

Cargese - Bridging Classical and Superfluid Turbulence - July 2023

Intermittency and Lagrangian dynamics of velocity gradients in fluid turbulence

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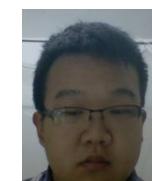
Intermittency and Lagrangian dynamics of velocity gradients in fluid turbulence

Charles Meneveau (JHU)

reporting on work by
Perry Jonson (now at UC Irvine)
&
Yuan Luo (Beijing Univ.)



Perry



Luo

based on past contributions by:

Laurent Chevillard (now ENS Lyon)
& **Michael Wilczek** (now U. Bayreuth)



Laurent



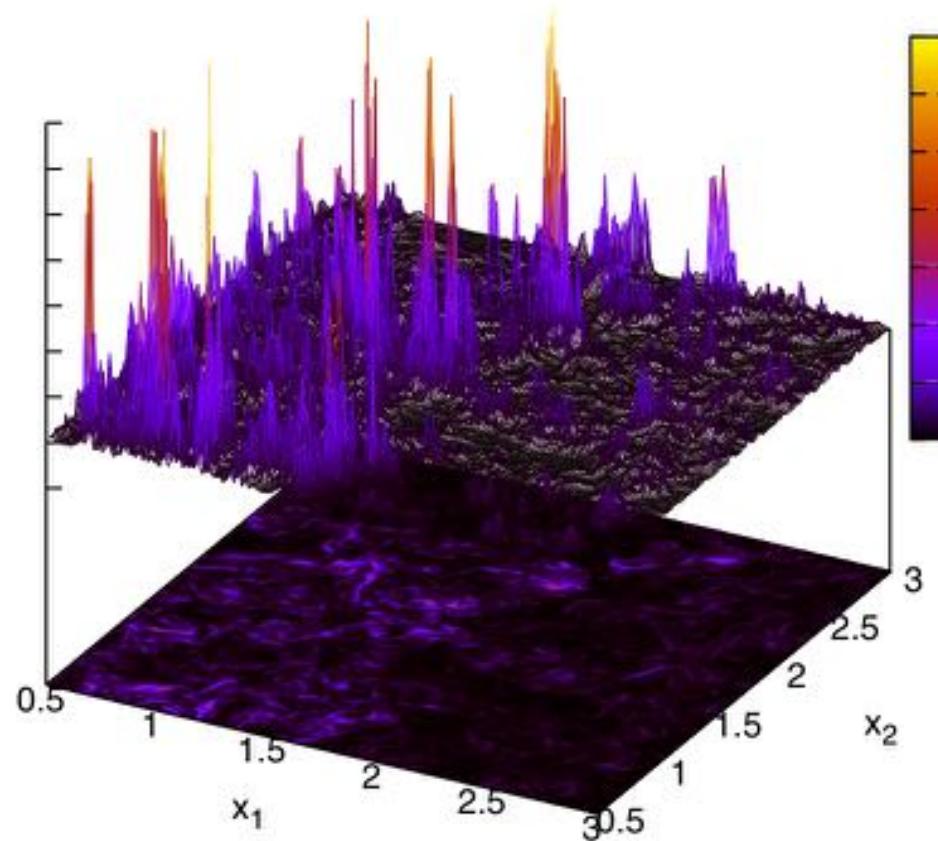
Michael

Extreme events in hydrodynamic turbulence (inner intermittency, isotropic turbulence)

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + \Omega_{ij}$$

$$\varepsilon = 2\nu S_{ij} S_{ij}$$

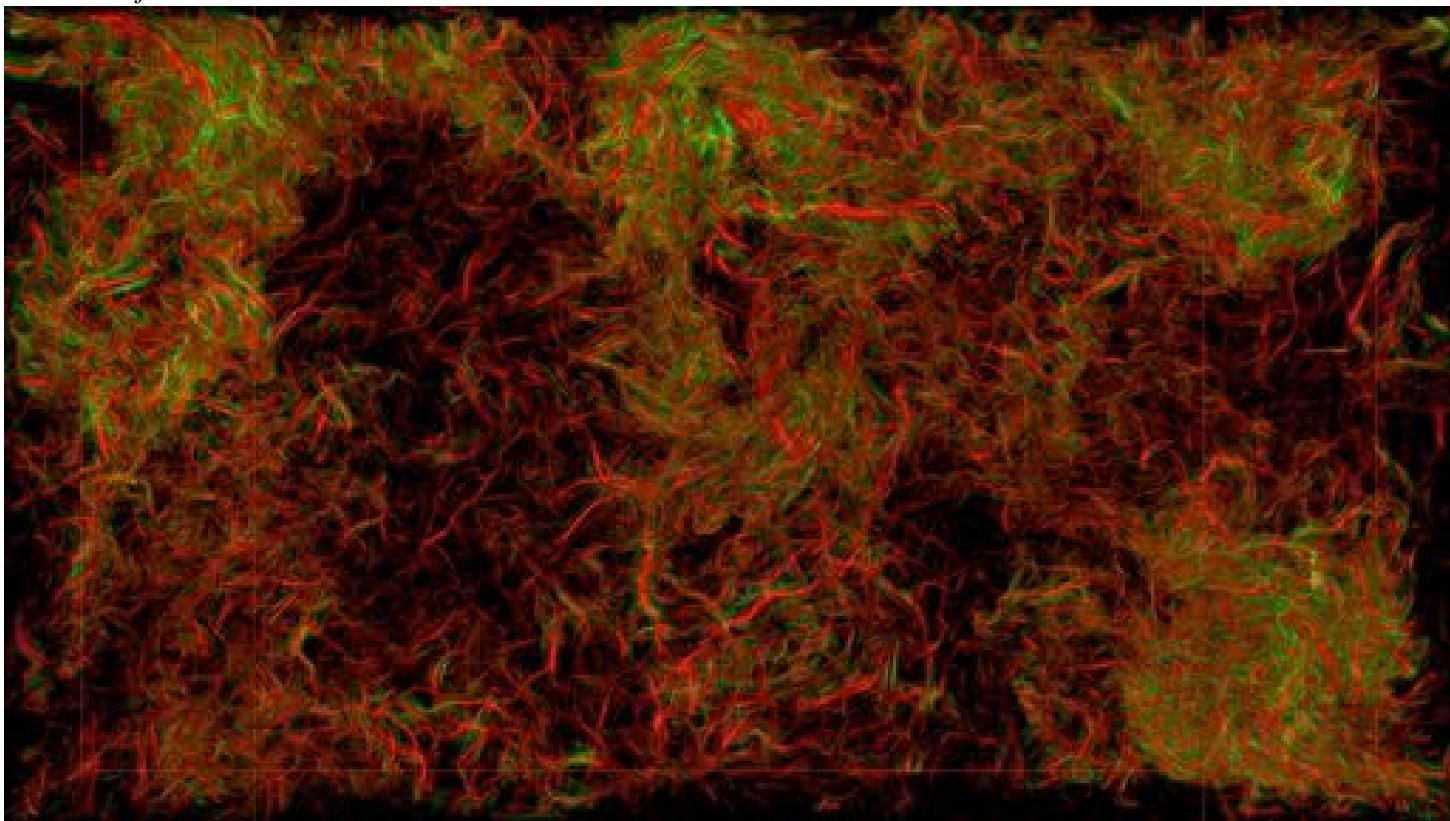
Rate of energy dissipation on a 512x512 plane
in $Re_\lambda=433$, 1024^3 DNS of isotropic turbulence



Extreme events in hydrodynamic turbulence

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + \Omega_{ij} \quad \omega^2 \propto \Omega_{ij} \Omega_{ij}$$

*Enstrophy density plots in $Re_\lambda=433$
 1024^3 DNS of isotropic turbulence*



JHU database, Dr. Kai Buerger visualization

The multiscale aspect of turbulence: clustering of vortices.. vortices within vortices

2 & 3 scale vorticity iso-contours in $Re_\lambda=433$, 1024^3 DNS of isotropic turbulence (JHTDB)



Bürger, K., Treib, M., Westermann, R., Werner, S., Lalescu, C.C., Szalay, A., Meneveau, C. and Eyink, G.L., 2012. Vortices within vortices: hierarchical nature of vortex tubes in turbulence. arXiv preprint arXiv:1210.3325.

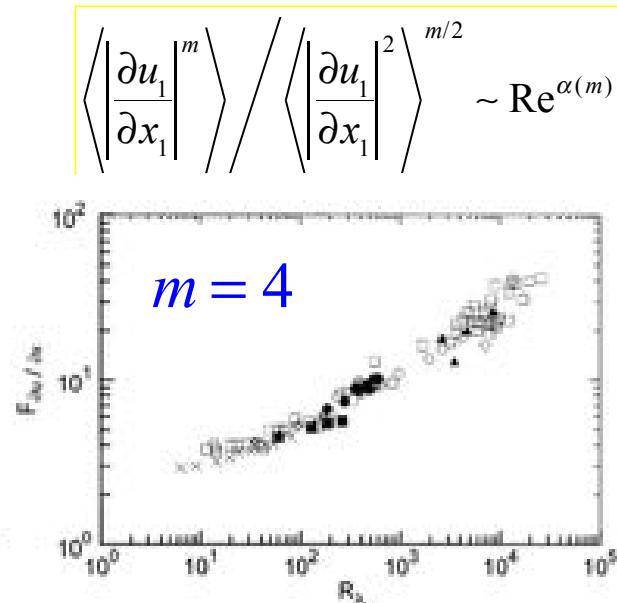
K41: assuming that mean dissipation tells entire story

$$\langle \varepsilon \rangle \sim \frac{u'^3}{\ell} \text{Re}^0 \quad \& \quad \langle \varepsilon^{m/2} \rangle \sim \left(\frac{u'^3}{\ell} \right)^{m/2} \text{Re}^0 \quad \Rightarrow \quad \left\langle \left| \frac{\partial u_1}{\partial x_1} \right|^m \right\rangle \Bigg/ \left\langle \left| \frac{\partial u_1}{\partial x_1} \right|^2 \right\rangle^{m/2} \sim \text{Re}^0$$

