Massively Parallel Pseudo-Spectral DNS and LES for Particle-Laden Turbulent Flows under Two-Way Momentum Coupling

(MSc Thesis Defense Presentation)

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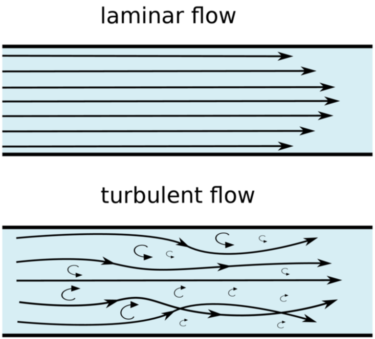
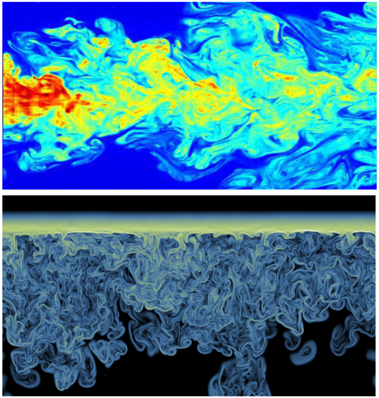
Outline

Introduction

Turbulent Flow



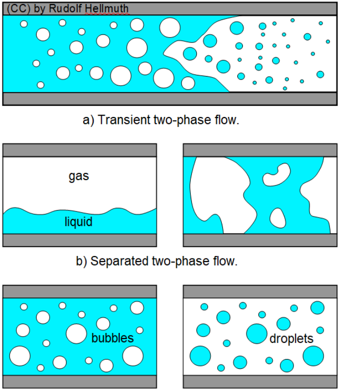
Source: www.cfdsupport.com/OpenFOAM-Training-by-CFD-Support/node334.html



Source: https://www.nortekgroup.com/knowledge-center/wiki/new-to-turbulent-flow-1

Turbulent flow, "not steady", involves fluctuations and vortices at different scales, that get smaller when energy is dissipated due to viscosity (*energy cascade*).

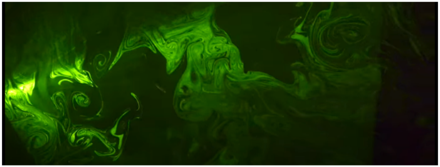
Particle-Laden Flow



a) Transient two-phase flow.

b) Separated two-phase flow.

c) Dispersed two-phase flow.



Source:https://www.youtube.com/watch?v=_UoTTq651dE&ab_channel=3Blue1Brown

Source: https://www.infectioncontroltoday.com/view/sneezing-produces-complex-fluid-cascade-not-simple-spray

Particle-laden flow, with two phases interacting with each other: *continuous* (fluid) and *disperse* (particles, that are insoluble and immiscible).

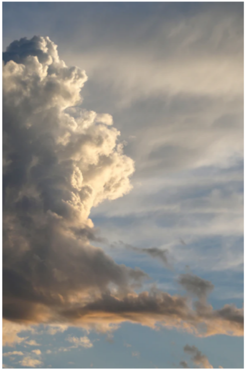
Real-Life Applications

INDUSTRY TECHNOLOGY

– combustion of pulverized coal
– transport in pipelines (bubbles)
– combustion of liquid fuel
– furnace dust handling

ECOLOGY AGRICULTURE

– spraying of fertilizers, etc.
– transport of pollutants
– transport of sediments in water



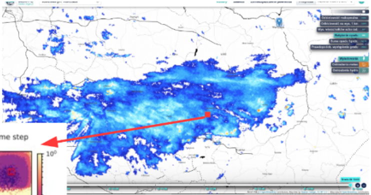
METEOROLOGY CLIMATE SCIENCE

– modelling of atmospheric clouds (i.e. small aerosol particles dispersed in the air)

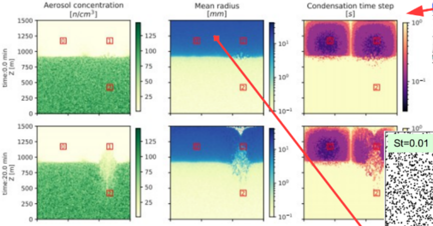
Sources: http://www.chinaeaf.com/products/Dust-collection-system.html; https://www.agairupdate.com/birtle-crop-dusters-add-firefighting-to-their-profile/; Photo by David Ballew (see: https://unsplash.com/photos/pH6-eomaijQ)

Scales in Cloud Modelling (I)

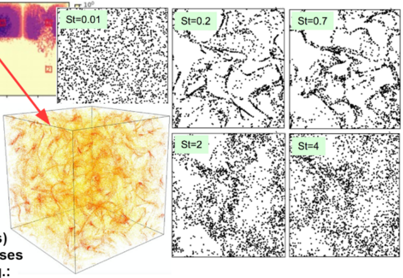
Atmospheric Cloud Modelling



IMGW-PIB METEO Forecasting Model
Domain size: hundreds/thousands of kms
Grid cell size (horizontal): ~2km
(B. Rosa et al.)



