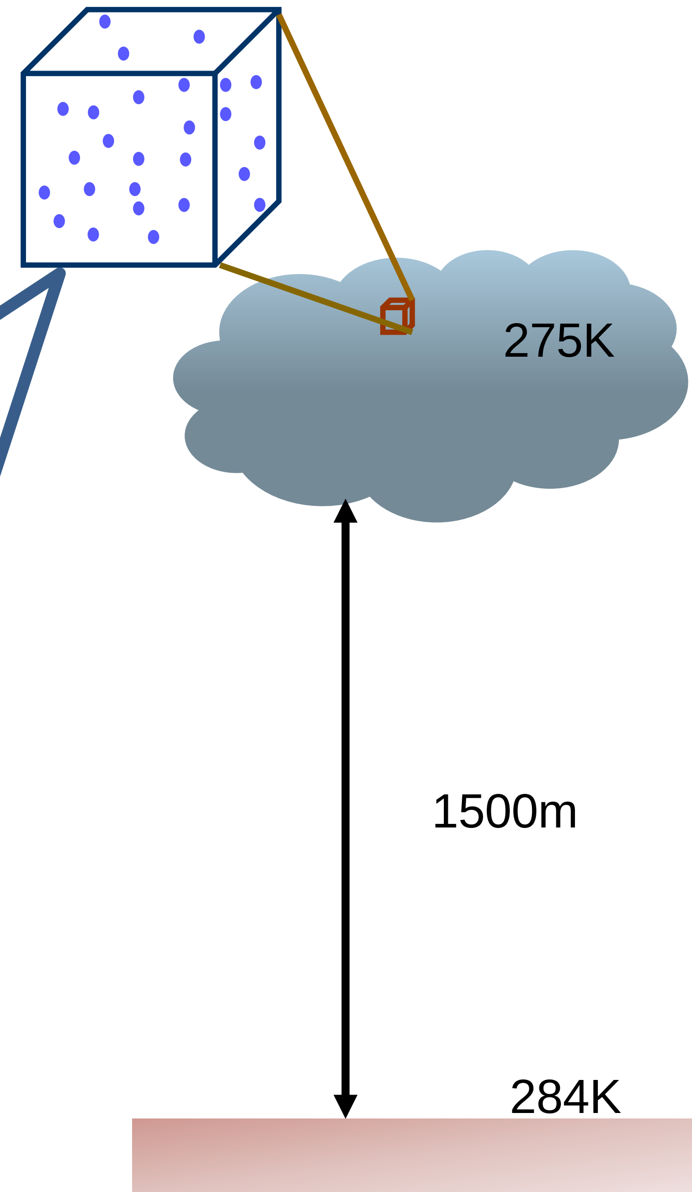
DNS : turbulence + scalar

pseudo spectral method
3DFFT + MPI + Open MP

interpolation for droplets

PIC + TS13 (or linear)

4th order Runge-Kutta-Gill



Initial Condition

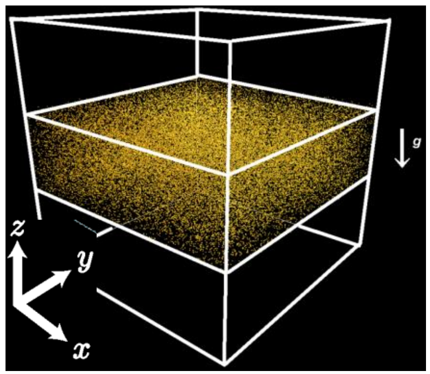
Turbulence

Isotropic Steady turbulence

Temperature fluctuation

θ : 275 K + zero fluctuation

Droplets



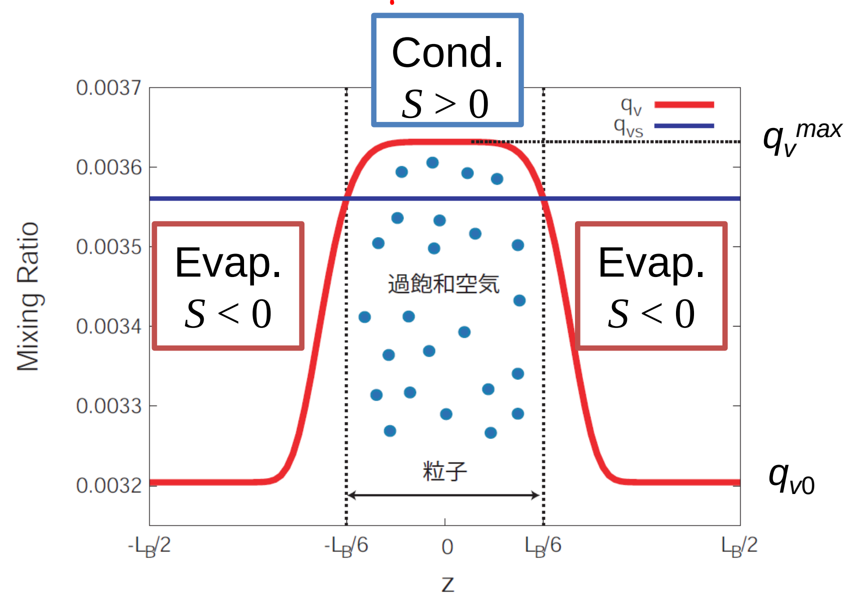
- Random in space in the range
  $-L_B/6 \leqq z \leqq L_B/6$
- No. of droplets : $2^{21} \fallingdotseq 2 \times 10^6$
  $2^{27} \fallingdotseq 1.3 \times 10$
- No.Density of droplets 31～125/cm^3
- Initial radius : 10 ～20 μm

Water vapor mixing ratio q_v

$$q_v(x, t=0) = (q_v^{max} - q_{v0}) \exp(-Az^6) + q_{v0}$$

$$q_v^{max} = 1.02 q_{vs} \qquad q_{v0} = 0.90 q_{vs}$$

$$q_v = q_{vs} \quad \text{at} \quad z = \pm L_B / 6$$



Re数、計算領域、格子数、粒子数を増大

Taylor micro scale Re 数 : R_λ	92	2.7倍	252
立方体の1辺の長さ: L	25.6cm	4倍	102.4cm
格子点数: N^3	128^3	8倍	1024^3
雲粒子数: N_p	2^{22} 個	2倍	2^{27} 個