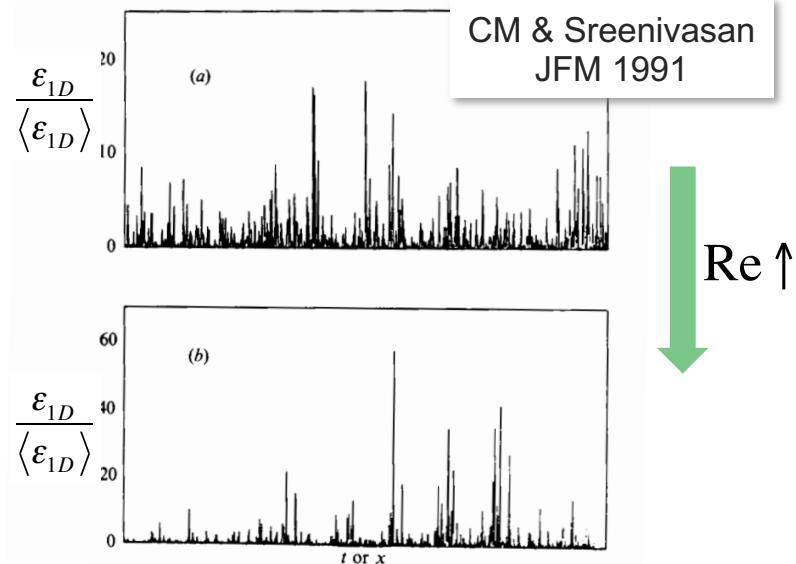
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$$\langle \varepsilon \rangle \sim \frac{u'^3}{\ell} \text{Re}^0 \quad \& \quad \langle \varepsilon^{m/2} \rangle \sim \left(\frac{u'^3}{\ell} \right)^{m/2} \text{Re}^0 \quad \Rightarrow \quad \left\langle \left| \frac{\partial u_1}{\partial x_1} \right|^m \right\rangle \Bigg/ \left\langle \left| \frac{\partial u_1}{\partial x_1} \right|^2 \right\rangle^{m/2} \sim \text{Re}^0$$

But: Intermittency in small-scale turbulence



Sreenivasan & Antonia ARFM 1997



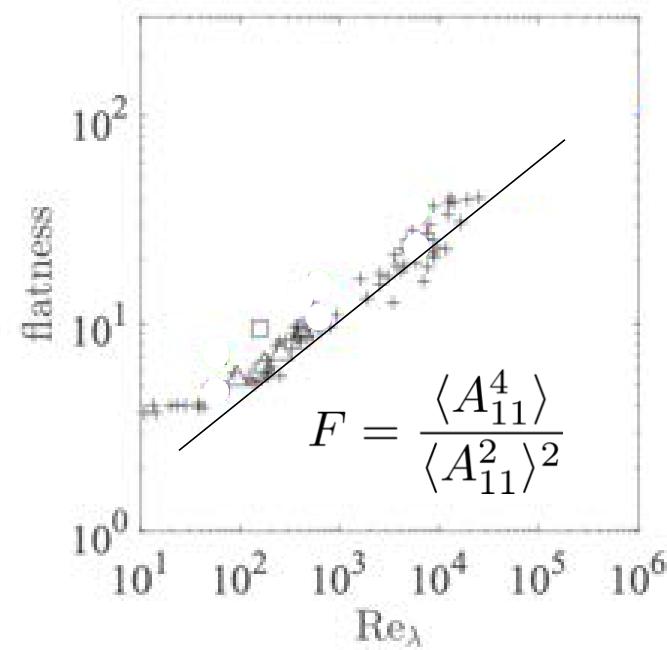
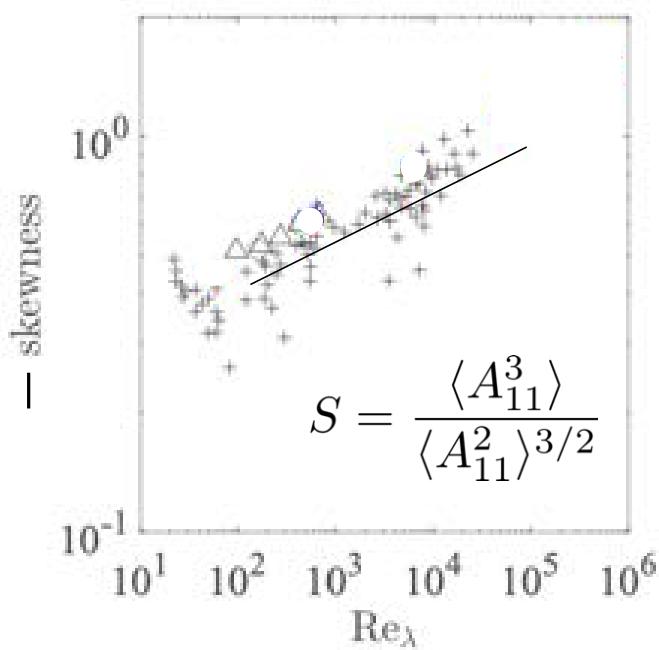
Also: anomalous scaling of structure functions in inertial range (Frisch 1995, etc..)

The velocity gradient tensor

Phenomenology (incompressible, NS):

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + \Omega_{ij}$$

intermittency: power-law increase of skewness and flatness with Re_λ

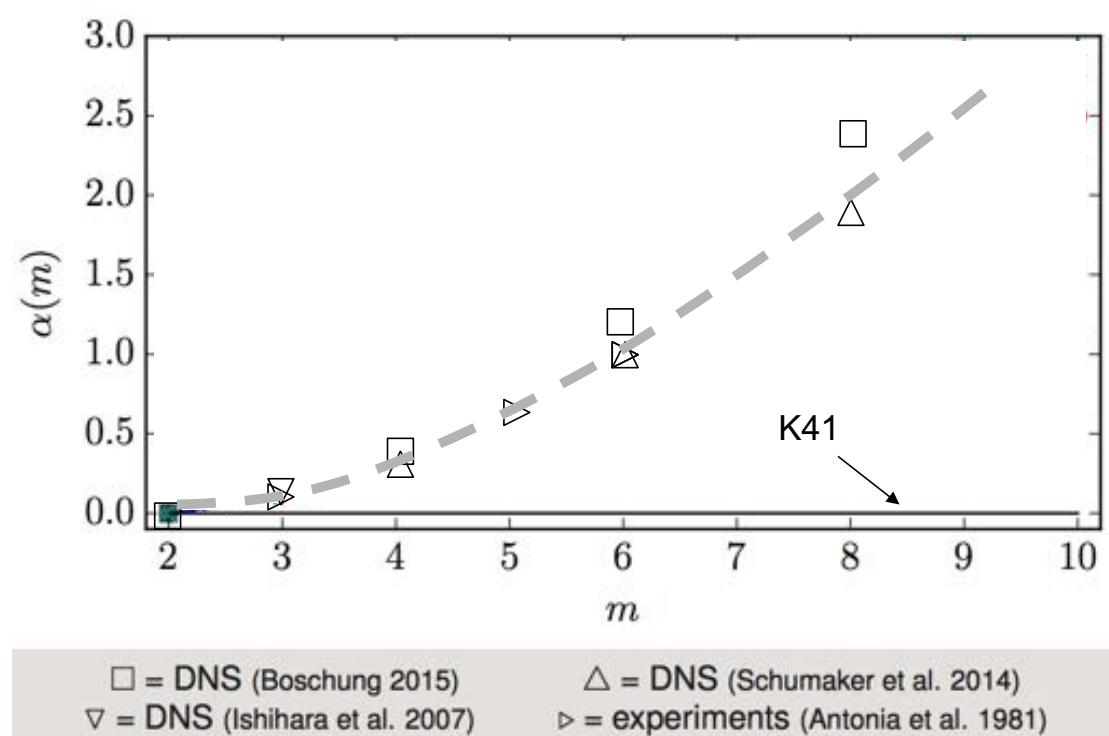


Data:

- + Sreenivasan & Antonia
(Ann. Rev. Fluid Mech. 1997)
- o Johnson & M (JFM, 2016)
- △ Ishihara et al. (JFM, 2007)

Anomalous gradient exponents: data

$$\frac{\langle |A_{11}|^m \rangle}{\langle |A_{11}|^2 \rangle^{m/2}} \sim \text{Re}^{\alpha(m)}$$

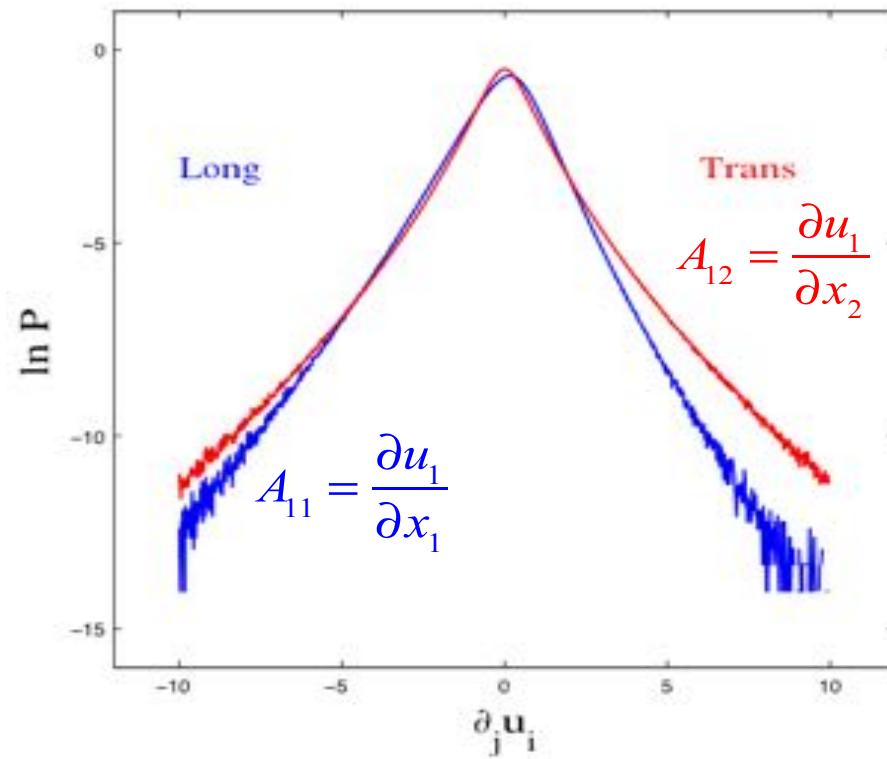


The velocity gradient tensor

Phenomenology (incompressible, NS):

intermittency: long tails in PDFs of gradients

$$A_{ij} = \frac{\partial u_i}{\partial x_j}$$



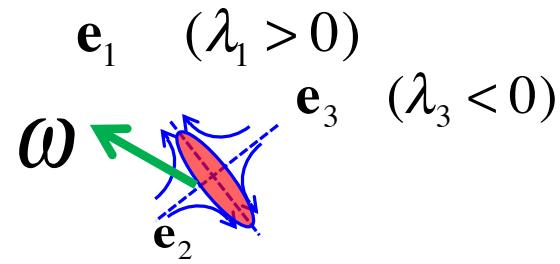
The velocity gradient tensor

Phenomenology (incompressible, NS):

