Numerical study of droplet growth by condensation by means of massive DNS simulations

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Eulerian vs. Lagrangian methods for cloud microphysics Workshop

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Rain formation

- Activation of Cloud Condensation Nuclei (CCN)
- Growth by condensation
- Growth by mixing/collision due to turbulence
- Growth by gravitational collision

Turbulence and droplet Condensation DNS: a Brief Excursus

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- turbulence has been indicated as the key missing link to solve condensation/ collision coalescence problem
- first DNS of turbulence/cloud interactions done by Vaillancourt et al. 2002. Domain 10cm, resolution 80^3 grid points, droplets 50000→ Conclusion: negligible effect of the small-scale turbulence on droplet spectra broadening
- Celani et al. 2007, resolving large-scale fluctuations 2D cloud→ Conclusion: dramatic increase in the width of the droplet spectrum is qualitatively found although the dynamics of the small scales is not resolved
- Paolo & Sharif, 2009, same conclusions but 3D simulation obtained adding an arbitrary large-scale forcing on the supersaturation equation field.
- Current state of the art: Lanotte et al 2009, 3D DNS simulations increasing size of the cloud up to 70 cm→ turbulence affects droplet spectra broadening mechanism by increasing the cloud size.

Spectral broadening due to turbulence

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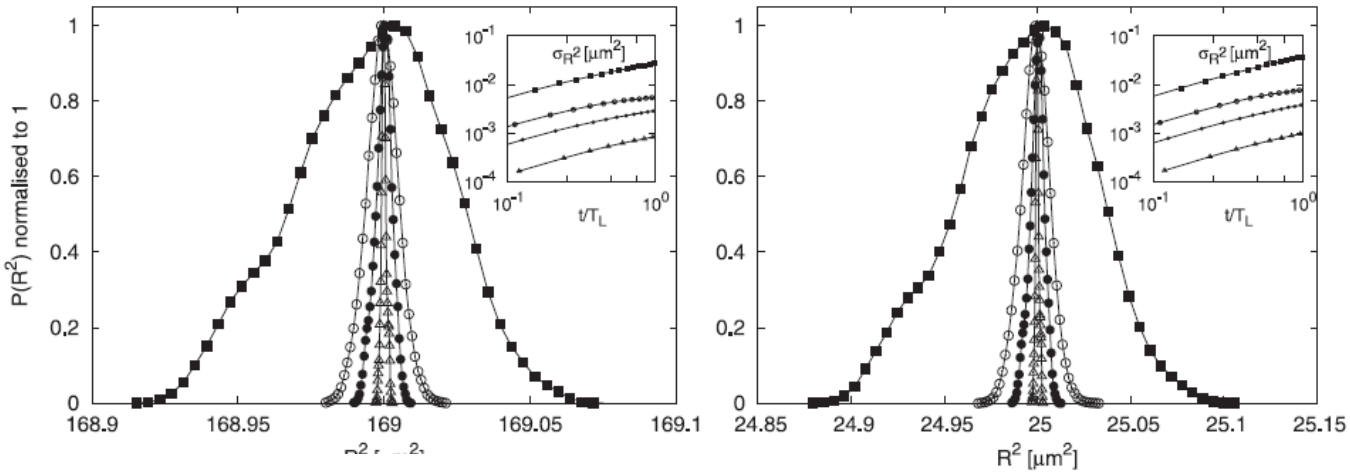

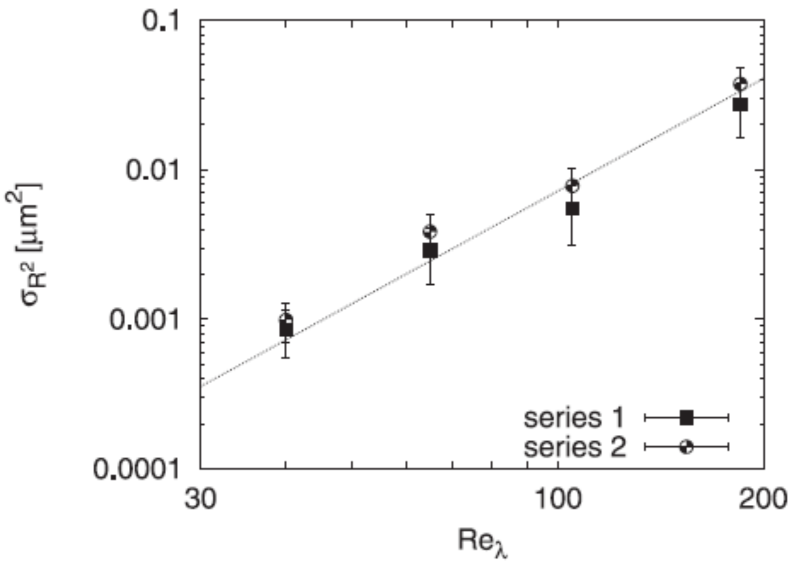

- Increase of standard deviation with Reynolds number : Importance of large scales
- Upper limit $T_L < \tau_s$