Simulations of Decay wet, Decay dry

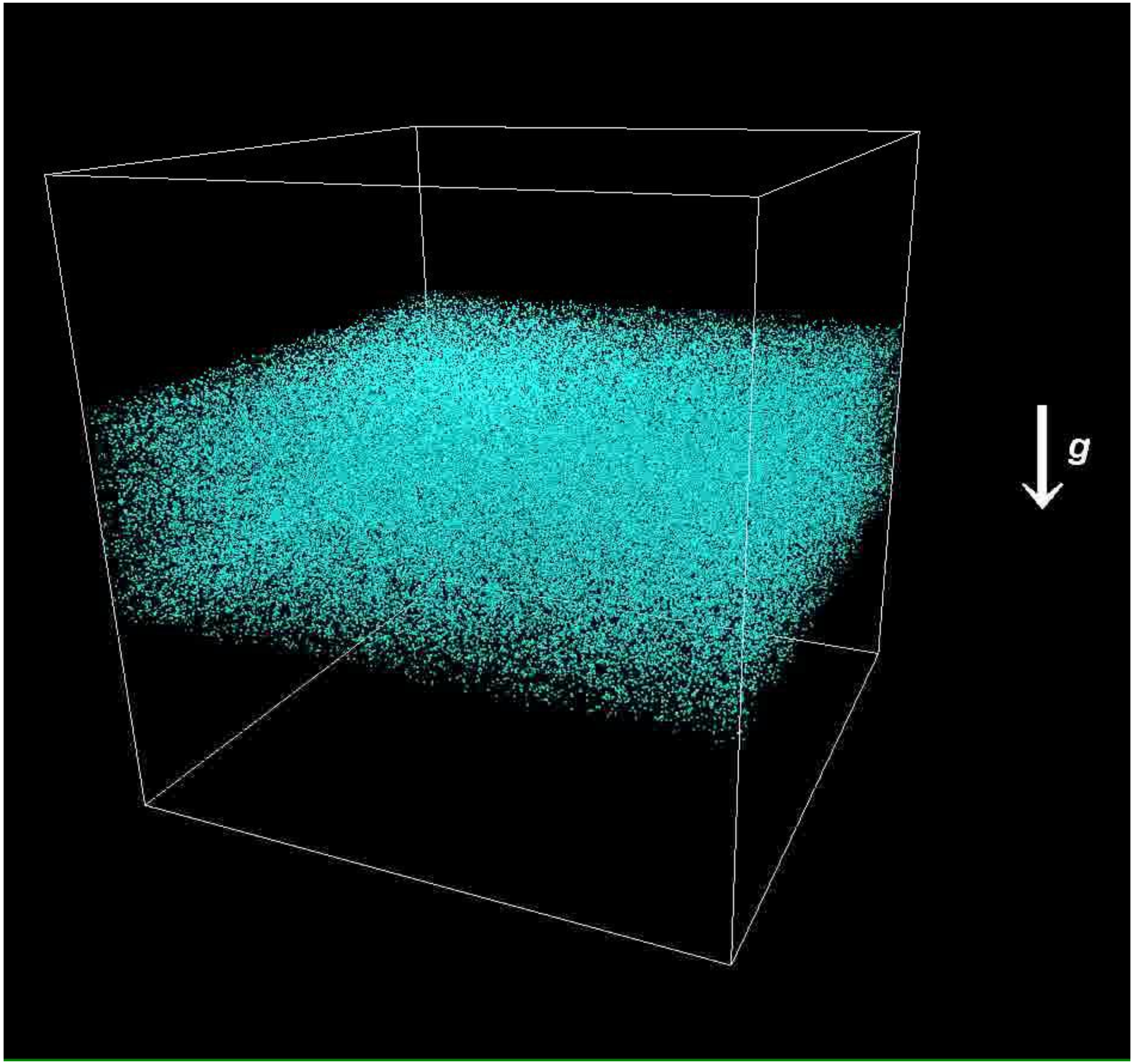
$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{1}{\rho_a}\nabla p + \nu_a \nabla^2 \boldsymbol{u} + B\boldsymbol{e}_3 + \boldsymbol{f}$$

	Initially steady	Decay wet	Decay dry
External force F	ON	OFF	OFF
Buoyancy B	OFF	ON	OFF

	A	B	C’	C”	C	D(A)	E(B)
N^3	128^3	128^3	128^3	128^3	1024^3	1024^3	1024^3
N_p	2^{21}	2^{21}	2^{22}	2^{19}	2^{25}	2^{27}	2^{27}
n_p [cm^{-3}]	125	125	250	31	31	125	125
q_v	やせる	ふとる	ふとる	ふとる	ふとる	やせる	ふとる
θ‘	0	0	0	0	0.05K	0	0
R_λ	92	92	92	92	252	252	252
$K_{max}\eta$	1.2	1.2	1.2	1.2	2.1	2.1	2.1
r(0) [μm]	20	20	15	15	15	20	20