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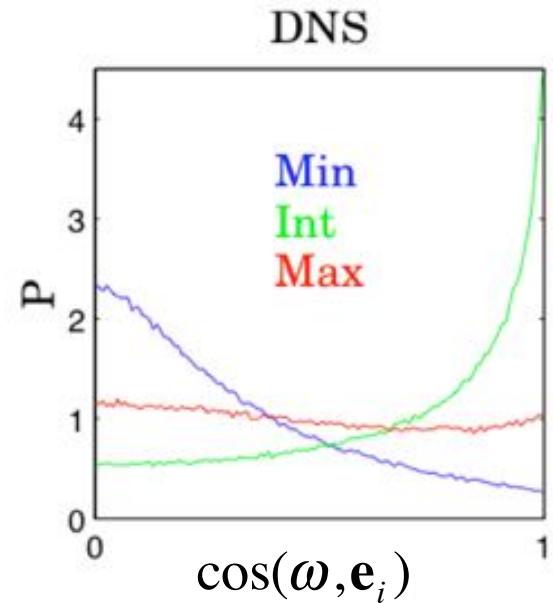
Strain-rate tensor:
eigen-values,
eigen-vectors

Rotation tensor
Vorticity vector



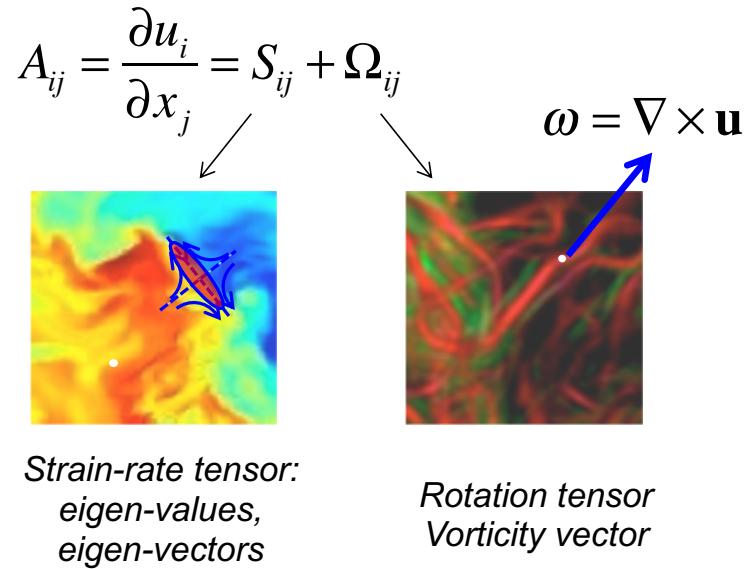
Geometric aspects:

E.g. preferential alignment of vorticity with intermediate strain-rate eigenvector
(Ashurst et al. 1987, Kerr 1988, etc.):



The velocity gradient tensor

Phenomenology (incompressible, NS):

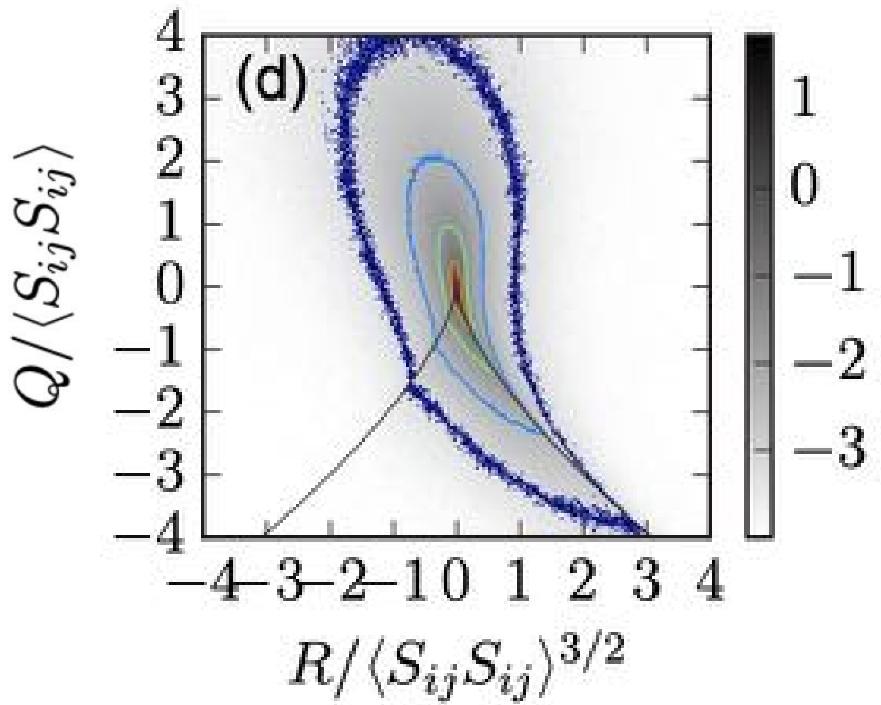


$$Q = -\frac{1}{2} A_{ij} A_{ji} \quad R = -\frac{1}{3} A_{ij} A_{jk} A_{ki}$$

Viellefosse 1982, Cantwell 1992

Geometric aspects:

Joint PDF of invariants: tear-drop shape



Also, many practical engineering motivations:

Small scale intermittency of turbulence generates extreme events, difficult to characterize based on local averages

Small scale intermittency affects:

- droplet and bubble deformations in turbulence
- flame structure (quenching) in combustion
- micro-organism motility and nutrient uptake
- polymer stretching–relaxation dynamics

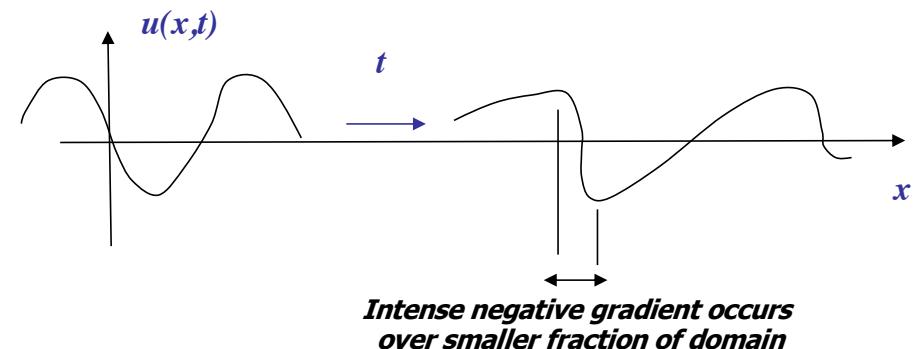
The velocity gradient tensor

in its Lagrangian evolution

Trivial case: 1-D inv Burgers equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0$$

$$A = \frac{\partial u}{\partial x}$$



The velocity gradient tensor

in its Lagrangian evolution

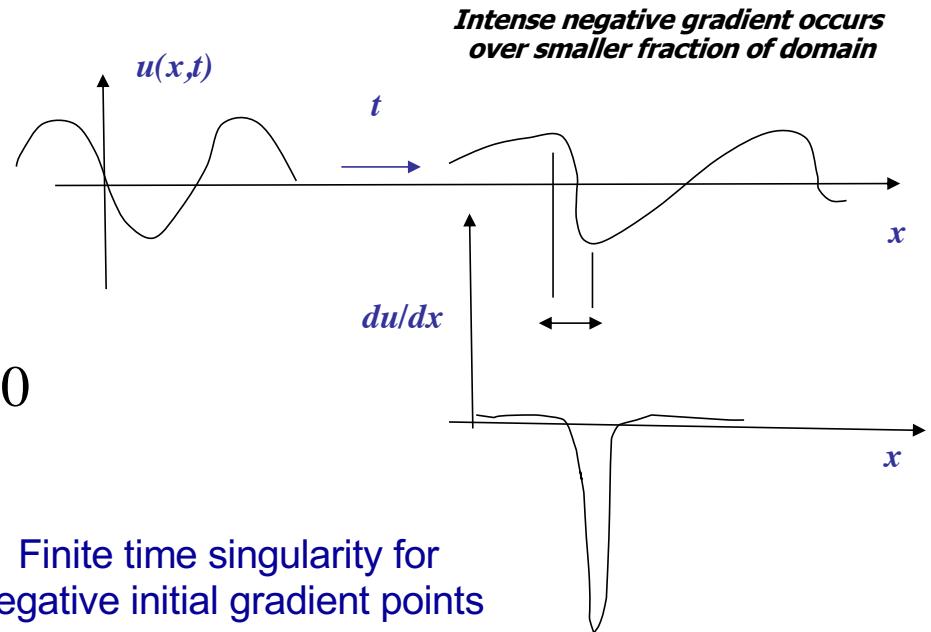
Trivial case: 1-D inv Burgers equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0$$

$$A = \frac{\partial u}{\partial x}$$

$$\frac{\partial}{\partial x} \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right) = \frac{\partial A}{\partial t} + u \frac{\partial A}{\partial x} + AA = 0$$

$$\frac{dA}{dt} = -A^2 \quad \Rightarrow A = \frac{1}{t - (-A_0^{-1})}$$



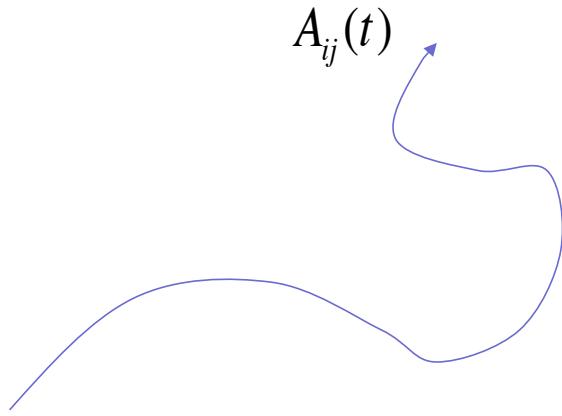
The velocity gradient tensor: 3D

in its Lagrangian evolution

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + \Omega_{ij}$$

$$\frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial t} + \frac{\partial u_k u_i}{\partial x_k} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \nabla^2 u_i + g_i$$

System of 9 (8) ODEs (not closed)
if viewed in Lagrangian frame
(dependent on non-local variables)



$$\frac{dA_{11}}{dt} = \dots$$

$$\frac{dA_{12}}{dt} = \dots$$

$$\frac{dA_{13}}{dt} = \dots$$

...