$$\sigma_{R^2} \propto A_3 A_1 v_\eta \tau_\eta^2 Re_\lambda^{5/2}$$

- Lower limit $T_L > \tau_s$

$$\sigma_{R^2} \propto A_3 A_1 v_\eta \tau_\eta \tau_s Re_\lambda^{3/2}$$

Lanotte, Seminara, Toschi, JAS 2009

Our objectives

1) Has Droplet spectra variance in warm cloud been well approximated so far?

2) Metodologies: -Direct Numerical Simulation DNS

3) Current simulation time seconds/2 minutes→ up to 20 minutes

Turbulence and condensation: mathematical model

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Eulerian framework: Navier-Stokes + supersaturation field s
→ s>0 condensation s<0 evaporation

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{f}, \quad \nabla \cdot \mathbf{u} = 0$$

$$\partial_t s + \mathbf{u} \cdot \nabla s = \kappa \nabla^2 s + A_1 w - \frac{s}{\tau_s}$$

$$\tau_s^{-1} = \frac{4\pi \rho_w A_2 A_3}{V} \sum_{i=1}^{N} R_i$$

Possible large scale forcing of supersaturation

Phase relaxation time scale

Lagrangian framework: droplet dynamics

$$\frac{d\mathbf{V}_i(t)}{dt} = -\frac{\mathbf{V}_i - \mathbf{v}_i[\mathbf{X}_i(t), t]}{\tau_d} + g\mathbf{z}$$

$$\frac{d\mathbf{X}_i(t)}{dt} = \mathbf{V}_i(t)$$

$$\frac{dR_i(t)}{dt} = A_3 \frac{s[\mathbf{X}_i(t), t]}{R_i(t)}$$

Droplet modeled as point particles

Force acting on droplets: Stokes drag and gravity

Same formulation of Lanotte et al., JAS 2009

Numerical Methodology

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- Combined Eulerian/Lagrangian Solver
- Pseudo-spectral code
- 2/3 rule for dealiasing
- Tri-linear interpolation to evaluate fluid velocity and saturation field at the droplet position
- Tri-linear extrapolation to calculate droplet feedback on the saturation field
- Full MPI parallelization for both carrier and dispersed phase
- Computational time step linearly scales up to 10000 cores → huge simulations

Simulations parameters

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Label	N^3	L_{box} $[m]$	v_{rms} $[m/s]$	T_L $[s]$	T_0 $[s]$	Re_λ	N_d
DNS A1/2	64^3	0.08	0.035	2.3	0.64	45	6×10^4
DNS B1/2	128^3	0.2	0.05	4	0.95	95	9.8×10^5
DNS C1/2	256^3	0.4	0.066	6	1.5	150	9×10^6
DNS D1	1024^3	1.5	0.11	14	3	390	4.4×10^8
DNS E1	2048^3	3	0.12	30	4	600	$3. \times 10^9$
LES E1	512^3	100	0.7	142	33	5000	1.3×10^{14}

- Dissipation rate: $\varepsilon = 10^{-3} \quad m^2 s^{-3}$
- Kolmogorov scale: $\eta = 1 \quad mm$
- Kolmogorov time: $\tau_\eta = 0.1 \quad s$
- Initial Radius: 13 µm (1) 5 µm (2) $St_\eta = 3.5E - 2 \div 5E - 3$
- Phase relaxation time: 2.5 s (1) 7 s (2) $C = 130/cm^3$