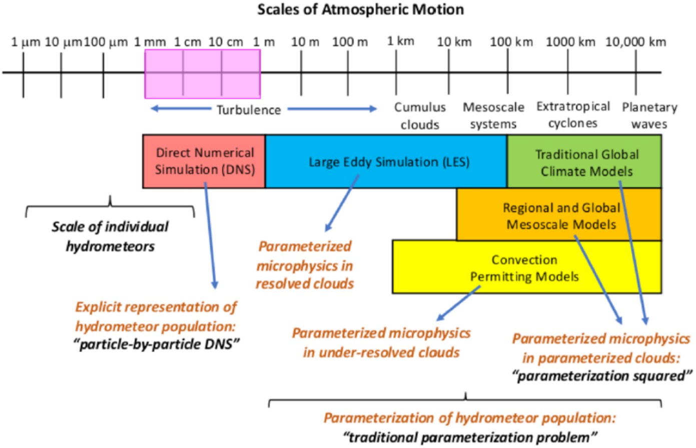
PySDM Cloud Modelling Package (P. Bartman)
Domain size: few kms
Grid cell size: less then m to few m



Our interest:
Domain size: less then m to few m
Grid cell size: order of mm and less

- homogeneous and isotropic turbulence (HIT)
- observation of phenomena specific to this system (e.g. droplet/particle clustering)
- calculation of statistics (e.g. collision kernels) that are needed to parametrize cloud processes In Numerical Weather Prediction models (e.g.: COSMO, WRF, Aladin)

Scales in Cloud Modelling (II)



Modelling Fluid-Particle Interactions

FLOW-ONLY SIMULATION

– uses 3D Navier-Stokes equation (momentum equation for fluids):

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{U}\times\boldsymbol{\omega} - \nabla\left(\frac{P}{\rho}+\frac{1}{2}\mathbf{U}^2\right) + \nu\nabla^2\mathbf{U} + \mathbf{f}(\mathbf{x},t) + \mathbf{f}^{(p)}$$

– due to simple domain shape (3D box) and boundary conditions (periodic), very convenient *spectral method* may be used to solve N-S equation

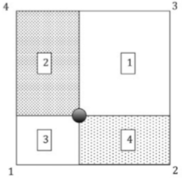
ONE-WAY MOMENTUM COUPLING

– momentum is transferred from fluid to particles

$$\frac{d\mathbf{V}^i(t)}{dt} = -f(Re_p)\frac{\mathbf{V}^i(t)-\mathbf{U}(\mathbf{Y}^i(t),t)}{\tau_p} + \mathbf{g} \quad \Big\| \quad \frac{d\mathbf{Y}^i(t)}{dt} = \mathbf{V}^i(t)$$

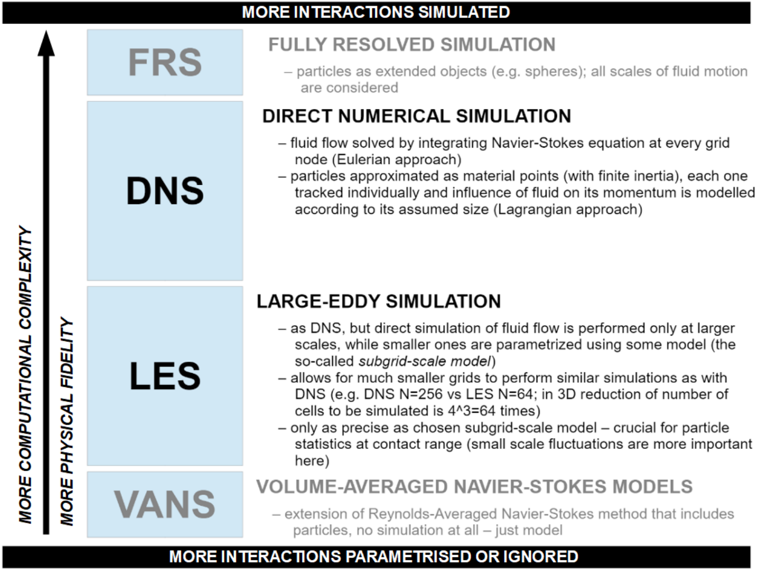
TWO-WAY MOMENTUM COUPLING

– momentum is also transferred from particles to fluid in neighbouring grid nodes (split according to proximity of tracked particle to surrounding 8 grid nodes (projection onto neighbouring nodes (PNN) method)

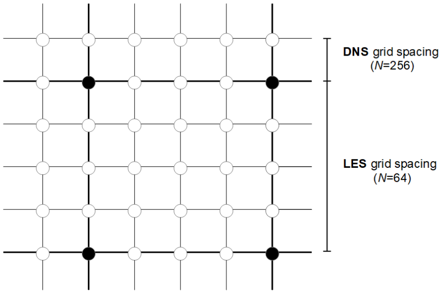


FOUR-WAY MOMENTUM COUPLING

Simulation Methods



Large Eddy Simulations (LES)



- small–scale structures are not directly resolved in simulations (N is smaller, but $k_{\max}$ is smaller as well), but they are parametrised using **subgrid–scale model**,
- quality of that model is important – small–scale interactions are most important for statistics we are calculating.

Rationale

- DNS simulations require a lot of computational resources, hence they are limited to grid sizes that may be insufficient;
- atmospheric air in some conditions exhibit turbulence charcterised by R_λ of around 10^4;
- for DNS with pseudo-spectral method it was shown theoretically (and confirmed by simulations) the attained R_λ increases with N sublinearly ($\propto N^{2/3}$) while node count increases as N^3;
- some larger values recently obtained:
  - $R_\lambda = 597$ for $N = 2048$ (see Ireland, Bragg, Collins, *J. Fluid Mech. 2016*)
  - $R_\lambda = 1300$ for $N = 12\,288$ (without particles; see Buaria, Bodenschatz, Pumir, *Phys. Rev. Fluids* 2020);
- values of order 10^4 seem to be currently out of reach for DNS, therefore another method may be necessary – LES that allows to obtain larger R_λ on smaller grids.

Specific Goals

Two-fold comparison of both methods, DNS and LES, in order to establish LES as a viable alternative in this domain of studying atmospheric phenomena.

In particular:

1. ensure whether the physical fidelity of results obtained by LES are in line with expectations, and are they qualitatively and quantitatively comparable to those from DNS;
2. analyse computational performance of both methods to ascertain advantages of LES and identify its bottlenecks and possible deficiencies.