...

$$\frac{dA_{33}}{dt} = \dots$$

The velocity gradient tensor: 3D

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + \Omega_{ij} \quad \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial t} + \frac{\partial u_k u_i}{\partial x_k} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \nabla^2 u_i + g_i$$

$$\frac{dA_{ij}}{dt} = -\underbrace{\left(A_{iq} A_{qj} - \frac{1}{3} A_{mn} A_{nm} \delta_{ij} \right)}_{\text{Self-stretching}} - \underbrace{\left(\frac{\partial^2 p}{\partial x_i \partial x_j} - \frac{1}{3} \nabla^2 p \delta_{ij} \right)}_{\text{unclosed}} + \nu \underbrace{\frac{\partial^2 A_{ij}}{\partial x_q \partial x_q}}_{\text{forcing}} + W_{ij}$$

“ $\frac{dA}{dt} = -A^2$ ” in 3D

The velocity gradient tensor: 3D

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + \Omega_{ij} \quad \frac{\partial}{\partial x_j} \left(\frac{\partial u_i}{\partial t} + \frac{\partial u_k u_i}{\partial x_k} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \nabla^2 u_i + g_i$$

$$\frac{dA_{ij}}{dt} = -\underbrace{\left(A_{iq} A_{qj} - \frac{1}{3} A_{mn} A_{nm} \delta_{ij} \right)}_{\text{Self-stretching}} - \underbrace{\left(\frac{\partial^2 p}{\partial x_i \partial x_j} - \frac{1}{3} \nabla^2 p \delta_{ij} \right)}_{\text{unclosed}} + \underbrace{\nu \frac{\partial^2 A_{ij}}{\partial x_q \partial x_q} + W_{ij}}_{\text{forcing}}$$

Restricted Euler Equation
 Viellefosse 1982, Cantwell 1992:

$$\frac{dA_{ij}}{dt} = -\left(A_{iq} A_{qj} - \frac{1}{3} A_{mn} A_{nm} \delta_{ij} \right) \quad A_{ii} = \frac{\partial u_i}{\partial x_i} = 0$$

System of 8 independent ODEs
 if viewed in Lagrangian frame

The velocity gradient tensor: 3D

Restricted Euler Equation

Viellefosse 1982, Cantwell 1992:

$$\frac{dA_{ij}}{dt} = - \left(A_{iq} A_{qj} - \frac{1}{3} A_{mn} A_{nm} \delta_{ij} \right)$$

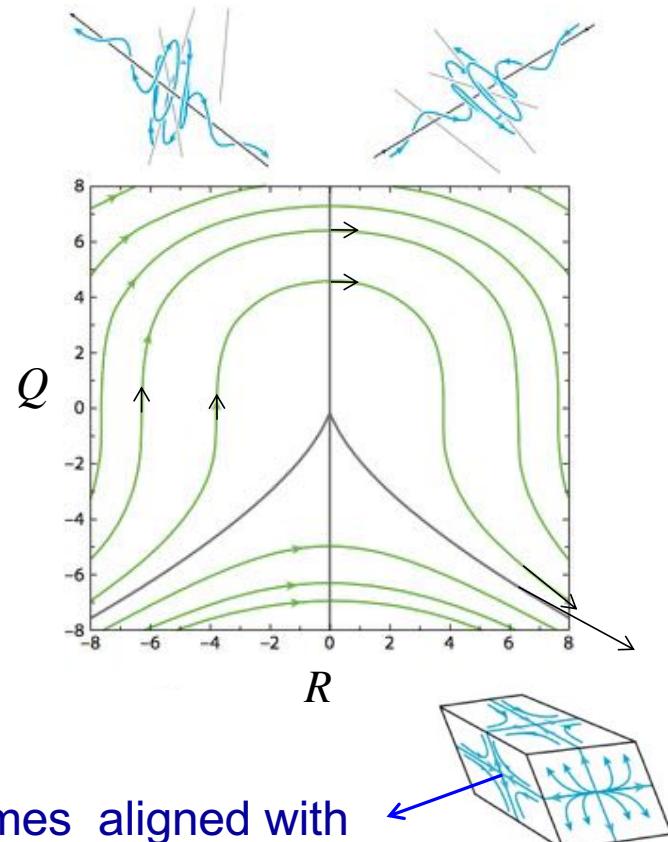
$$Q = -\frac{1}{2} A_{mn} A_{nm} \quad R = -\frac{1}{3} A_{mn} A_{np} A_{pm}$$

Two very “special” invariants, R, Q :

$$\frac{dQ}{dt} = -3R, \quad \frac{dR}{dt} = \frac{2}{3}Q^2,$$

En-route to singularity, RE reproduces several very realistic trends, e.g.

vorticity becomes aligned with intermediate eigenvector



The velocity gradient tensor: how to damp RE?

Restricted Euler Equation with **linear damping: not enough!**

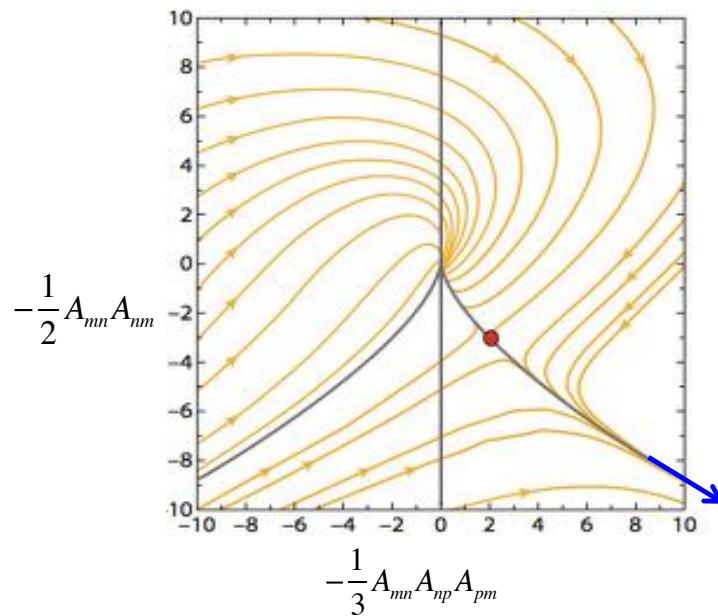
Martin et al. Phys Fluids 1998:

$$\frac{dA_{ij}}{dt} = -\left(A_{iq}A_{qj} - \frac{1}{3}A_{mn}A_{nm}\delta_{ij} \right) - \frac{1}{T}A_{ij}$$

$$A_{ii} = \frac{\partial u_i}{\partial x_i} = 0$$

Still, most initial conditions
have finite-time **divergence** to infinity

Goal: develop **Lagrangian** model
for missing physics keeping
simplicity of 8 ODEs (or SDE if with
stochastic ingredients)



Families of models (review: Annu Rev Fluid Mech, 2011):

$$\frac{dA_{ij}}{dt} = - \left(A_{iq} A_{qj} - \frac{1}{3} A_{mn} A_{nm} \delta_{ij} \right) - \left(\frac{\partial^2 p}{\partial x_i \partial x_j} - \frac{1}{3} \nabla^2 p \delta_{ij} \right) + \nu \frac{\partial^2 A_{ij}}{\partial x_q \partial x_q} + W_{ij}$$

- Restricted Euler Equation (1982 Viellefosse, 1992 Cantwell..)
- Linear relaxation (Martin et al.. 1998)
- Specified lognormal and stochastic (Chen, Pope, Girimaji)
- Tetrads.. (Chertkov, Pumir)
- Recent Fluid Deformation closure (Chevillard & CM, 2006)
- Linear combination, with a shell-model approach (Biferale et al.)
- Gaussian and “enhanced” Gaussian (Wilczek & CM, JFM 2014)
- Deformed Gaussian Fields Model (Johnson & CM, JFM 2017)

Pressure Hessian model: assume pressure is slowly varying along Lagrangian trajectories over short time-period τ

$$\frac{dp}{dt} \approx 0 \rightarrow$$

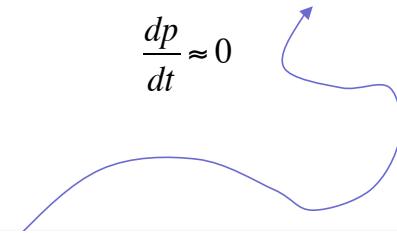
$$\nabla \nabla \left(\frac{dp}{dt} \right) = \frac{d \nabla \nabla p}{dt} + \nabla \mathbf{u} \nabla \nabla p + \nabla \mathbf{u}^T \nabla \nabla p$$

$$\rightarrow \frac{d \nabla \nabla p}{dt} \approx -\nabla \mathbf{u} \cdot \nabla \nabla p - \nabla \mathbf{u}^T \cdot \nabla \nabla p$$

$$\rightarrow \nabla \nabla p(t) \approx e^{-\tau \nabla \mathbf{u}} \cdot \nabla \nabla p(0) \cdot e^{-\tau \nabla \mathbf{u}^T}$$

$$A_{ij}(t)$$

$$\frac{dp}{dt} \approx 0$$



Olroyd (upper convective) derivative = zero

Chevillard & CM (2006): Recent Fluid Deformation Map

Also assumed I.C. is an isotropic tensor
(Lagrangian restricted Euler)

$$\langle \nabla \nabla p(0) | \mathbf{A} \rangle = \langle \frac{\partial^2 p(0)}{\partial x_i \partial x_j} | \mathbf{A} \rangle \approx C \delta_{ij}$$