Typical value found in stratocumuli

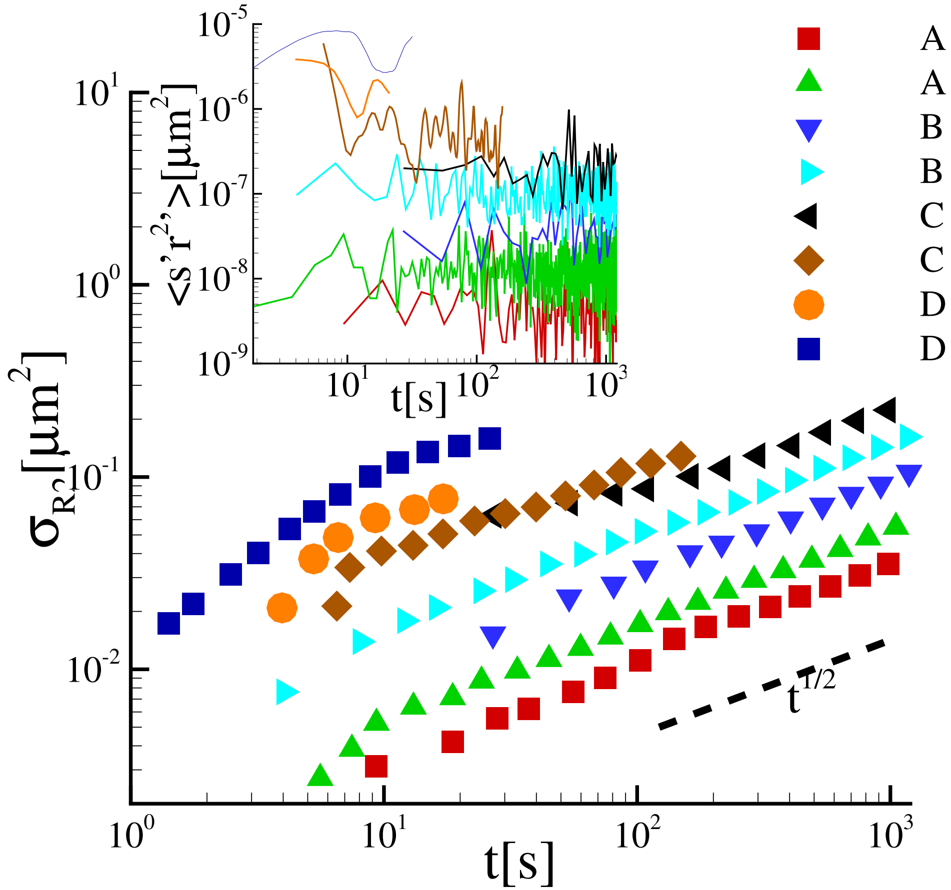
DNS E1: state of the art with 1024^3 grid point resolution corresponding to a domain length of 1.5 meters with 10^9 droplets evolved. First DNS with cloud size order meter.

E1, C2 and D1 do not reach 20 minutes of simulation

Conservative hypothesis

- We assume <s>=0 → all is due to s fluctuations
- No mean updraft
- Consequently $<R^2>=R_0^2$
- Entrainment effects are not considered (Kumar, Schumacher and Shaw, JAS 2014)
- Adiabatic approximation→ small temperature fluctuations (DNS D1 T_rms=0.005 K)→ A_1, A_2, A_3 costants
- Effects due to inhomogeneity are not captured
- Collisions not included
- Our results represent a lower limit on droplet growth

DNS results



- σ_{R^2} standard deviation of square radius fluctuations
- Standard deviation increases continuosly even if s has reached the quasi steady state
- Power law $t^{1/2}$
- Proportional to Re_λ and τ_s
- Larger scales are responsible for variance growth
- Correlation $\langle s' R^{2'} \rangle$ reaches a quasi-steady state

$$\frac{d\langle (R_i^{2'})^2 \rangle}{dt} = \frac{d\sigma^2_{R^2}}{dt} = 4A_3 \langle s' R^{2'} \rangle$$

1-D stochastic model/1

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$$w_i'(t+dt) = w_i'(t) - \frac{w_i'(t)}{T_0}dt + v_{rms}\sqrt{2\frac{dt}{T_0}}\xi_i(t)$$

$$s_i'(t+dt) = s_i'(t) - \frac{s_i'}{T_0}dt + A_1 w_i' dt - \frac{s_i'}{\langle \tau_s \rangle}dt +$$
$$+\sqrt{(1-C_{ws}^2)\langle s'^2\rangle \frac{2dt}{T_0}}\eta_i(t) + C_{ws}\sqrt{\langle s'^2\rangle\frac{2dt}{T_0}}\xi_i(t)$$

$$R_i^{2'}(t+dt) = R_i^{2'}(t) + 2A_3 s_i' dt$$

$$C_{ws} = \langle w's'\rangle / (v_{rms}\sqrt{\langle s'^2\rangle})$$

velocity/supersaturation auto-correlation

$$T_0$$

Large eddy turn over time

1-D stochastic model/2

$$\frac{d\langle s' R^{2'} \rangle}{dt} = A_1 \langle w' R^{2'} \rangle + 2A_3 \langle s'^2 \rangle - \frac{\langle s' R^{2'} \rangle}{\langle \tau_s \rangle}$$

$$\frac{d\langle w' R^{2'} \rangle}{dt} = 2A_3 \langle w' s' \rangle - \frac{\langle w' R^{2'} \rangle}{T_0}$$

$$\frac{d\langle s'^2 \rangle}{dt} = 2A_1 \langle w' s' \rangle - 2\frac{\langle s'^2 \rangle}{\langle \tau_s \rangle}$$

$$\frac{d\langle w' s' \rangle}{dt} = A_1 v_{rms}^2 - \frac{\langle w' s' \rangle}{\langle \tau_s \rangle}$$