NOTE: The focus is mainly on the analysis of results for LES under two-way momentum coupling, which constitute major original contribution of this thesis.

Physical Fidelity of DNS and LES

Flow-only Simulations

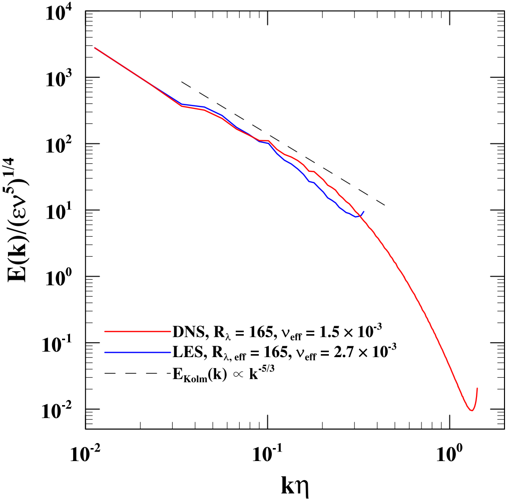
- common initial step is to perform simulations without any particles, only integrating fluid flow so it reaches statistically stationary state;
- fluid–only smulations are dimendsionless;
- it has two main purposes:
    - acquire statistically stationary velocity field to serve as input for further particle-laden simulations,
    - calculate scale statistics that are used as parameters in further simulations;
- key flow parameters:
    - N – *grid nodes per dimension*, determine size of the grid, here: 256 for DNS, and 64 for LES;
    - ν – *numerical viscosity*, dimensionless quantity that simulates viscosity (internal friction) of a fluid which influences creation and dissipation of vortices in the flow (turbulence);
    - Δt – *size of time step in seconds*, needs to be tuned to achieve numerical stability of a system (small enough CFL, Courant number).

Flow Statistics

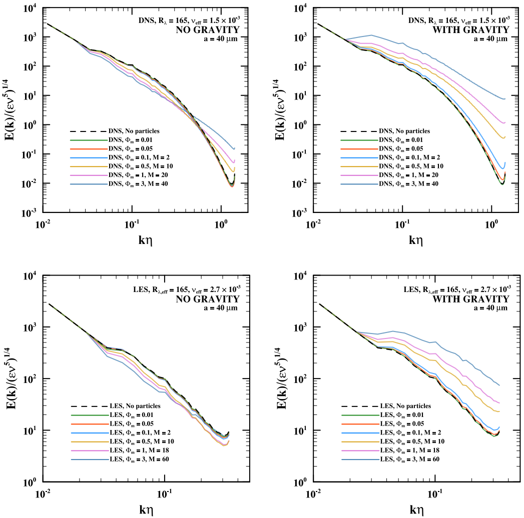
	DNS	LES*	Rosa et al. (2013) DNS
N	256	64	256
$\Delta t \cdot 10^4$	9.0	9.0	9.0
$\nu \cdot 10^3$	1.5	1.5	1.1
u'	0.871 ± 0.001	0.861 ± 0.001	0.868 ± 0.002
ϵ	0.212 ± 0.002	0.200 ± 0.001*	0.200 ± 0.003
$\eta \cdot 10^2$	1.125 ± 0.003	2.078 ± 0.007*	0.903 ± 0.037
$\tau_k \cdot 10^2$	8.436 ± 0.043	15.755 ± 0.122*	7.420 ± 0.620
L_s	1.462 ± 0.003	1.501 ± 0.004	1.496 ± 0.005
$\lambda \cdot 10$	2.851 ± 0.011	5.252 ± 0.014*	2.494 ± 0.015
T_e	3.616 ± 0.028	3.697 ± 0.025*	3.774 ± 0.045
$k_{\max}\eta$	1.423 ± 0.004	—	1.143 ± 0.005
R_λ	165.91 ± 0.51	165.01 ± 0.11*	196.87 ± 0.78

Table 2.1: Parameters and statistics of background turbulent flows in spectral units simulated in this study (first two columns) and these by Rosa et al. (2013), shown for result validation (third column). All listed simulations used deterministic forcing scheme. (* – in LES, statistics marked with * are "effective", i.e. calculated using viscosity adjusted by subgrid-scale model; for more details see Appendix B.

Energy Spectra



Modulated Energy Spectra (TWC)



Radial Distribution Function (1)

"measure of the effect of preferential concentration of droplets on the collision rate"

Basic computation method at contact distances, i.e. for $r = R := a_1 + a_2$. In such case, RDF may be directly computed from definition as:

$$g_{ii}(r;t) = \frac{2N_{pairs}}{N_i(N_i - 1)} \frac{V_s}{V_B}$$

where:

- i – particle radius category;
- N_{pairs} – total number of pairs detected with separation distance r falling into spherical shell of radii $R - \delta$, $R + \delta$ (with small δ, e.g. $\delta = 0.01r$);
- N_i – total number of particles with radius i;
- V_s – volume of probed spherical shell;
- V_B – volume of entire domain (here: $8\pi^3$).

Finally, $g_{ii}(r;t)$ is averaged over time to get $g_{ii}(r = R)$.