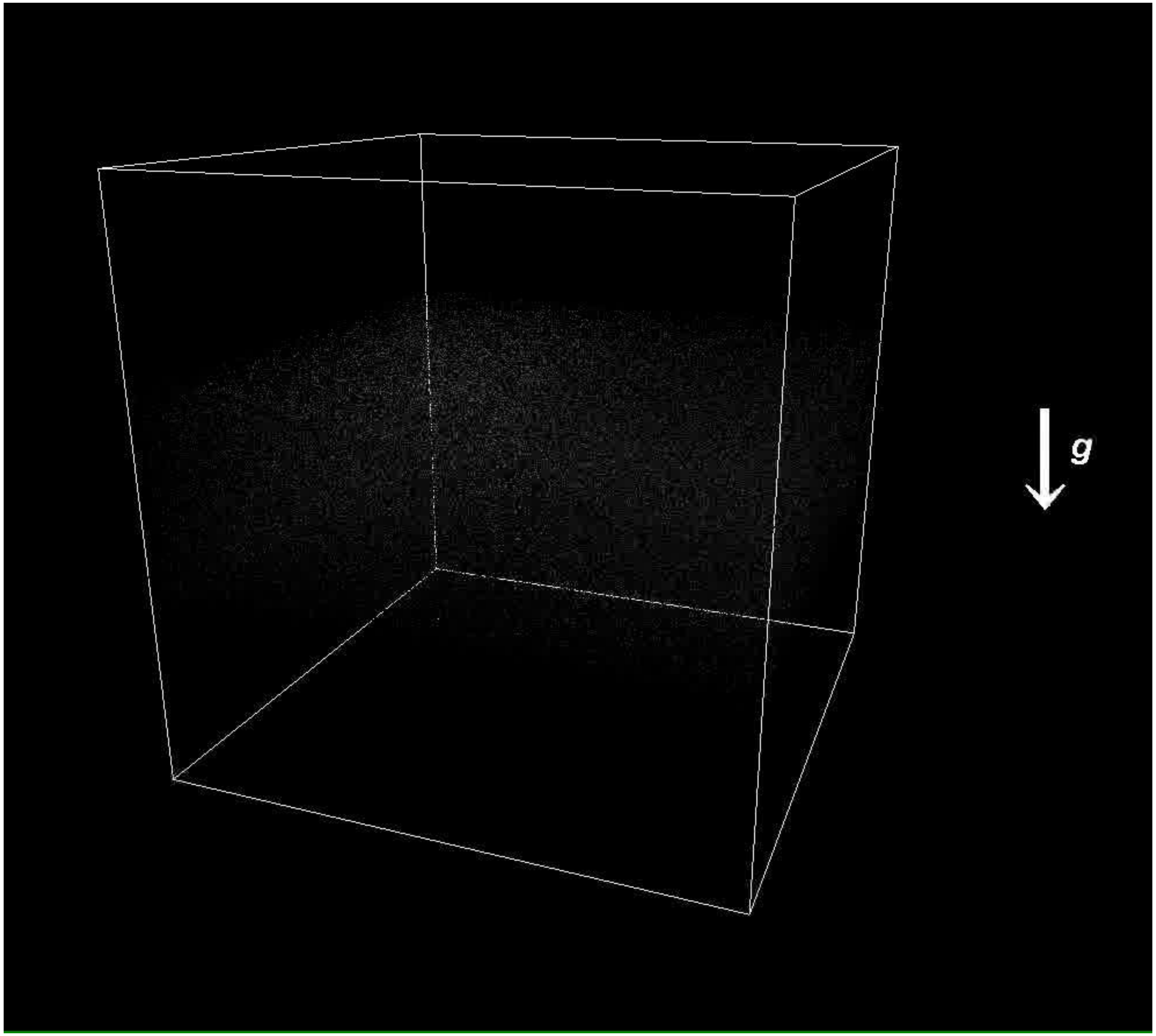
雲粒子　ふとる　$M_{\rm vs} \leq M_{\rm v} + M_{\rm l} \Longleftrightarrow \rho_{\rm a}\int_V q_{\rm vs} {\rm d}V \leq \rho_{\rm a}\int_V q_{\rm v}(x,t){\rm d}V + \frac{4}{3}\pi\rho_{\rm l}\sum_{j=1}^{N_{\rm p}} r_j^3$

雲粒子　やせる　$M_{\rm vs} \geq M_{\rm v} + M_{\rm l}$



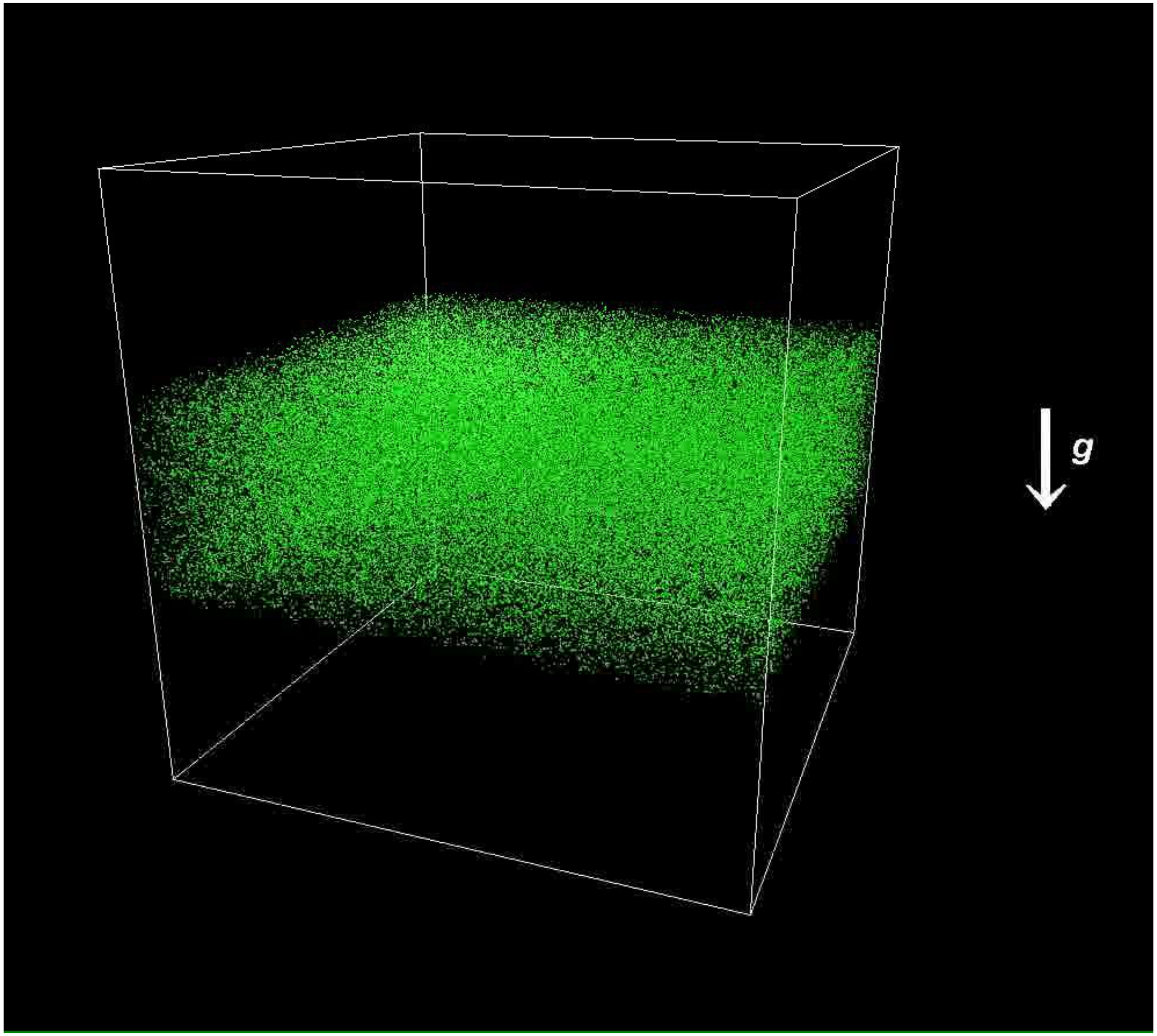
$R_\lambda = 92$

- 境界:3軸方向周期境界条件
- 雲粒子の個数：4×10^6個
- 可視化粒子数：10^5個
- 初期雲粒子半径: 15 μm
- 粒子の色:粒子半径
  赤⇒半径大、 青⇒半径小
- 0s～4sまで可視化