Steady state→

$$\langle s'^2 \rangle_{qs} = A_1^2 v_{rms}^2 \langle \tau_s \rangle^2$$

$$\langle s' R^{2'} \rangle_{qs} = 2A_3 A_1^2 v_{rms}^2 \langle \tau_s \rangle^2 T_0 = 2A_3 \langle s'^2 \rangle_{qs} T_0$$

and consequently

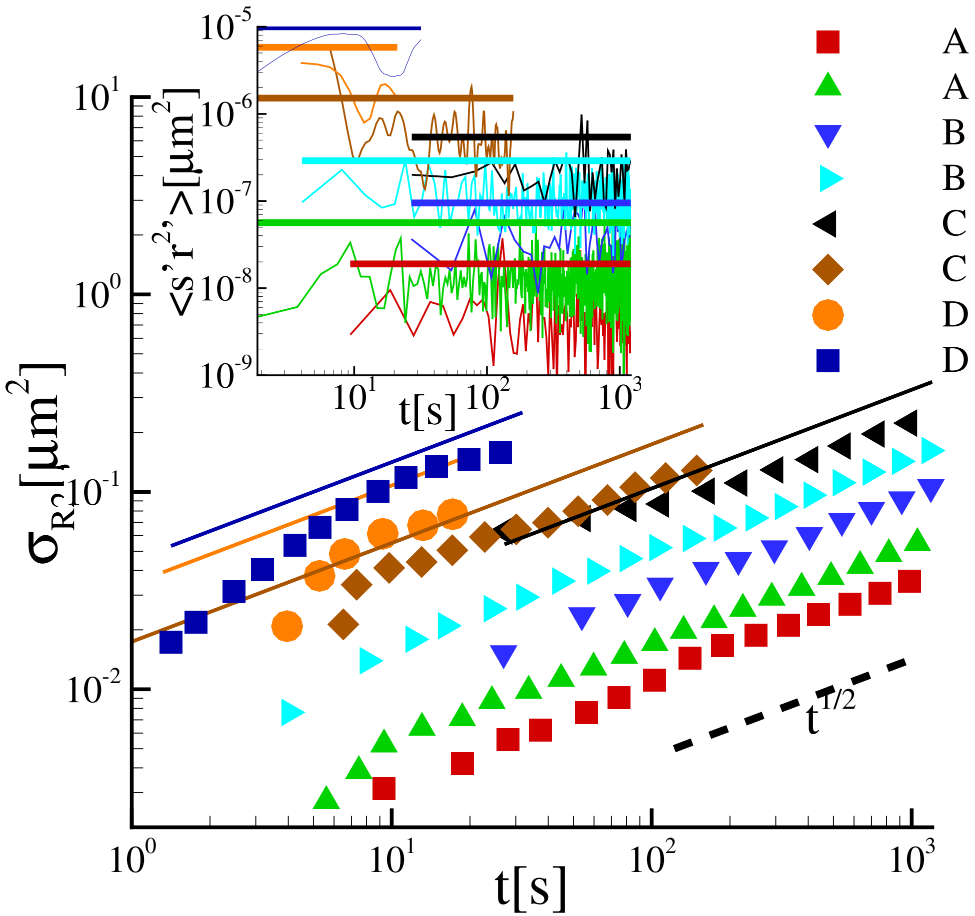
$$\sigma_{R^2} = \sqrt{8} A_3 A_1 v_{rms} \langle \tau_s \rangle (T_0 t)^{1/2} = \sqrt{8 \langle s'^2 \rangle_{qs}} A_3 (T_0 t)^{1/2}$$

since $v_{rms} \simeq Re_\lambda^{1/2} v_\eta$ and $T_0 \simeq 0.06 Re_\lambda \tau_\eta$

$$\sigma_{R^2} \simeq 0.7 A_3 A_1 \nu^{1/2} \langle \tau_s \rangle Re_\lambda t^{1/2}$$

Standard deviation does not depend on dissipation and so on small scales but is proportional to scale separation

Comparisons with DNS results



- The model approximates the largest simulation
- Smallest simulations are influenced by viscous effects of the smallest scales
- In general the stochastic model tends to overestimate