Radial Distribution Function (2)

Here, to achieve better results, we calculate above quantity, but for more separation distances than only R (180 shells/bins in range of $[R, 10R]$), then we fit obtained data into power–law dependency:

$$g(r) = c_0(\eta/r)^{c_g(St,S_V)} ,$$

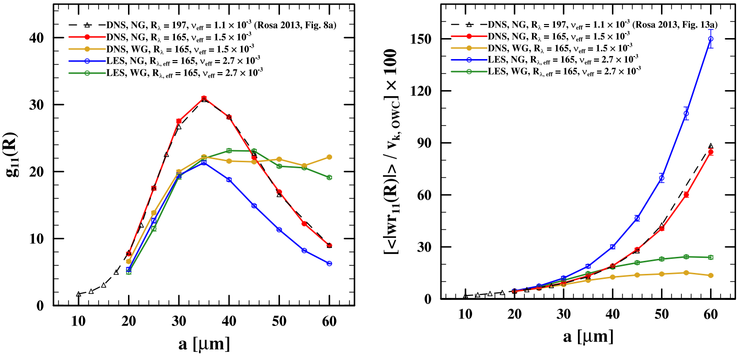
where exponent depends on Stokes' number $(St = \tau_p/\tau_k)$ and settling velocity $(S_V = v_p/v_k)$; c_0 – power law pre–factor.
This allows for more precise estimation of g_{11} at contact distance (R).

Relative Radial Velocity

- statistic measuring relative velocities of particles, more precisely, for any particles: $w_r = \frac{\mathbf{w} \cdot \mathbf{r}}{|\mathbf{r}|}$, where: $\mathbf{w}$ – their relative velocity vector, and $\mathbf{r}$ – their separation;
- computation is similar to that for RDF – velocity bins are fitted to similar power law;
- power law for RRV (normalized by Kolmogorov velocity) is given by:

$$\frac{\langle |w_r(r)| \rangle}{v_k} = c_0(\eta/r)^{c_w(St, S_V)},$$

Kinetic statistics (RDF, RRV) for OWC Simulations



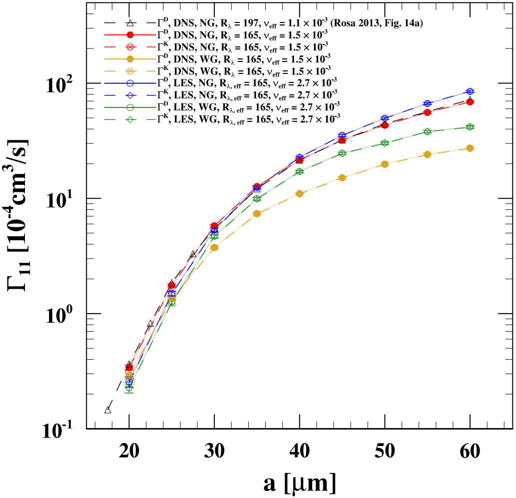
Collision Kernels

- dynamic collision kernel (Γ_{11}^{D}) is defined as the ratio of collision rate to particle pair concentration;
- it can be calculated during simulation by detecting all collision events at each time stem and then averaging it over time;
- alternatively, it was shown that collision kernel, this time referred to as kinematic (Γ_{11}^{K}), may be computed using previously obtained quantities of RDF and RRV at contact distance using following simple formula:

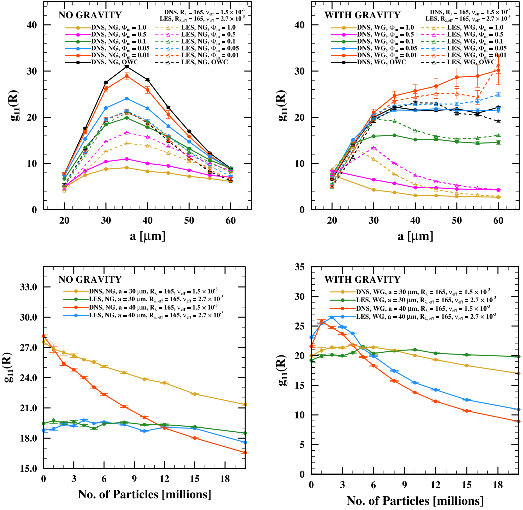
$$\Gamma_{11}^{K} = 2\pi R^2 \langle |w_r|(r = R)\rangle g_{11}(r = R)$$

- values of collision kernels computed using both methods should give same results, which is confirmed by this and previous results.

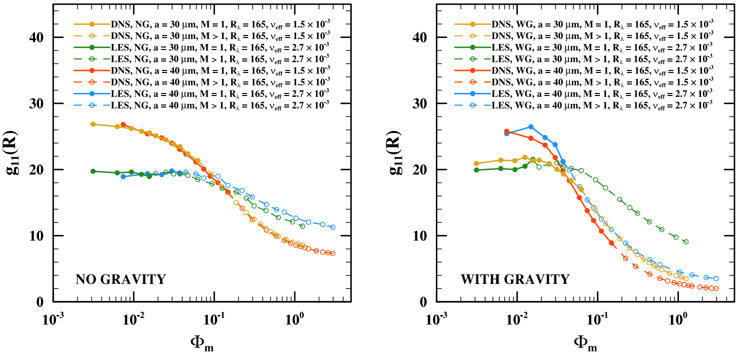
Collision kernels for OWC Simulations



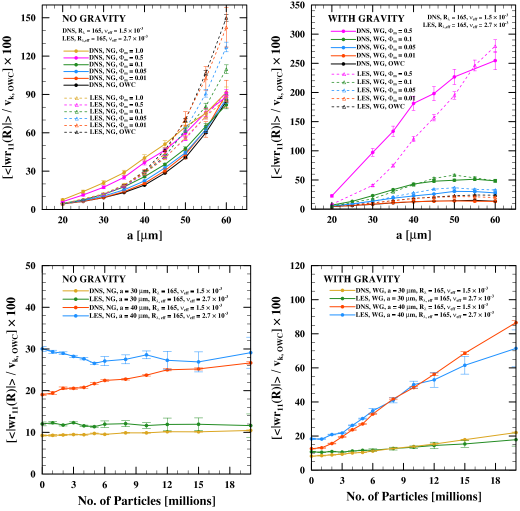
RDF for TWC Simulations (1)