$R_{\lambda} = 252$

- 境界:3軸方向周期境界条件
- 雲粒子の個数：1.3×10^8個
- 可視化粒子数：10^5個
- 初期雲粒子半径: 20 μm
- r >20 μm を黒から白色
- 0s～6s まで可視化

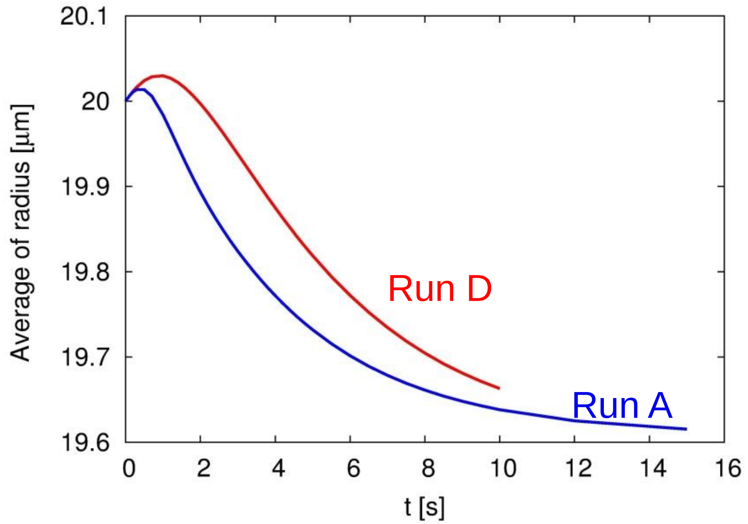


$R_\lambda = 252$

- 境界:3軸方向周期境界条件
- 雲粒子の個数：1.3×10^8個
- 可視化粒子数：10^5個
- 初期雲粒子半径: 20 μm
- 粒子の色:粒子半径
  赤⇒半径大、 青⇒半径小
- 0s～6sまで可視化

Effects of Reynolds number

Run A ($R_\lambda = 92$) and D ($R_\lambda = 252$)

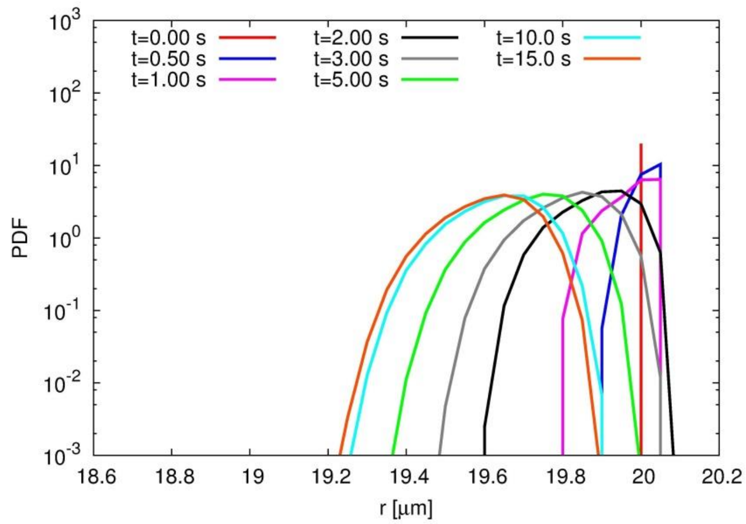


When R_λ increases

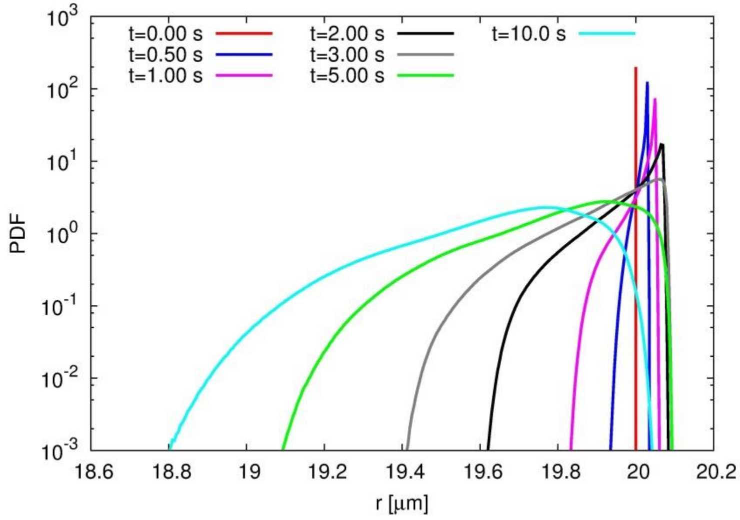
<r> → slowly decrease

PDF → broad

Run A

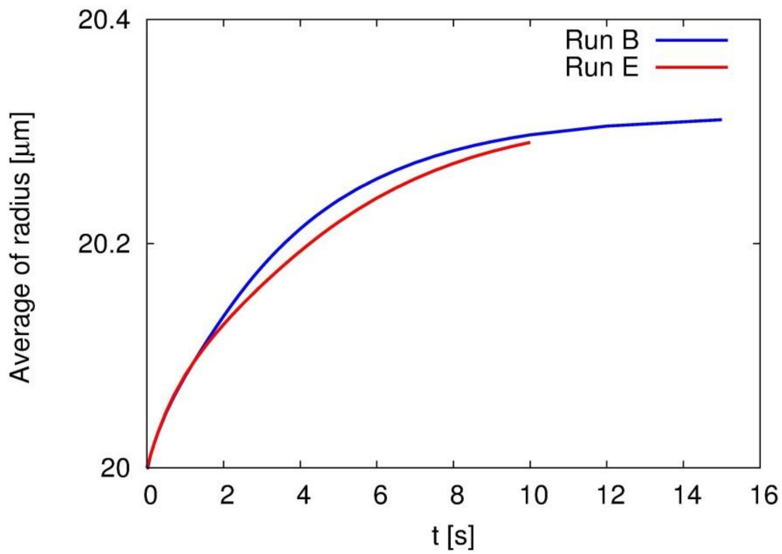


Run D



Effects of Reynolds number

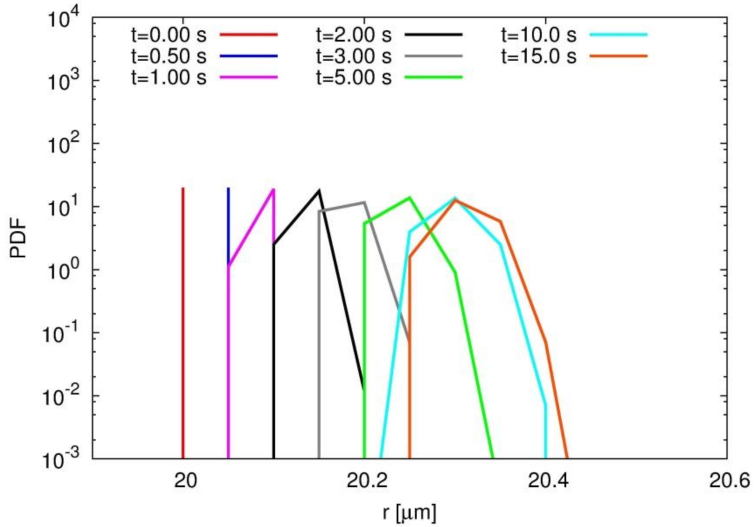
Run B (R_λ=92) and E(R_λ=252)