Error estimation

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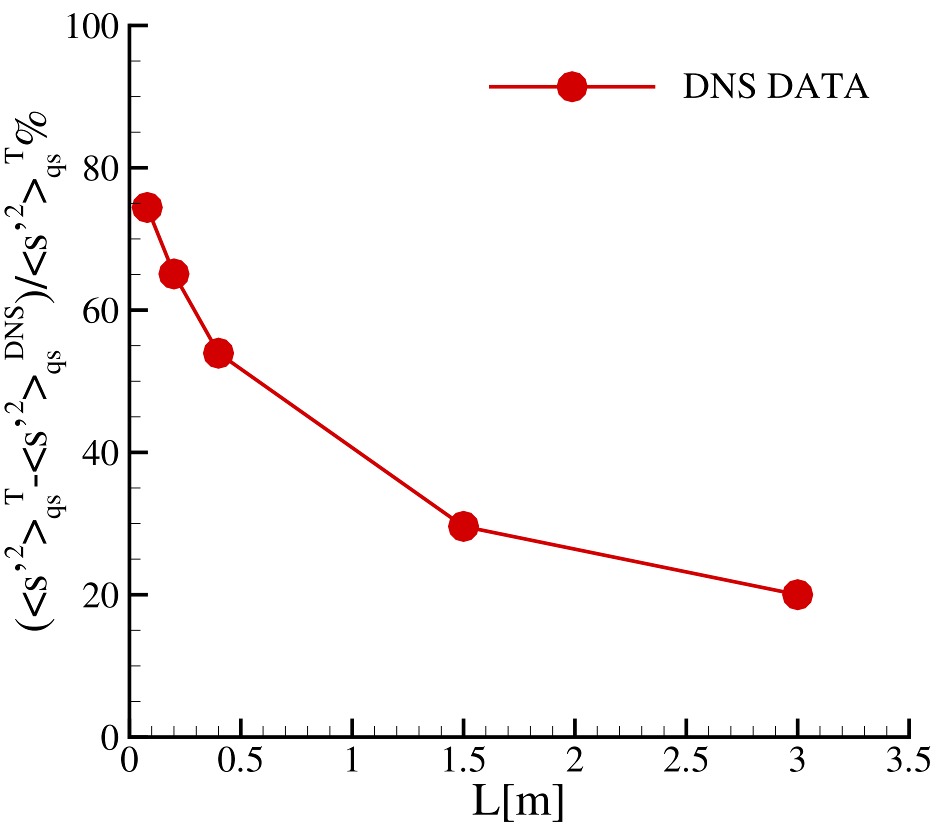
- DNS/Stochastic model comparison
- Estimate of the supersaturation fluctuations



- Stochastic models overestimates but….
- The error tends to diminishing by increasing the large turbulent scales
- 20% is already a good approximation for evaluating the order of magnitude
- We found an upper limit at no cost

Why these differences?

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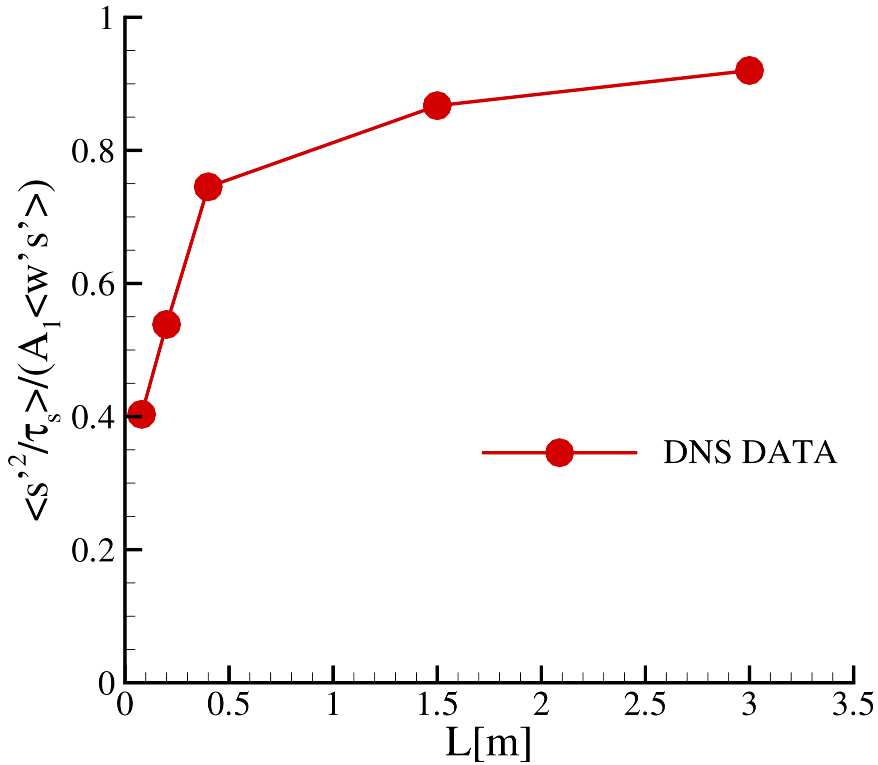
Supersaturation variance equation