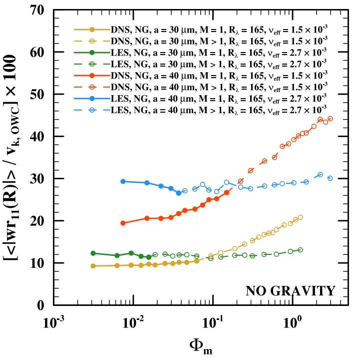
RDF for TWC Simulations (2)

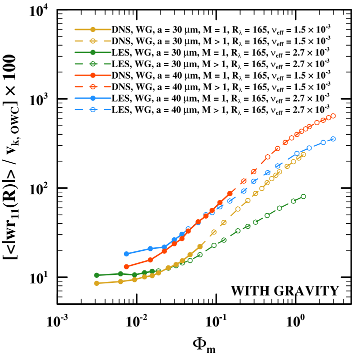


RRV for TWC Simulations (1)

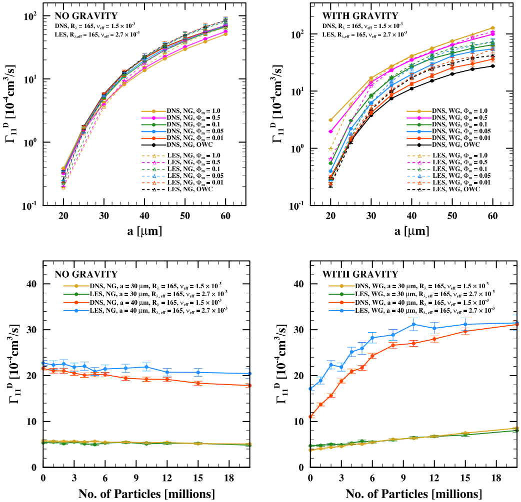


RRV for TWC Simulations (2)

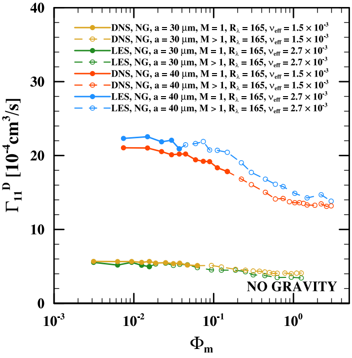


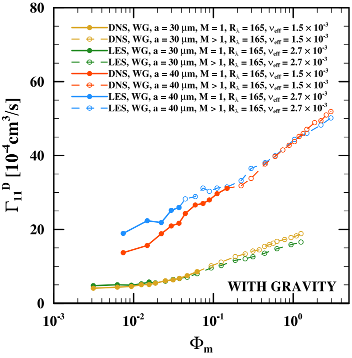


Collision kernels for TWC Simulations (1)



Collision kernels for TWC Simulations (2)





Physical Fidelity - Conclusions (1)

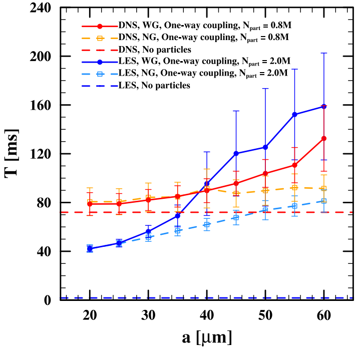
- in general, LES may be considered as a promising alternative to DNS;
- similar effects of subgrid-scale model on TWC as was observed for OWC (e.g. underestimation of the RDF and overestimation of RRV; mostly cancelling each other in case of collision kernel);
- in TWC, such discrepancies diminish with increasing mass loading (esp. for $a = 30\,\mu$);
- results of DNS and LES are more aligned in simulations with gravity.

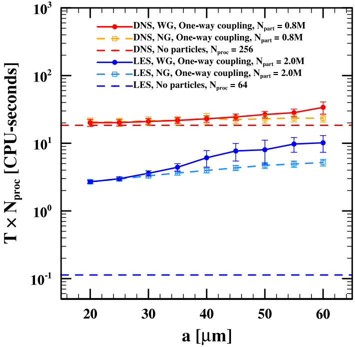
Physical Fidelity - Conclusions (2)

- there are specific cases where mispredictions of LES accumulate – e.g. systems with large amounts of relatively small settling particles that tend to strongly modulate small-scale turbulence, which is filtered in LES, thus leading to significant discrepancies in kinematic particle statistics and collision kernel;
- main challenge - quality of subgrid-scale model and the fact that it is agnostic to the influence of particles on the fluid (any turbulence modulation that affects predominantly small scales has no effect).

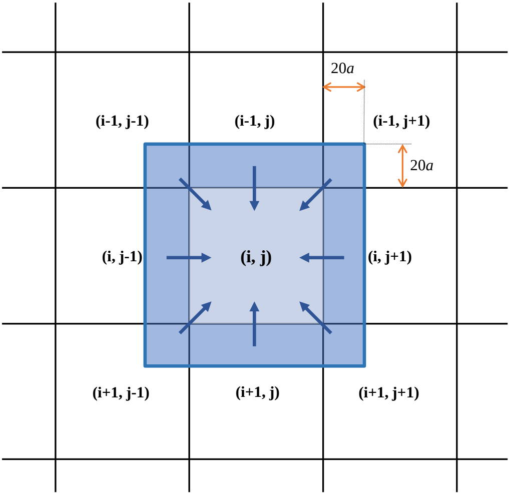
Computational Performance of DNS and LES

Basic Timings – OWC)