Another view: Gaussian closure for conditional pressure Hessian

(Wilczek & CM, JFM, 2015)

$$\langle \nabla \nabla p(0) | \mathbf{A} \rangle = \left\langle \frac{\partial^2 p(0)}{\partial x_i \partial x_j} | \mathbf{A} \right\rangle \approx \alpha (\mathcal{S}_1^2 - \frac{1}{3} \text{Tr}(\mathcal{S}_1^2) I) + \beta (\mathcal{W}_1^2 - \frac{1}{3} \text{Tr}(\mathcal{W}_1^2) I) + \gamma (\mathcal{S}_1 \mathcal{W}_1 - \mathcal{W}_1 \mathcal{S}_1)$$

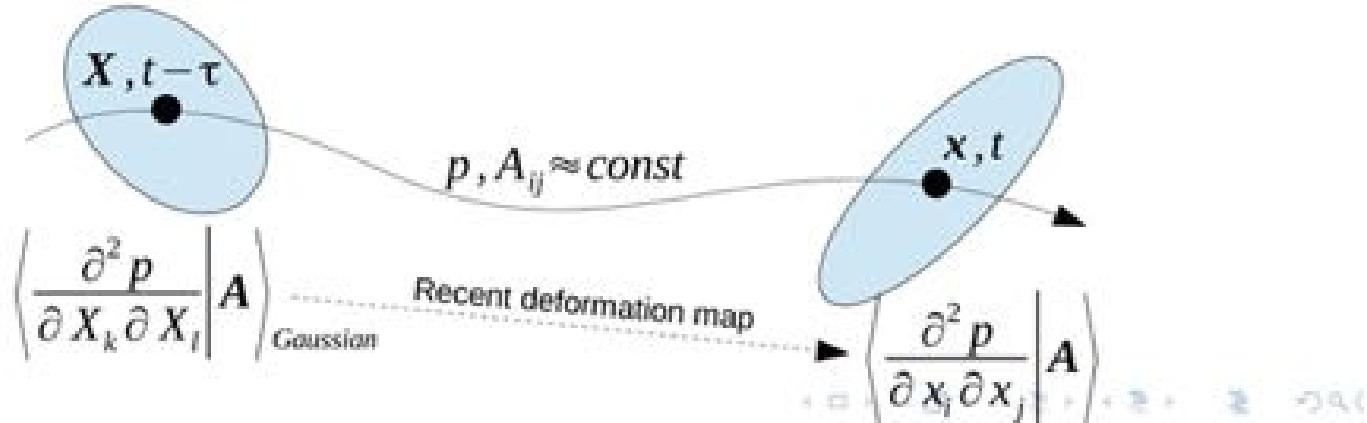
with

$$\begin{aligned}\alpha &= -\frac{4}{105f_u''(0)^2} \int dr \left(8\frac{f_u'^2}{r^3} - 4\frac{f_u'f_u''}{r^2} - 4\frac{f_u'f_u'''}{r} - 4\frac{f_u''^2}{r} + f_u''f_u'''\right) \\ \beta &= -\frac{4}{125f_u''(0)^2} \int dr \left(16\frac{f_u'^2}{r^3} - 12\frac{f_u'f_u''}{r^2} - 4\frac{f_u'f_u'''}{r} - 4\frac{f_u''^2}{r} - f_u''f_u'''\right) \\ \gamma &= \frac{4}{75f_u''(0)^2} \int dr \left(4\frac{f_u'f_u''}{r^2} - 4\frac{f_u''^2}{r} - f_u''f_u'''\right).\end{aligned}$$

These terms can be significantly simplified by partial integration and identifying product rules, which then leads to

$$\begin{aligned}\alpha &= -\frac{2}{7} \\ \beta &= -\frac{2}{5} \\ \gamma &= \frac{6}{25} + \frac{16}{75f_u''(0)^2} \int dr \frac{f_u'f_u'''}{r}.\end{aligned}$$

The Recent Deformation of Gaussian Fields (RDGF) closure (P. Johnson & CM, JFM 2016)



$$\langle \nabla \nabla p(t) | \mathbf{A} \rangle = \langle \frac{\partial^2 p(t)}{\partial x_i \partial x_j} | \mathbf{A} \rangle \approx \exp(-\tau \mathbf{A}) \cdot \langle \nabla \nabla p(0) | \mathbf{A} \rangle \cdot \exp(-\tau \mathbf{A}^T)$$

$$\langle \nabla \nabla p(0) | \mathbf{A} \rangle \approx \alpha (\mathcal{S}_1^2 - \frac{1}{4} \text{Tr}(\mathcal{S}_1^2) I) + \beta (\mathcal{W}_1^2 - \frac{1}{4} \text{Tr}(\mathcal{W}_1^2) I) + \gamma (\mathcal{S}_1 \mathcal{W}_1 - \mathcal{W}_1 \mathcal{S}_1)$$

The Recently-Deformed Gaussian Fields (RDGF) Model

- Langevin equation, $dA_{ij} =$

$$\left[- \left((\mathbf{A}^2)_{ij} - \frac{C_{ij}^{-1}}{C_{kk}^{-1}} \text{tr}(\mathbf{A}^2) \right) - \left(G_{ij} - \frac{C_{ij}^{-1}}{C_{kk}^{-1}} \text{tr}(\mathbf{G}) \right) + V_{ij} \right] dt + dF_{ij}$$

where

$$G_{ij} = D_{mi}^{-1} \left[-\frac{2}{7} (\mathbf{S}^2)_{ij}^{(d)} - \frac{2}{5} (\boldsymbol{\Omega}^2)_{ij}^{(d)} + \frac{86}{1365} (S_{ik}\Omega_{kj} - \Omega_{ik}S_{kj}) \right] D_{nj}^{-1},$$

$$V_{ij} = \frac{-7}{10\sqrt{15}} \frac{C_{kk}}{3} \tau_K^{-1} \left(T_{ij} C_{kk}^{-1} + 2T_{ik} B_{kj}^{-1} - \frac{4}{21} B_{ik}^{-1} S_{kj} - \frac{2}{21} B_{k\ell}^{-1} S_{k\ell} \delta_{ij} \right)$$

$$S_{ij} = \frac{(A_{ij} + A_{ji})}{2}, \quad \Omega_{ij} = \frac{(A_{ij} - A_{ji})}{2}, \quad T_{ij} = \frac{23}{105} A_{ij} + \frac{2}{105} A_{ji}.$$

- Recent deformation tensor:

$$D_{ij}^{-1} = \exp(-A_{ij}\tau), \quad C_{ij}^{-1} = D_{ki}^{-1} D_{kj}^{-1}, \quad B_{ij}^{-1} = D_{ik}^{-1} D_{jk}^{-1}.$$

$$\tau = 0.13 \tau_K$$

0.13 chosen such that $\langle 2S_{ij}S_{ij} \rangle^{-1/2} = \tau_K$

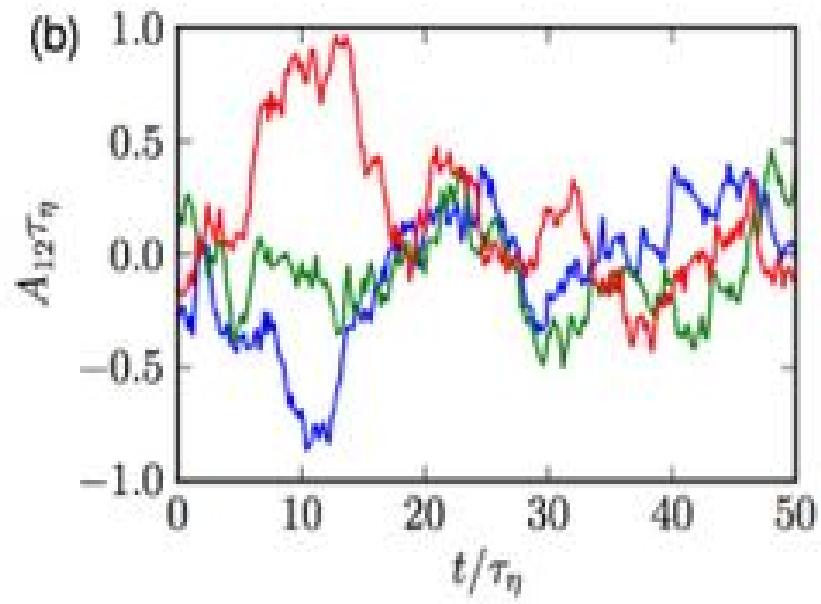
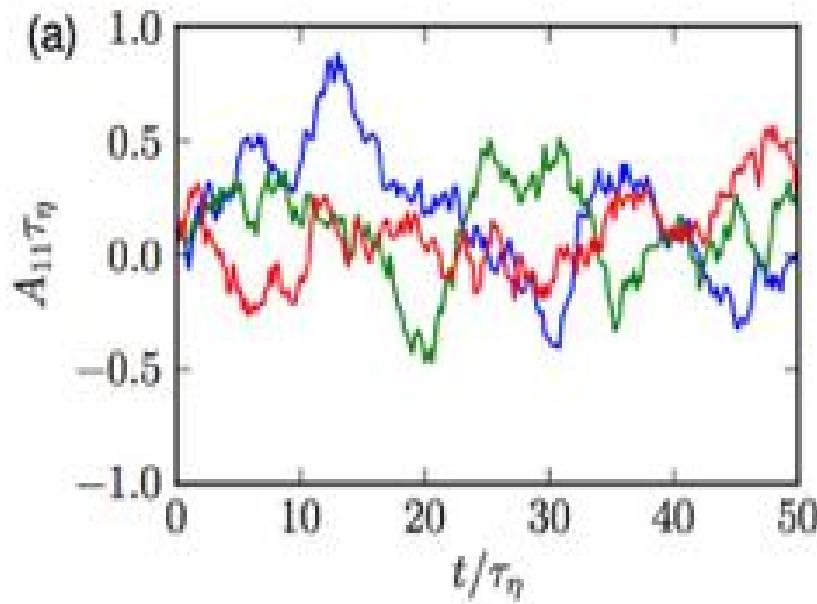
2 more parameters for
forcing strength D_a, D_s : $\langle Q \rangle = 0$
 fixed from 2 required $\langle R \rangle = 0$
 Betchov symmetries:

The Recently-Deformed Gaussian Fields (RDGF) Model

$$dA_{ij} = \left[-\left(A_{ik}A_{kj} - \frac{1}{3}A_{pq}A_{pq}\delta_{ij} \right) + h_{ij}(\mathbf{A}, \tau_K) \right] dt + dF_{ij}(\tau_K)$$

- 9 x SDE solver: 2nd order predictor-corrector method,
- $dt/\tau_K = 0.04, 0.02, 0.01$ for comparisons & checks
- 2^{16} trajectories advanced for 1000 τ_K .