$$\underbrace{\frac{D\langle s^2/2\rangle}{Dt}}_{=0,s.s.} = -\underbrace{\kappa\langle(\nabla s)^2\rangle}_{\text{viscous dissipation}<0} + \underbrace{A_1\langle ws\rangle}_{\text{production}>0} - \underbrace{\langle\frac{s^2}{\tau_s}\rangle}_{\text{droplet sink }<0}$$



- Balance between droplet sink and production
- At smallest scales viscous dissipation dominates
- Two different regime and supersaturation balance between small and large scales
- At large scale the s equation tend to the classical Twomey equation

Comparison with Large Eddy Simulation

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- We want to see the effects of the large scale on droplet condensation
- Maximum cloud size in homogeneous conditions order 100 meters
- Classic Smagorinsky model for the fluid velocity and supersaturation field
- Droplet number: order 10^{15} → unfeaseable→ use of renormalization as described in Lanotte et al., 2009
- Parameters $\varepsilon = 10^{-3} \quad m^2 s^{-3}$

$$v_{rms} = 0.7 \quad m/s$$

$$Re_\lambda = 5000$$

Large Eddy Simulation microphysics parametrization

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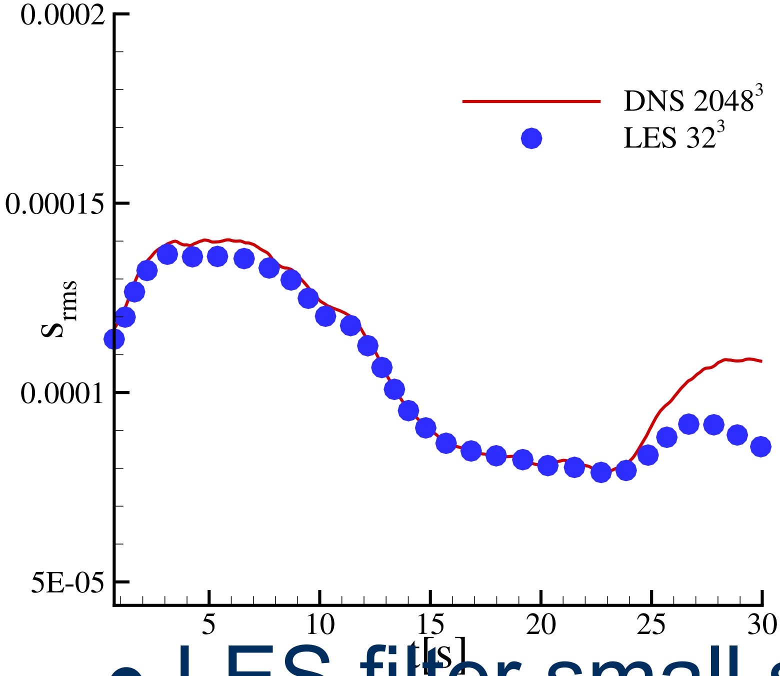
- We assume no sgs-model
- →Supersaturation value is not evaluated at the droplet scale
- LES does not evolve the correct number of droplet→ rescaling
- Equation for droplet radius