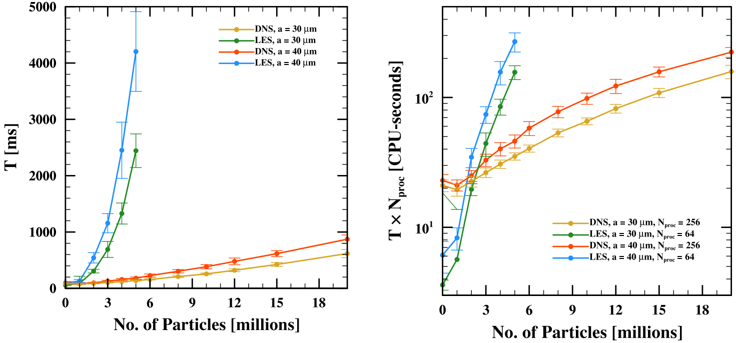




Halo Regions



Basic Timings – TWC

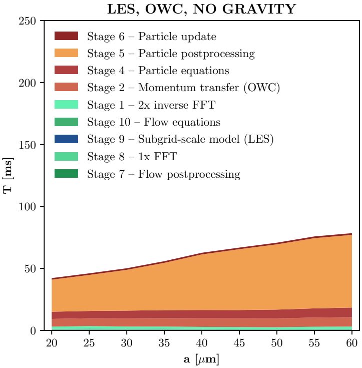


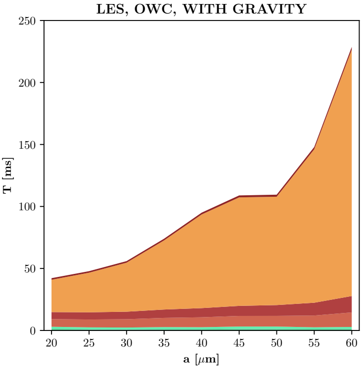
Stages of Single Iteration

No. (Cat.)	Name *Description*	Interdomain communication	Notes
1 (F)	**Transform $\hat{\mathbf{u}}$ and $\hat{\omega}$ to physical space** *Uses inverse 3D FFT twice; first two steps of pseudo-spectral method procedure.*	FFT	Eqn. A.6 and A.7.
2 (P)	**Calc. momentum transfer from fluid to particles** *Finds closest grid points to particles, and calculates momentum transfer using six-point Lagrange interpolation scheme (OWC).*	Local	—
3 (P)	**Calc. momentum transfer from particles to fluid** *Uses PNN kernel to apply momentum transfer projected from particles onto fluid at neighbouring grid points (TWC).*	Local	Eqn. 1.8. **(TWC only)**
4 (P)	**Calc. new particle velocities and positions** *Integrate equations of motion for particles to obtain their new velocities and positions; update data structures used to keep track of neighbouring particles.*	Local	Eqn. 1.5.
5 (Pd)	**Calculate and write particle collision statistics** *Detection a counting of particle collision (Γ_{11}^{D}) and relative particle pair data within radial shells necessary to compute RDF and RRV.*	Global (only to write data), Local	Sec. 2.2.1 and 2.2.2; every step; for steps > 30000 (after system relaxation).
6 (P)	**Update particle velocities and positions** *Change the state of particles as calculated in step 4; transfer data for particles crossing subdomain boundaries.*	Global, Local	—
7 (Fd)	**Calculate and write flow statistics and spectra** *Energy and dissipation spectra are obtained and stored; other base flow statistics (u' and ϵ) and derived statistics are calculated.*	Global, FFT, Local	Sec. 2.1.1 and 2.1.2; every 50 steps*.
8 (F)	**Transform $\mathbf{u} \times \omega$ to spectral space** *Uses 3D FFT to perform third step of pseudo-spectral method procedure; performs post-transform dealiasing.*	FFT	Eqn. A.8.
9 (F)	**Calc. effective viscosity using subgrid-scale model** *Uses fluid energy spectrum and subgrid-scale model formulation to adjust kinematic viscosity with spectral-eddy viscosity, i.e. $\nu + \nu_e(k\|k_c)$.*	Global	Eqn. 1.3 and 1.4. **(LES only)**
10 (F)	**Integrate fluid flow equations** *Fourth step of pseudo-spectral method; integrates 3D Navier-Stokes equation using Crank-Nicholson scheme; incorporates deterministic forcing and other external forces; performs necessary dealiasing and symmetrisation.*	Global, Local	Eqn. A.12

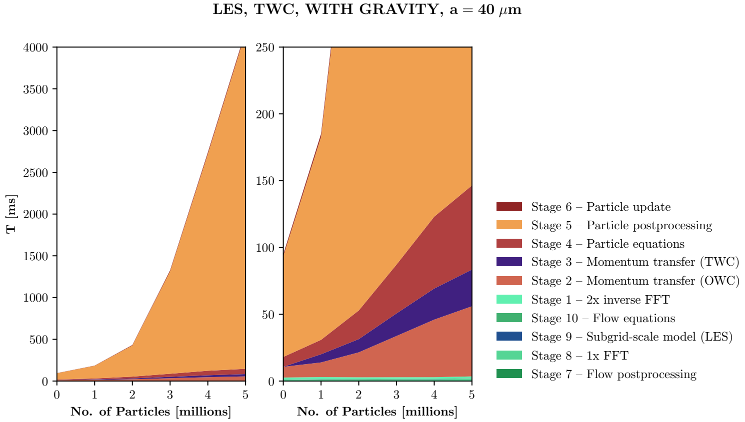
Profile Data – Flow-only and OWC

	N	Stage 7 Postprocessing T_7 [ms]	Stage 8 FFT of $(\mathbf{u} \times \omega)$ T_8 [ms]	Stage 9 SGS model T_{LES} [ms]	Stage 10 Flow eqns.) T_{10} [ms]	Stage 1 2x FFT^{-1} T_1 [ms]	TOTAL T_{F} [ms]
DNS	**256**	2.179 ± 9.571	18.027 ± 1.457	—	6.676 ± 0.371	30.826	55.708 ± 10.934
LES	256	2.193 ± 9.633	17.382 ± 0.902	1.501 ± 0.265	7.135 ± 0.272	31.768	59.981 ± 10.204
LES	**64**	0.067 ± 0.291	0.571 ± 0.055	0.052 ± 0.007	0.155 ± 0.008	0.964	1.808 ± 0.337