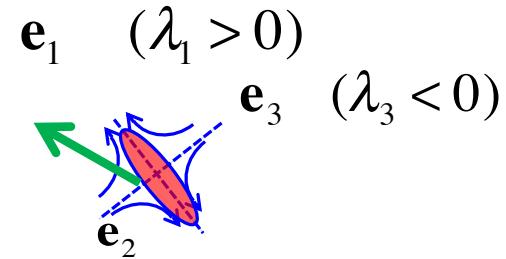
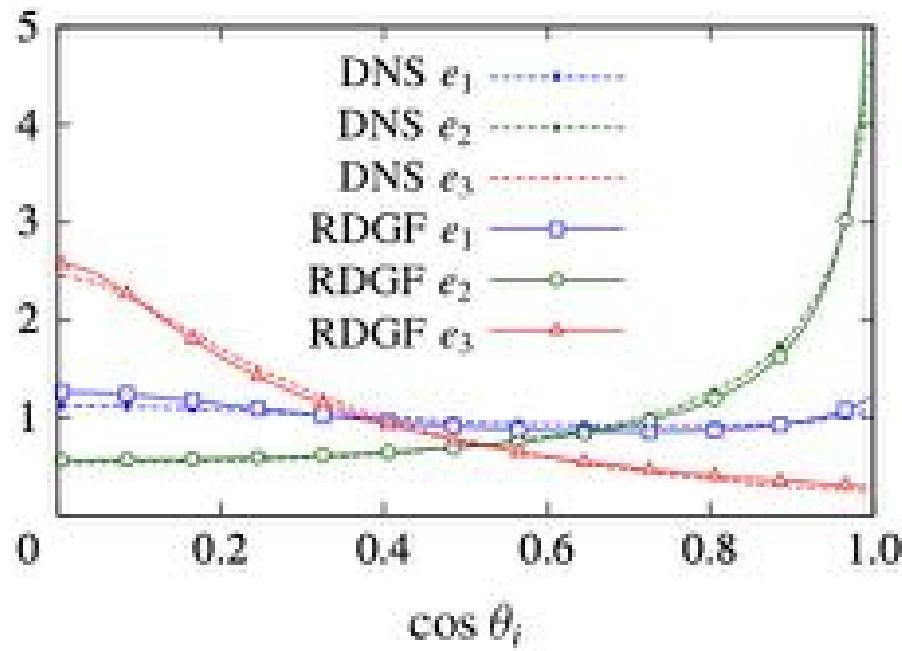
✓ Lagrangian time series (3 sample realizations)



The Recently-Deformed Gaussian Fields (RDGF) Model

$$dA_{ij} = \left[-\left(A_{ik}A_{kj} - \frac{1}{3}A_{pq}A_{pq}\delta_{ij} \right) + h_{ij}(\mathbf{A}, \tau_K) \right] dt + dF_{ij}(\tau_K)$$

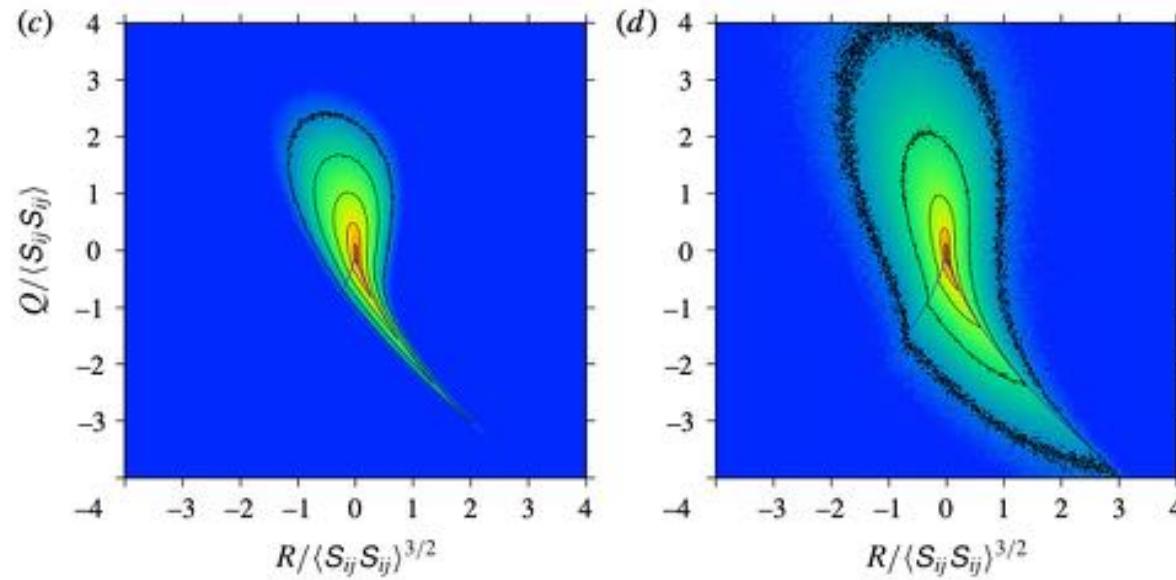
✓ Alignments



The Recently-Deformed Gaussian Fields (RDGF) Model

$$dA_{ij} = \left[-\left(A_{ik}A_{kj} - \frac{1}{3}A_{pq}A_{pq}\delta_{ij} \right) + h_{ij}(\mathbf{A}, \tau_K) \right] dt + dF_{ij}(\tau_K)$$

✓ tear-drop joint PDF

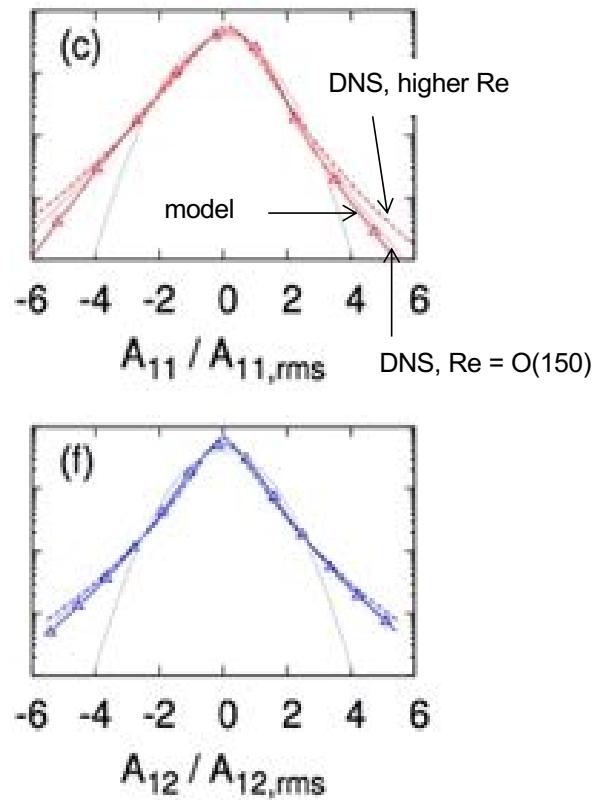


The Recently-Deformed Gaussian Fields (RDGF) Model

$$dA_{ij} = \left[-\left(A_{ik}A_{kj} - \frac{1}{3}A_{pq}A_{pq}\delta_{ij} \right) + h_{ij}(\mathbf{A}, \tau_K) \right] dt + dF_{ij}(\tau_K)$$

✓ gradient PDFs

Model ———
 Re = 430 DNS
 Re = 160 —— DNS

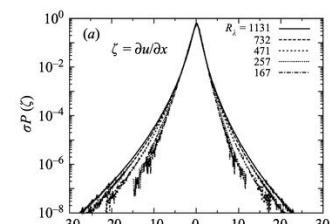


Summary:

- ✓ Skewness
- ✓ Alignments
- ✓ Joint PDF (Q,R)

However:

- Behavior like at a **fixed** Re ($\text{Re}_\lambda \sim 60 - 120$).
- Can't describe continued "widening" of tails in PDF at large Re



A multiple time-scale model

(Johnson & CM, Phys Rev Fluids, 2017, Luo, Shi & CM, Phys. Rev. Fluids 7, 2022):

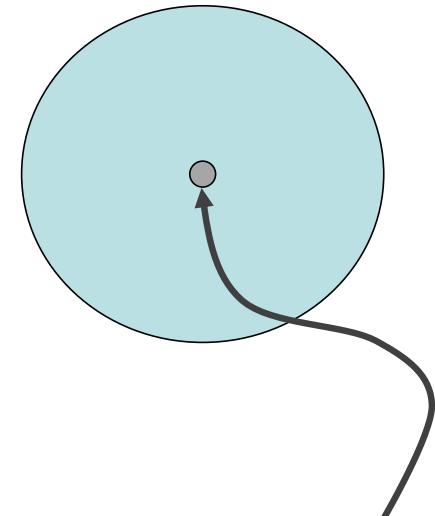
$$dA_{ij} = \left[-\left(A_{ik}A_{kj} - \frac{1}{3}A_{pq}A_{pq}\delta_{ij} \right) + h_{ij}(\mathbf{A}, \tau_K) \right] dt + dF_{ij}(\tau_K)$$

Instead of constant τ_K (constant $v/\langle\varepsilon\rangle$), “variable” background $v/\varepsilon(t)$:

$$dA_{ij}^{(n)} = \left[\underbrace{-\left(A_{ik}^{(n)}A_{kj}^{(n)} - \frac{1}{3}A_{pq}^{(n)}A_{pq}^{(n)}\delta_{ij} \right)}_{\text{local-in-scale interactions: from N-S}} + \underbrace{h_{ij}^n(\mathbf{A}, \tau_n) - \frac{\dot{\tau}_n}{\tau_n}A_{ij}}_{\text{non-local interactions}} \right] dt + dF_{ij}(\tau_n)$$