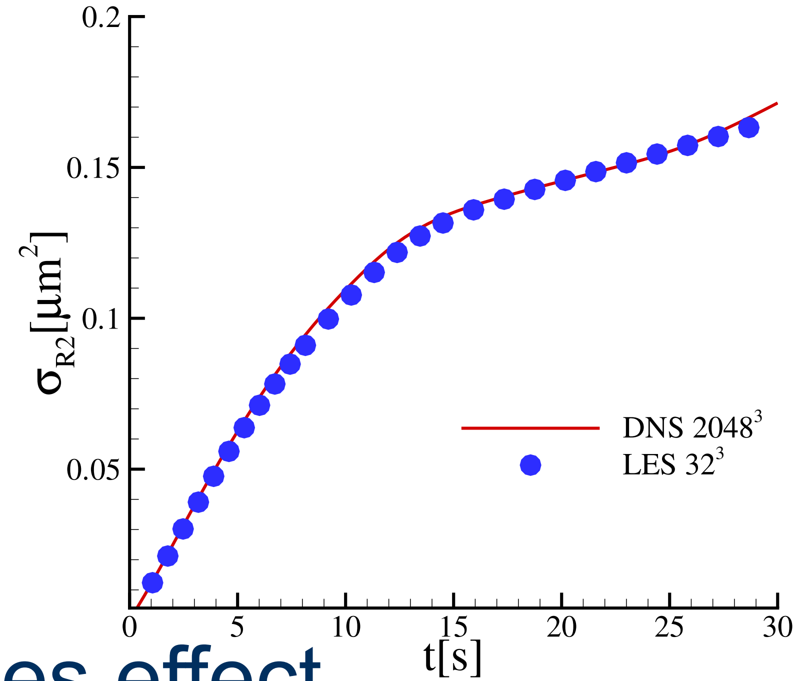
$$\frac{dR_i^2}{dt} = 2A_3(s_{res} + s_{sgs}) --> \frac{d\langle (R_i^{2'})^2 \rangle}{dt} = \frac{d\sigma^2_{R^2}}{dt} = 4A_3(\langle s' R^{2'} \rangle_{res} + \langle s' R^{2'} \rangle_{sgs})$$

- From DNS results $\langle s' R^{2'} \rangle_{res} >> \langle s' R^{2'} \rangle_{sgs}$
- Small scale dynamics is lost→ underestimation
- Now we have a lower limit at moderate cost