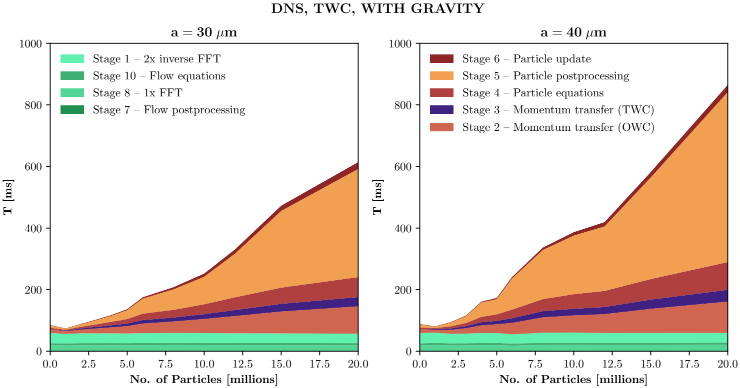




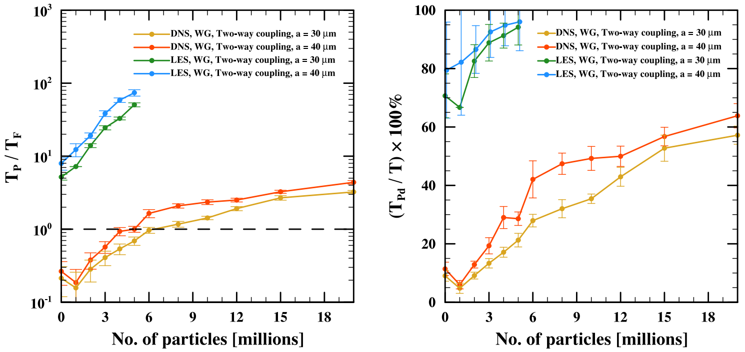
Profile Data – LES TWC



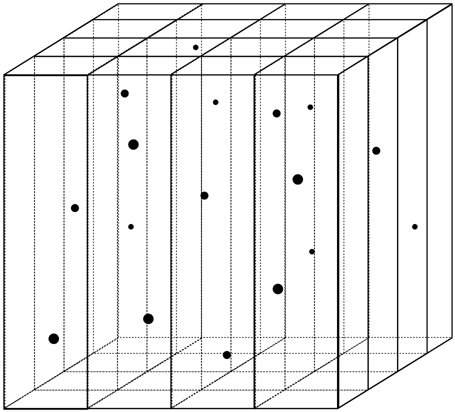
Profile Data – DNS TWC



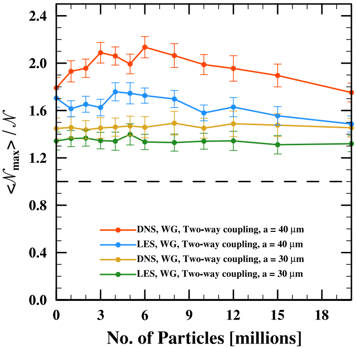
Bottleneck – Particle Postprocessing

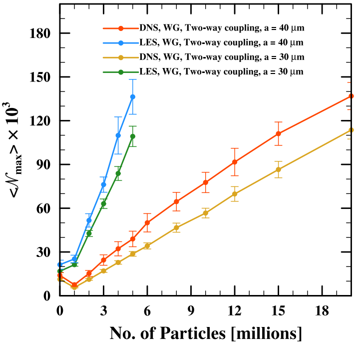


2D Domain Decomposition

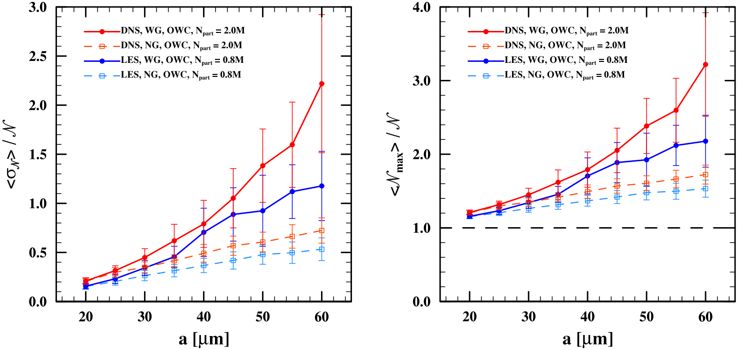


Particle Distribution in Subdomains – TWC

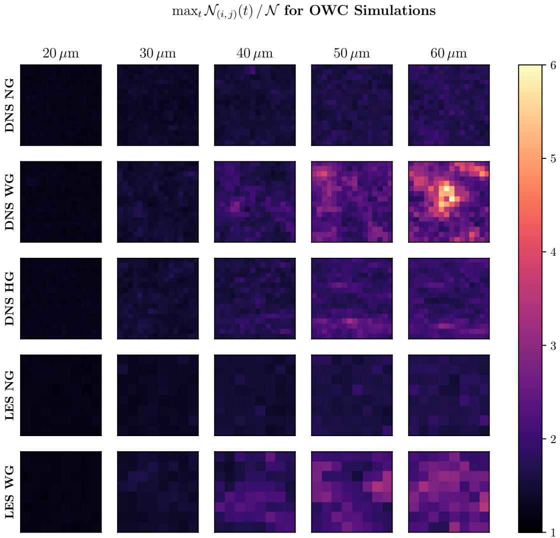




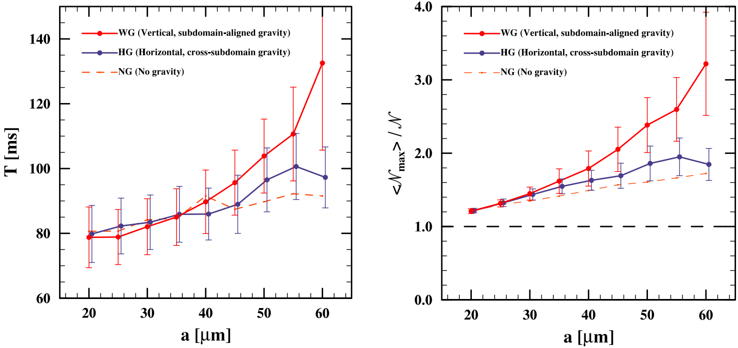
Particle Distribution in Subdomains – OWC (1)



Particle Distribution in Subdomains – OWC (2)



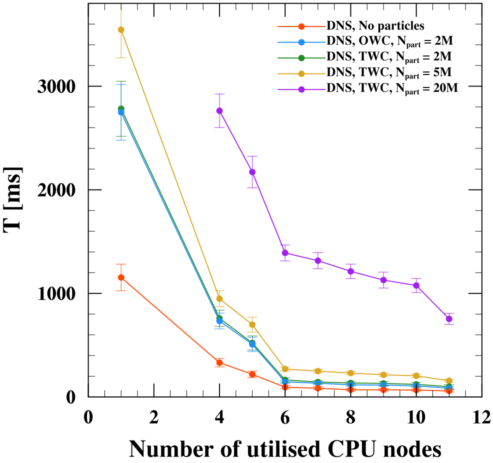
Experiment – "Horizontal" Gravity (OWC DNS only)



Particle Distribution in Subdomains – OWC (3)

Animation (Demo)

Extra – Resource-starved simulations (DNS)



Extra – Different sizes of subdomains

		Wallclock time per step [ms]				
		No particles	OWC	TWC	TWC	TWC
Subdomain size	N/SD		$N_{\text{part}} = 2\text{M}$	$N_{\text{part}} = 2\text{M}$	$N_{\text{part}} = 5\text{M}$	$N_{\text{part}} = 20\text{M}$
DNS, 8×8	2^{14}	24.6 ± 7.4	39.2 ± 8.1	41.9 ± 7.7	60.0 ± 11.0	2015.2 ± 29.4
DNS, 16×16	2^{16}	58.3 ± 10.2	89.7 ± 9.8	97.6 ± 9.4	180.0 ± 20.8	872.5 ± 76.2
DNS, 32×32	2^{18}	192.0 ± 43.2	310.6 ± 45.0	317.8 ± 44.0	551.8 ± 45.9	3046.2 ± 139.4
LES, 8×8	2^{12}	1.8 ± 0.3	—	338.4 ± 29.5	2539.7 ± 246.5	—
LES, 16×16	2^{14}	4.1 ± 0.5	1359.4 ± 49.1	1425.9 ± 52.4	9142.4 ± 290.8	—

		(WCT [s] $\times \text{N}_{\text{proc}}$) per step				
		No particles	OWC	TWC	TWC	TWC
Subdomain size	N_{proc}		$N_{\text{part}} = 2\text{M}$	$N_{\text{part}} = 2\text{M}$	$N_{\text{part}} = 5\text{M}$	$N_{\text{part}} = 20\text{M}$
DNS, 8×8	1024	25.2 ± 7.5	40.01 ± 8.2	42.9 ± 7.8	61.4 ± 11.3	220.4 ± 30.1
DNS, 16×16	256	14.9 ± 2.6	23.0 ± 2.5	25.0 ± 2.4	46.1 ± 5.3	223.4 ± 19.5
DNS, 32×32	64	12.3 ± 2.8	19.9 ± 2.9	20.3 ± 2.8	35.3 ± 2.9	195.0 ± 8.9
LES, 8×8	64	0.113 ± 0.022	—	21.7 ± 1.9	162.5 ± 246.5	—