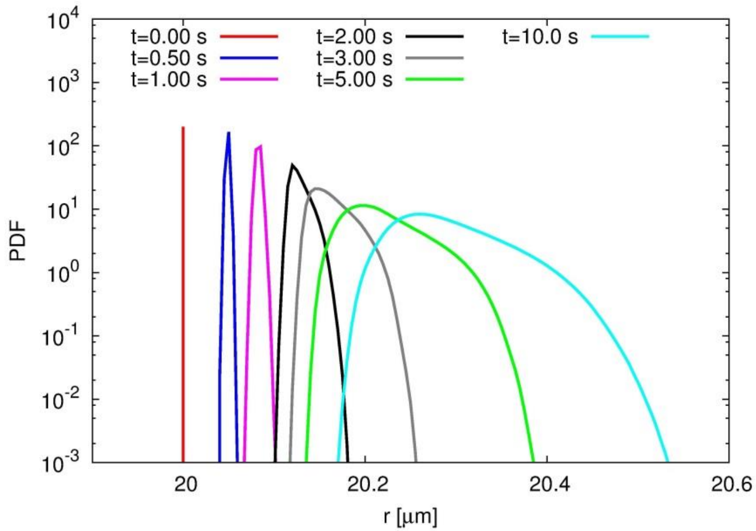
When R_λ increases

<r> → comparable
PDF → broad

Run B

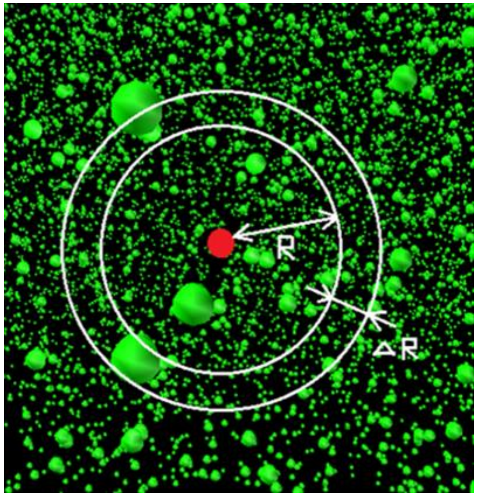


Run E



Radial distribution function of cloud droplets

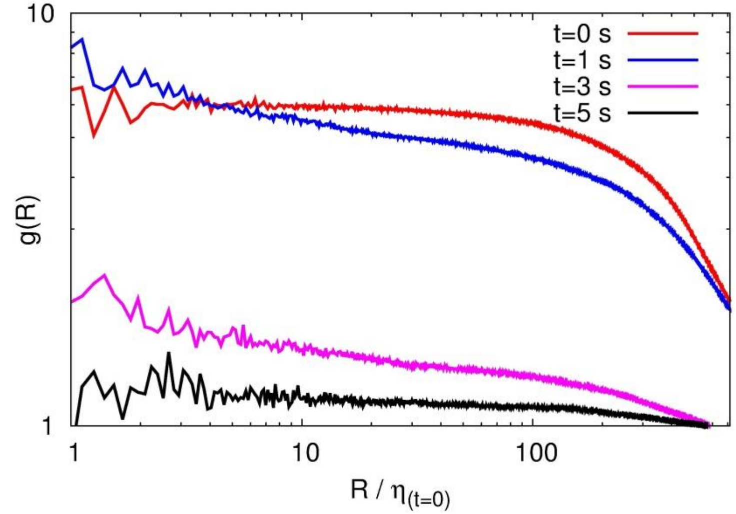
$$g(R) = \frac{G(R)}{4\pi R^2 n_d \Delta R}$$



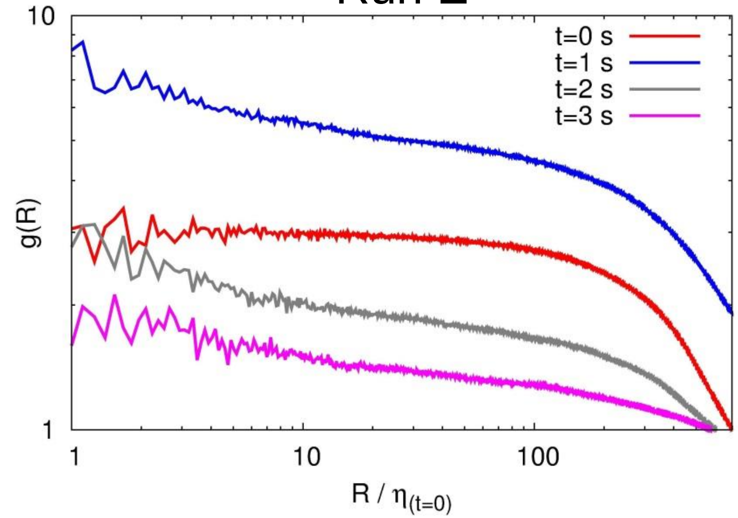
$G(R)\Delta R$: No. of particles within spherical shell between R and ΔR