$$LES < DNS < Stochastic \quad Model$$

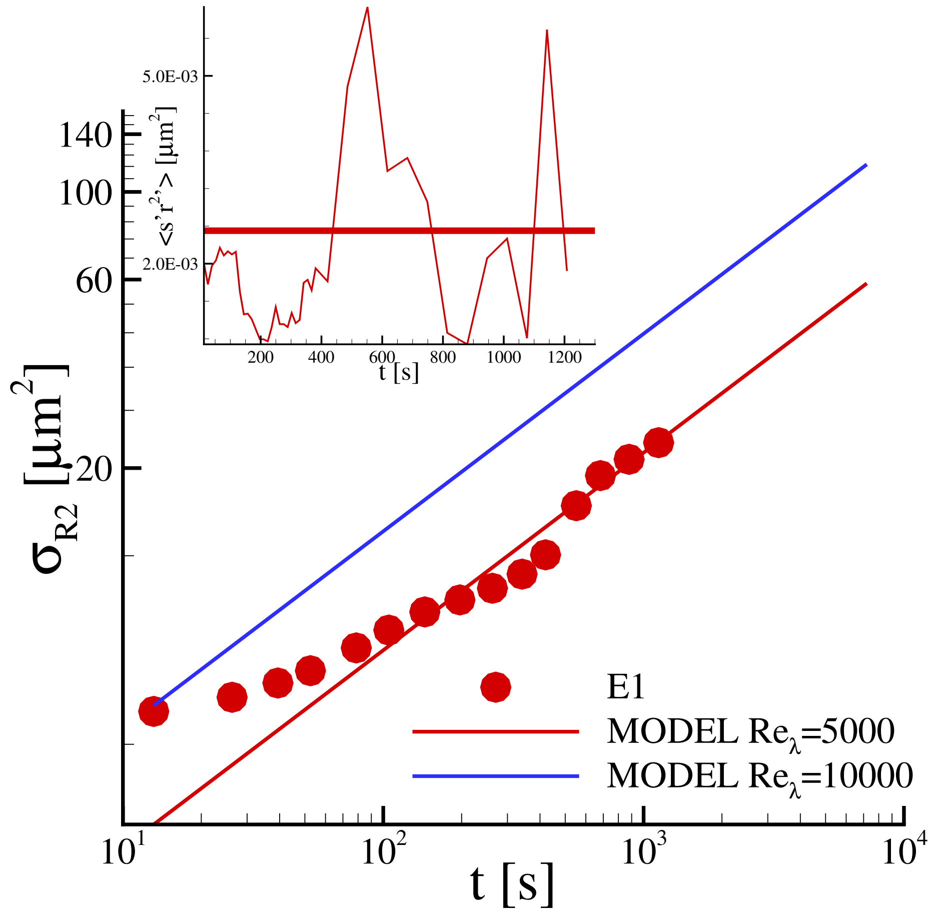
Comparison with large DNS 2048^3





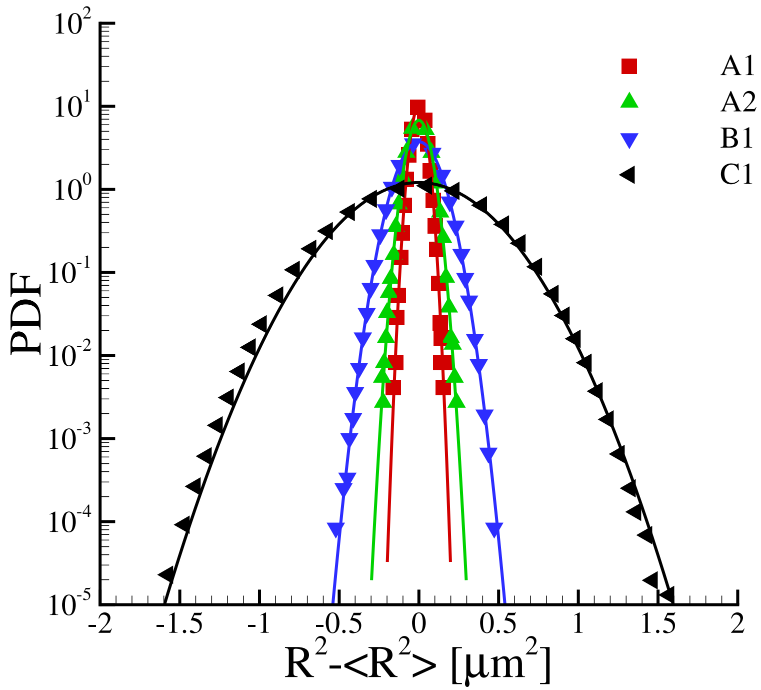
- LES filter small scales effect
- DNS 10 days of computations in 4096 cores on the 32nd TOP500 list supercomputer
- LES almost 1 hour in 1 core on my laptop

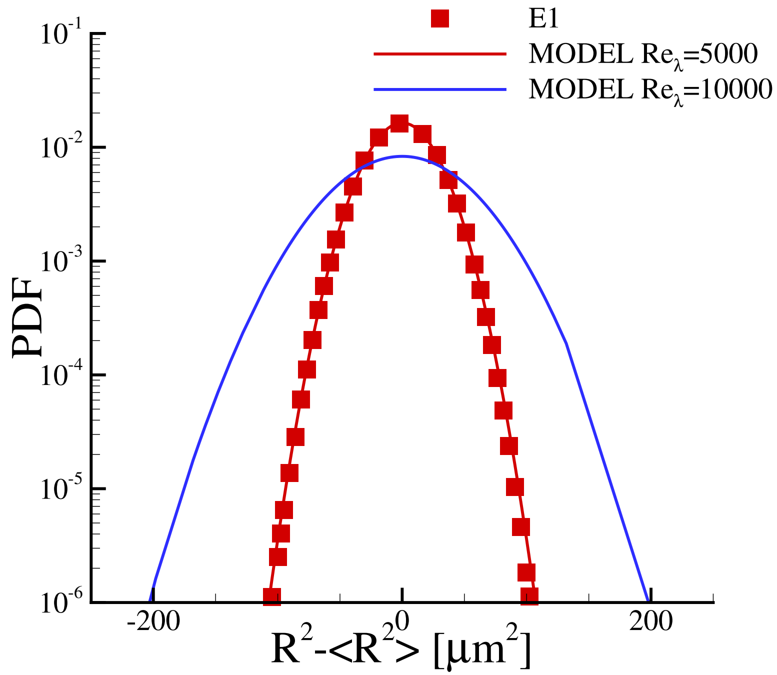
Model vs LES



- Very good agreement for both standard deviation and correlation
- Model extension for higher Reynolds number
- Significant values of standard variation found after several minutes
- Importance to have longer simulations
- Impact of condensation has been underestimated in the last years

Droplet distribution





- Gaussian distribution
- RMS is sufficient to characterize pdf

Conclusions and perspectives/1

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- New state of the art simulations able to reproduce condensation growth with time comparable with rain formation
- Standard deviation of square radius fluctuations increases continuously in time according to a power law
- Importance of large/small scale separation
- Validation of a simple stochastic model that is able to capture all the essential dynamics
- Droplet distribution seems to follow a Gaussian curve

Conclusions and perspectives/2

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- Limit of our study: smallest droplets
- Include Köhler model of nucleation of CCN in our model
- Will the rms continue to increase or the final droplet distribution will reach a steady state?
- Combining condensation+collisions
- Difficult but maybe more interesting since
- Condensation—>large scale
- Collision→ small scales and difficult to include in LES/stochastic models