LES, 16×16	16	0.066 ± 0.008	21.8 ± 0.8	22.8 ± 0.8	146.3 ± 4.7	—

Table 3.4: Time-averaged wallclock times per step by itself (top) and multiplied by the number of parallel processes used to execute code (bottom) for DNS and LES simulations with different sizes of computational subdomains. Entries in bold represent "standard" (see Table 3.1) sizes used in this study.

Computational Performance - Conclusions

- different bottlenecks for DNS and LES (fluid vs particle computations, respectively);
- current adaptation of solver designed for DNS infeasible for LES with even moderate particle counts (few million);
- adjustment of parallelisation strategy for LES is necessary;
- particle postprocessing stage does not scale well with number of particles and is very susceptible to nonuniformities in distribution of particles in subdomains;
- particle postprocessing stage is a good candidate for optimisation (e.g. improve data structures used to filter neighbouring particles);
- in extreme cases (e.g. high inertia settling particles under OWC) changing the direction of gravity helps to distribute particles more evenly among subdomains

Conclusions

Physical Fidelity

- in general, LES may be considered as a promising alternative to DNS;
- similar effects of subgrid-scale model on statistics for OWC and TWC, but discrepancies are smaller for larger Φ_m in TWC;
- results of DNS and LES are more aligned in simulations with gravity;
- in some cases, under TWC, the filtering of small-scale turbulence modulated by particles is significantly affecting results of LES (subgrid-scale model is agnostic to the effects of particles on fluid).

Computational Performance

- different bottlenecks for DNS and LES (fluid vs particle computations, respectively);
- current adaptation of solver designed for DNS infeasible for LES with even moderate particle counts (few million);
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Thank You