n_d : Average number density

Run D

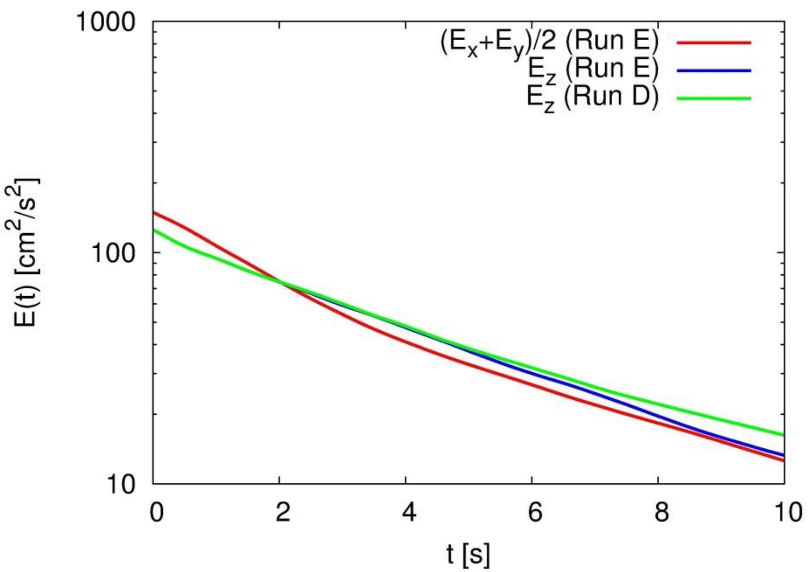


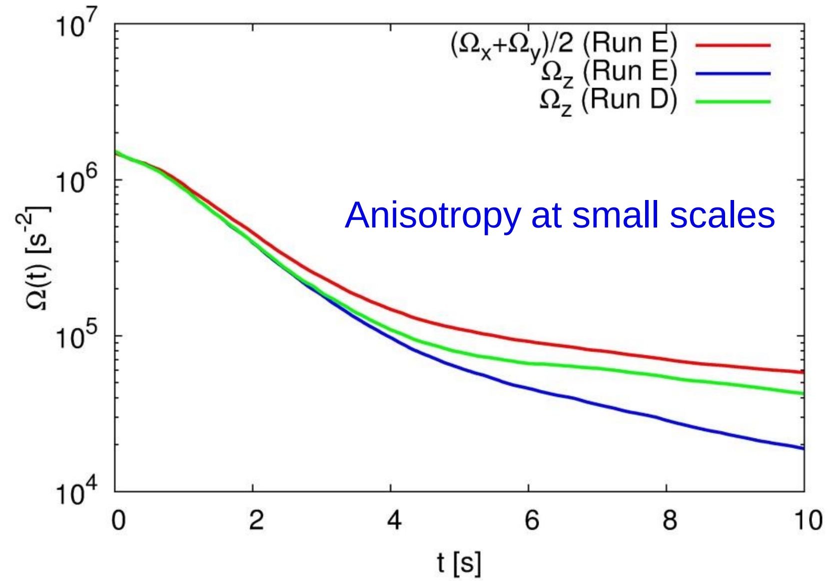
Run E



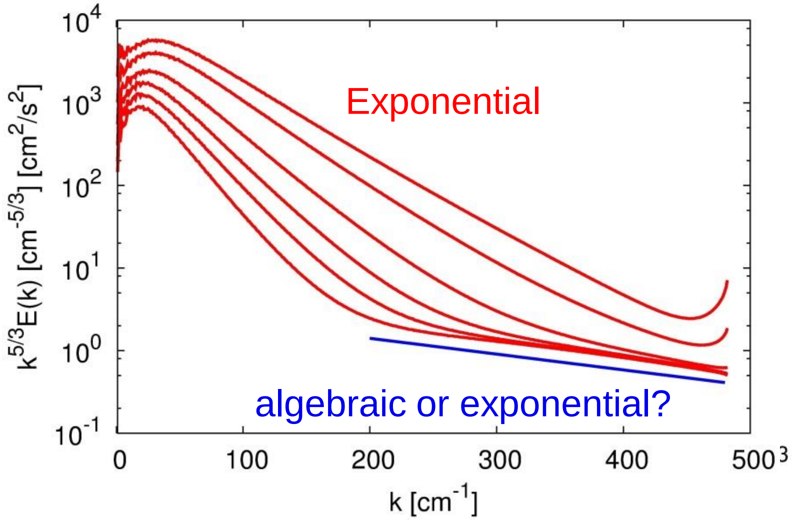
Power low $g(R) \propto R^{-\alpha}$

Turbulence modulation

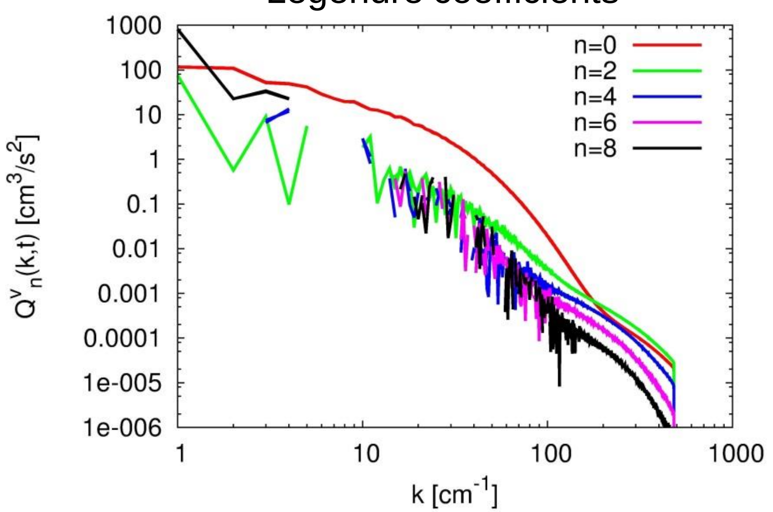




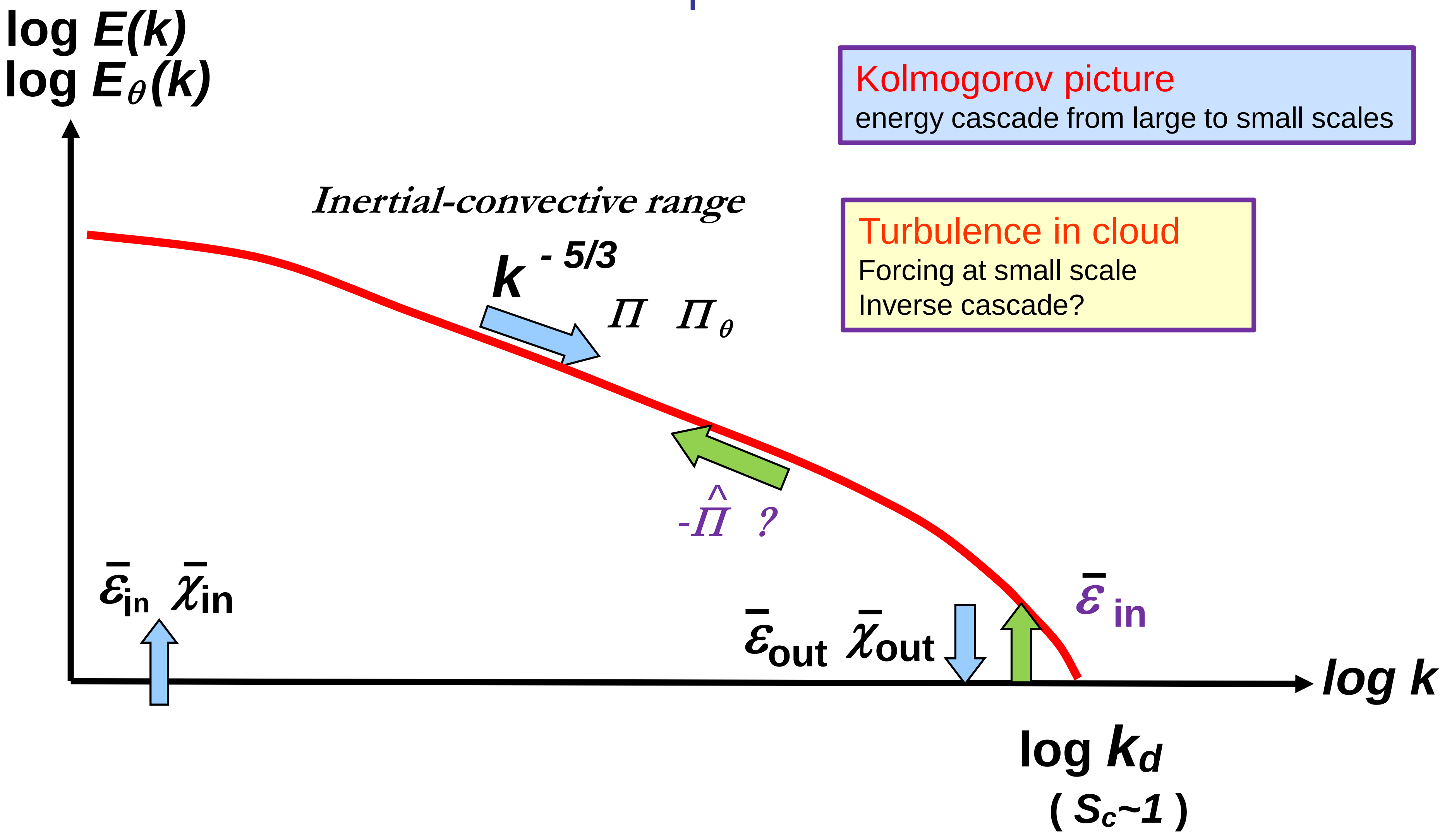
Spectrum modulation begins at high wavenumbers and proceeds low wavenumbers



Legendre coefficients



Turbulence spectrum



Contribution of buoyancy force

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = -\nabla p + \nu \nabla^2 u + e_z B + f, \qquad \nabla \cdot u = 0$$

$$B = g\left(\frac{T - T_0}{T_0} + \epsilon(q_v - q_{v0}) - q_l\right) = B_\theta + B_q + B_l$$

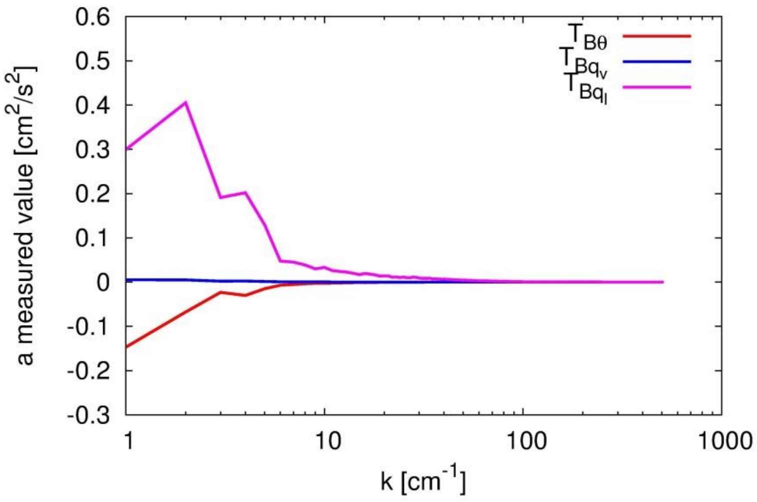
$$\frac{DE}{Dt} = -\epsilon + P_B, \qquad P_B = \langle B u_3 \rangle = \int T_B(k,t) dk$$

$$T_B(k,t) = 2 \sum_{\text{shell}} \text{Real}\left(\langle B_\theta(k,t) u_3(-k,t)\rangle + \langle B_q(k,t) u_3(-k,t)\rangle + \langle B_l(k,t) u_3(-k,t)\rangle\right)$$

$$= T_{B\theta}(k,t) + T_{Bq}(k,t) + T_{Bl}(k,t)$$

dominant

Run E



Summary

- Reynolds number effects (no collision)
  may be small on growth rate of the average particle radius
  broaden PDF of particle radius

- Average growth of cloud droplets governed by diffusion process is very slow
  Needs for particle collision process

- Turbulence modulation begins at small scales due to the cloud droplets and the anisotropic modulation is inversely transferred to large scales