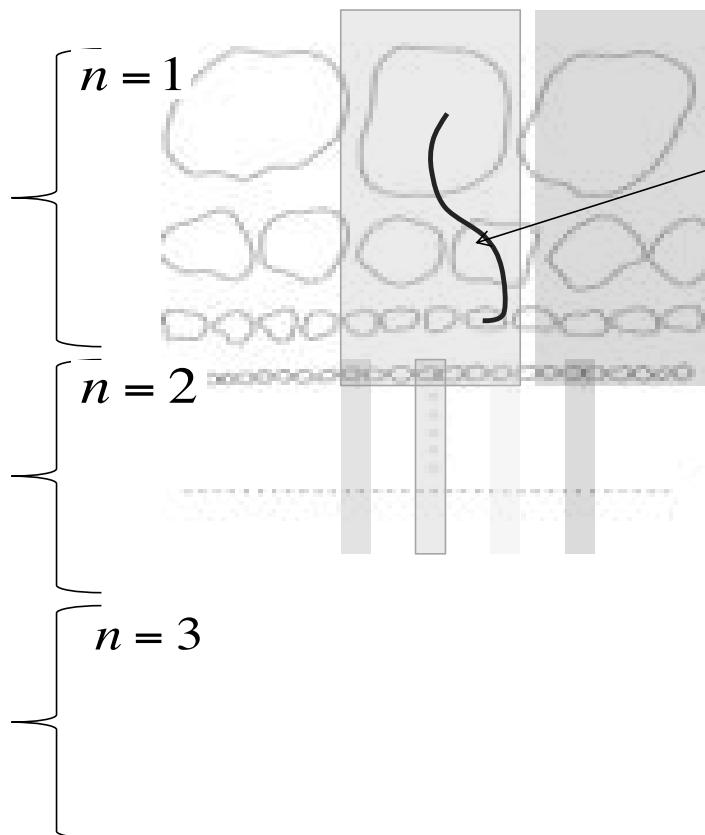
$$\begin{aligned} \tau_1 &= \beta^{N-1} \tau_K \\ \tau_n(t) &= \frac{1}{\beta} \left(2S_{ij}^{(n-1)}S_{ij}^{(n-1)} \right)^{-1/2}, \quad n = 2, 3, \dots, N \end{aligned}$$

- Free parameter – timescale ratio (fitted) $\beta=10$
- levels: scale-separation needed in model
- not a “shell cascade model” (scale ratio = 2)



“The combined local and nonlocal cascade”

Nonlocal dynamics,
modulated time-scales,
scale separation



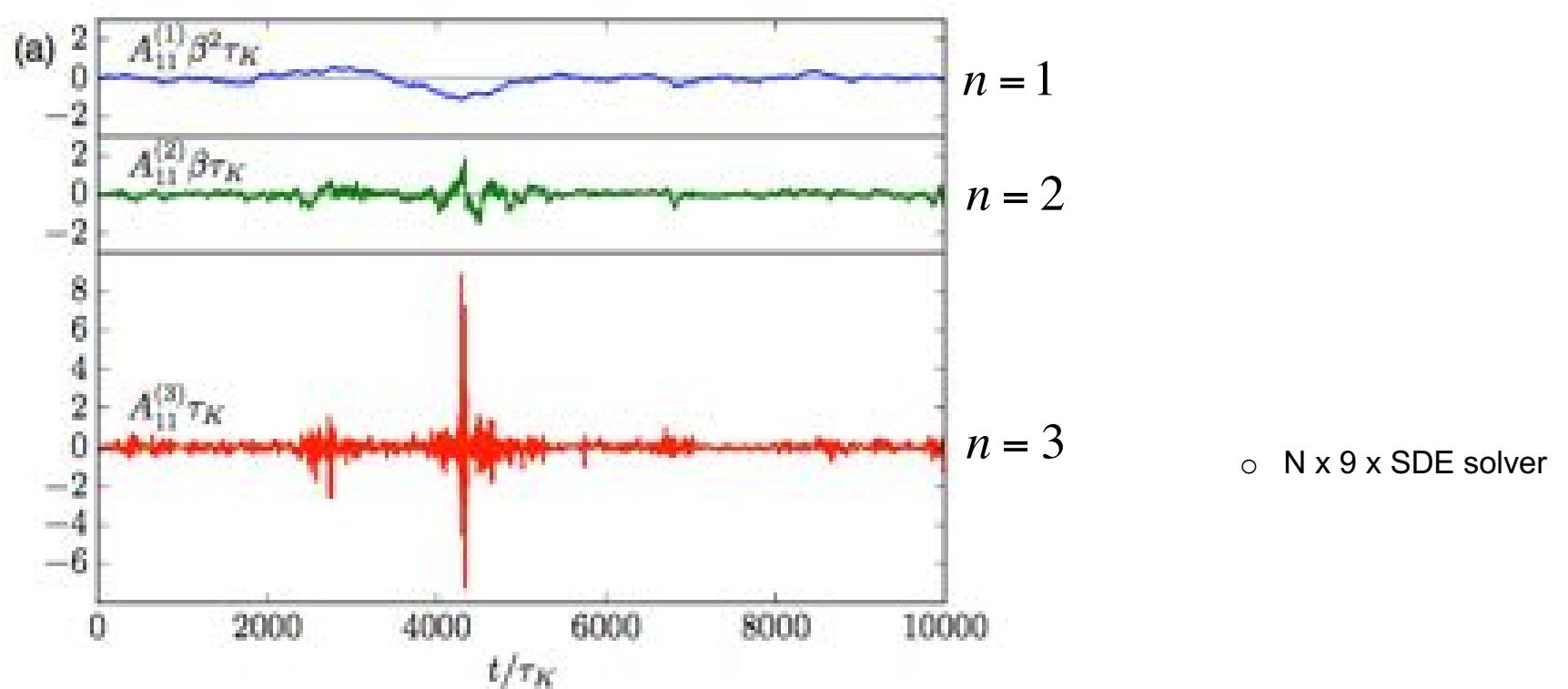
Local dynamics
from N-S
 $\frac{d\mathbf{A}}{dt} = -\mathbf{A}^2 + \dots \mathbf{F}$



Results: Time scale modulation

$\beta=10$

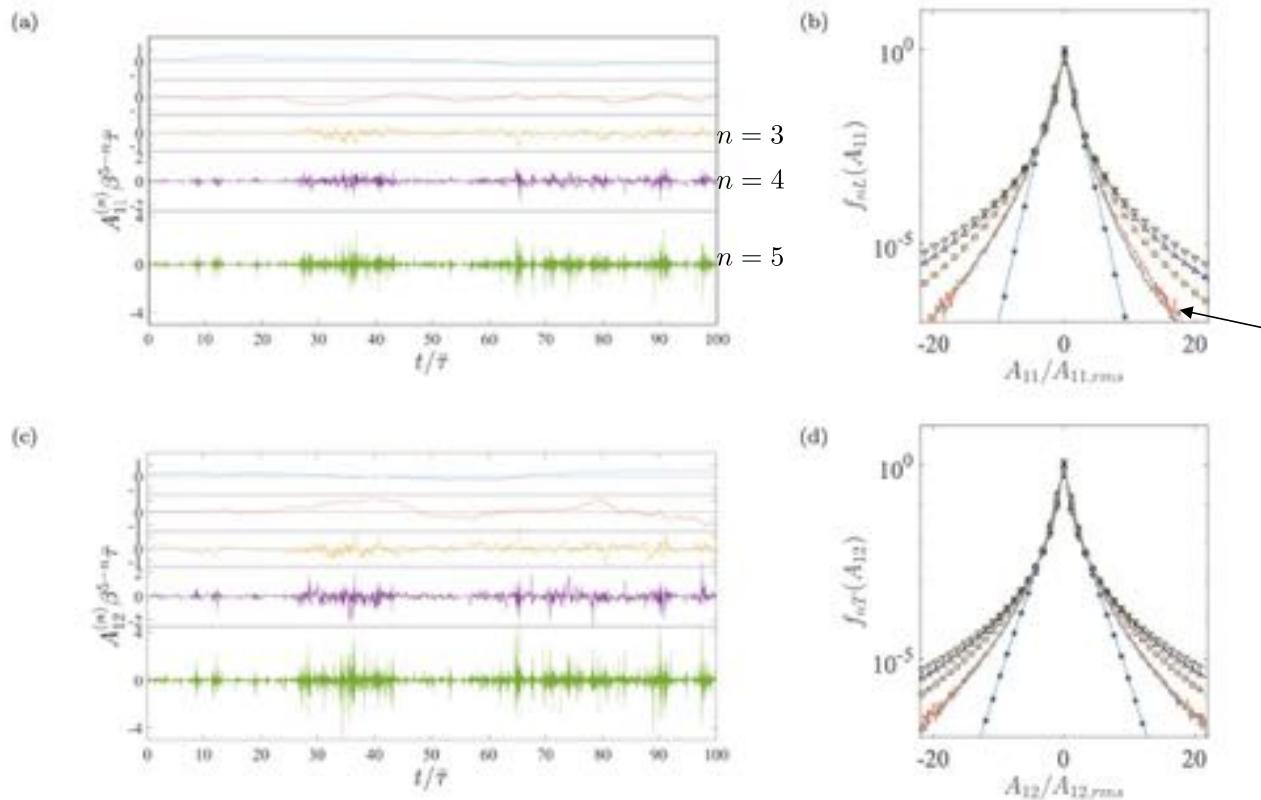
$$dA_{ij}^{(n)} = \left[-\left(A_{ik}^{(n)} A_{kj}^{(n)} - \frac{1}{3} A_{pq}^{(n)} A_{pq}^{(n)} \delta_{ij} \right) + h_{ij}^n(\mathbf{A}, \tau_n) - \frac{\dot{\tau}_n}{\tau_n} A_{ij} \right] dt + dF_{ij}(\tau_n) \quad \tau_n(t) = \frac{1}{\beta} (2S_{ij}^{(n-1)} S_{ij}^{(n-1)})^{-1/2}$$