雲粒子間衝突

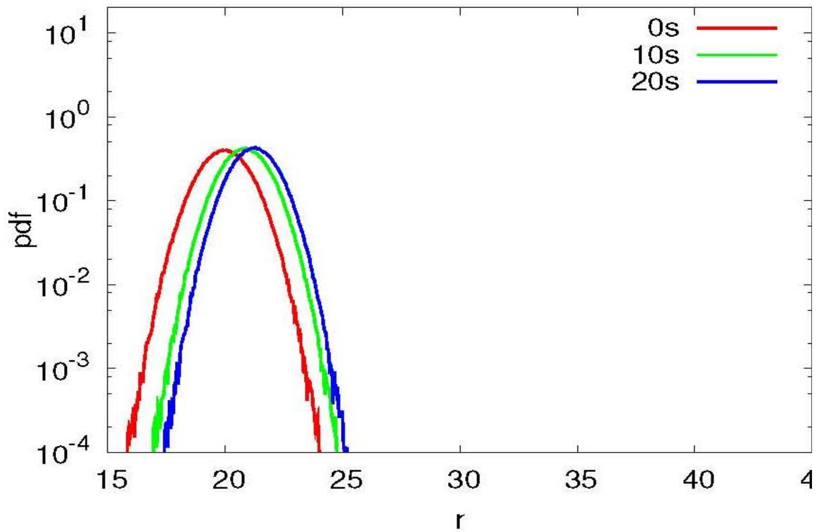
衝突条件

$$r = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} \leq r_i + r_j$$

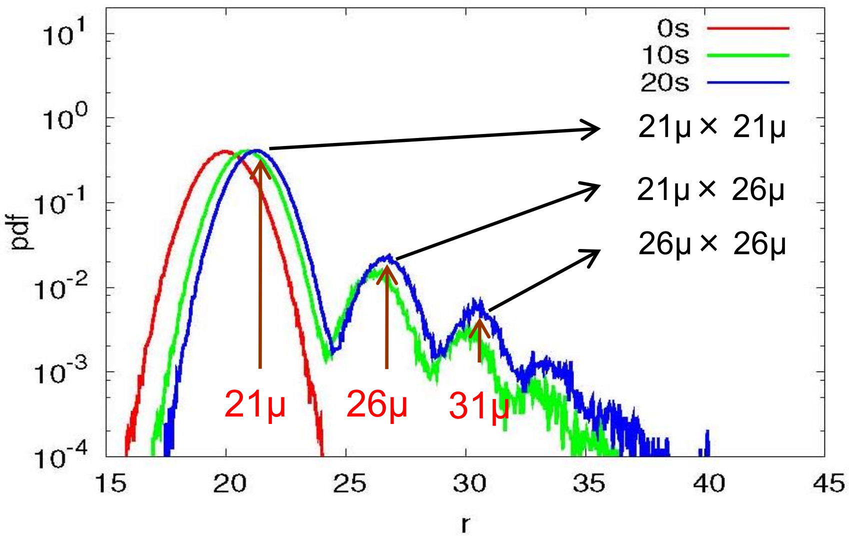
・質量保存 $M_p = M_i + M_j$ → $r_p^3 = r_i^3 + r_j^3$

・運動量保存 $M_p \boldsymbol{V}_p = M_i \boldsymbol{V}_i + M_j \boldsymbol{V}_j$ → $\boldsymbol{V}_p = \dfrac{M_i \boldsymbol{V}_i + M_j \boldsymbol{V}_j}{M_p}$

衝突・合体なし

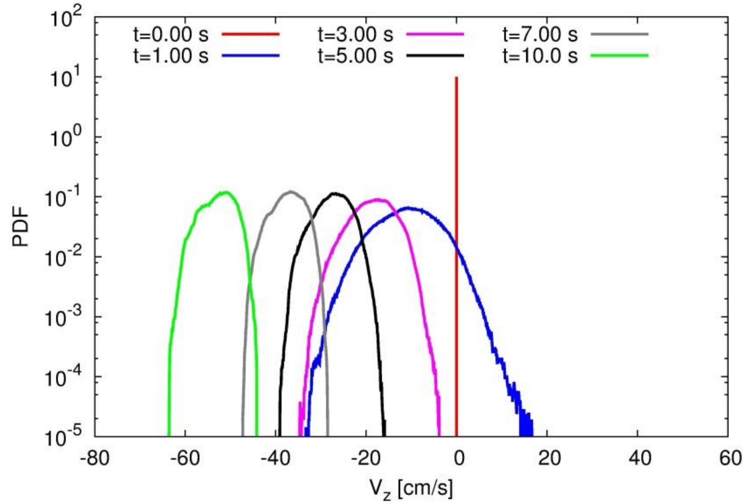


衝突・合体あり

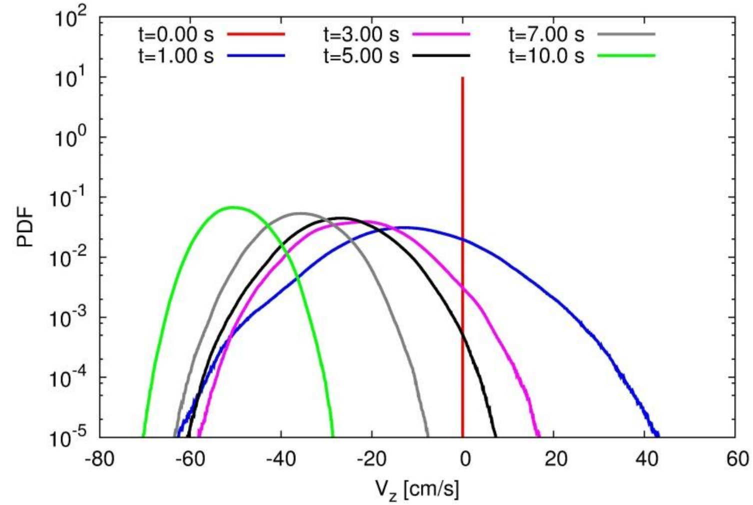


PDF of vertical velocity of cloud droplets

$R_\lambda = 92$



$R_\lambda = 252$



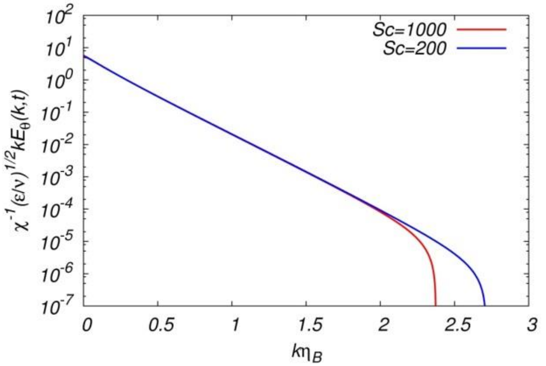
When R_λ increases

Wider PDF of u_3 → More chance to collide

Larger R_λ → Faster growth and wider PDF of r

Other progress

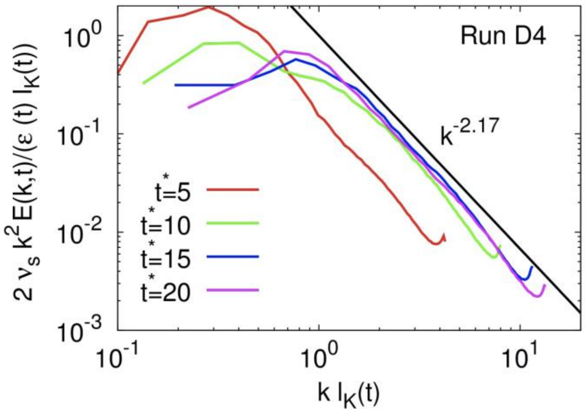
- Scalar spectrum at Sc=1000



$$E_{1\theta}(k) = C_B \chi (\epsilon/\nu)^{-1/2} k^{-1} \exp\left(-\sqrt{6C_B} k\eta_B\right)$$

Gotoh

- Polymer effects on turbulence



Power low behavior of the energy spectrum in the far dissipation range

Watanabe and Gotoh

- Fast Time-reversible method for MD of water molecules

Kajima and Ogata

Acknowledgements

HPC, CC at Nagoya Univ