Results: Widening tails in gradient PDF

$\beta=10$

$$dA_{ij}^{(n)} = \left[-\left(A_{ik}^{(n)} A_{kj}^{(n)} - \frac{1}{3} A_{pq}^{(n)} A_{pq}^{(n)} \delta_{ij} \right) + h_{ij}^n(\mathbf{A}, \tau_n) - \frac{\dot{\tau}_n}{\tau_n} A_{ij} \right] dt + dF_{ij}(\tau_n) \quad \tau_n(t) = \frac{1}{\beta} (2S_{ij}^{(n-1)} S_{ij}^{(n-1)})^{-1/2}$$

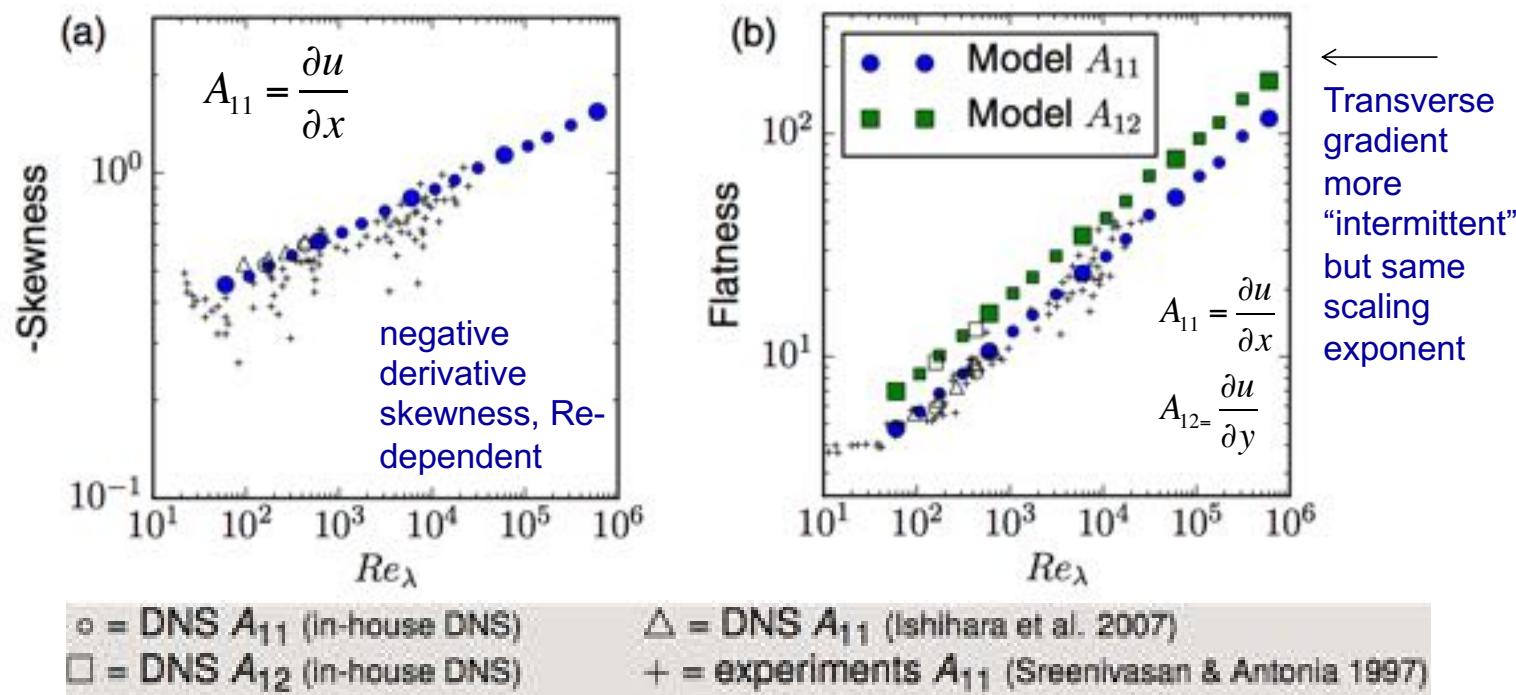


Luo, Shi & CM, Phys Rev.
Fluids 7, 04609 (2022)

Reynolds number scaling of $-S$ and F

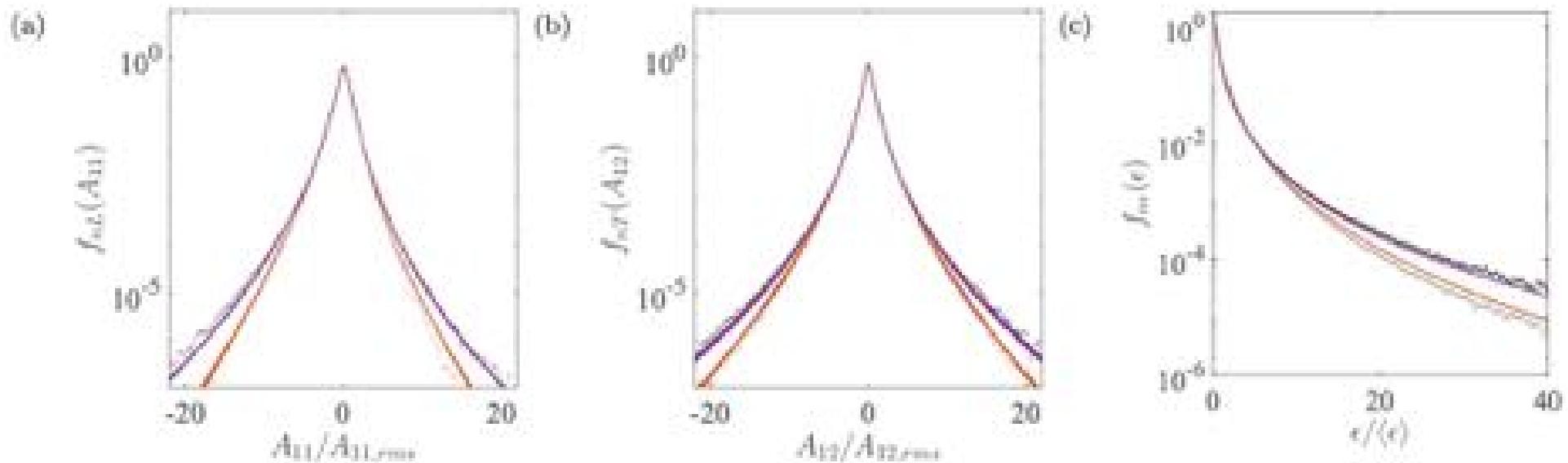
Choosing $\beta = 10$

$$dA_{ij}^{(n)} = \left[-\left(A_{ik}^{(n)} A_{kj}^{(n)} - \frac{1}{3} A_{pq}^{(n)} A_{pq}^{(n)} \delta_{ij} \right) + h_{ij}^n(\mathbf{A}, \tau_n) - \frac{\dot{\tau}_n}{\tau_n} A_{ij} \right] dt + dF_{ij}(\tau_n) \quad \tau_n(t) = \frac{1}{\beta} (2S_{ij}^{(n-1)} S_{ij}^{(n-1)})^{-1/2}$$



Detailed comparison with DNS at 2 Reynolds numbers:

Luo, Shi & CM, Phys Rev. Fluids 7, 04609 (2022)



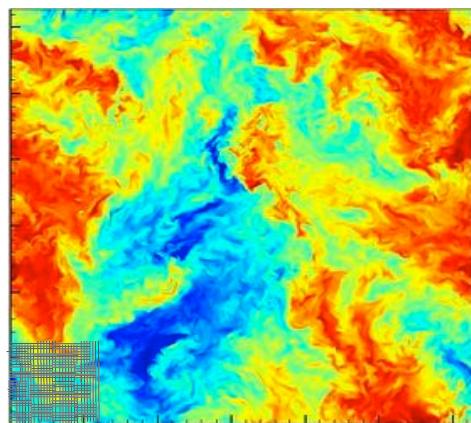
$R_\lambda=430$ (dots: JHTDB 1024^3 DNS data. Line = model, at $n=1.85$)

$R_\lambda=1,300$ (JHTDB, data from PK Yeung, Georgia Tech, 8193^3 DNS. Line = model, at $n=2.33$)

Engineering application: Large-Eddy-Simulation (LES)

Coarse-graining (local homogenization) for more affordable simulations

4×10^9
d.o.f.

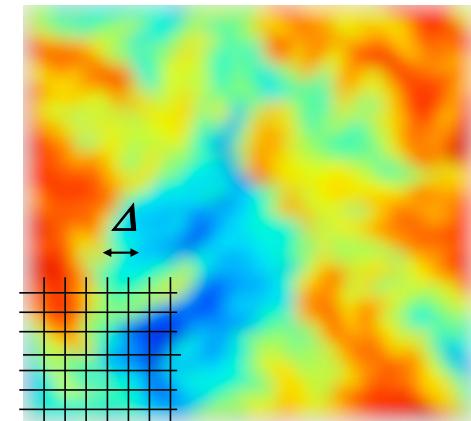


DNS

$$\frac{\partial u_j}{\partial t} + \frac{\partial u_k u_j}{\partial x_k} = -\frac{\partial p}{\partial x_j} + \nu \nabla^2 u_j$$

$$\frac{\partial u_j}{\partial x_j} = 0$$

$\tilde{u}_1(x, y, z_0, t_0)$

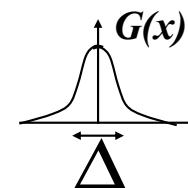


LES

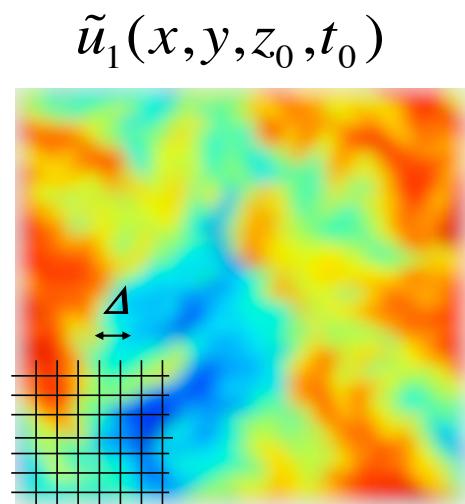
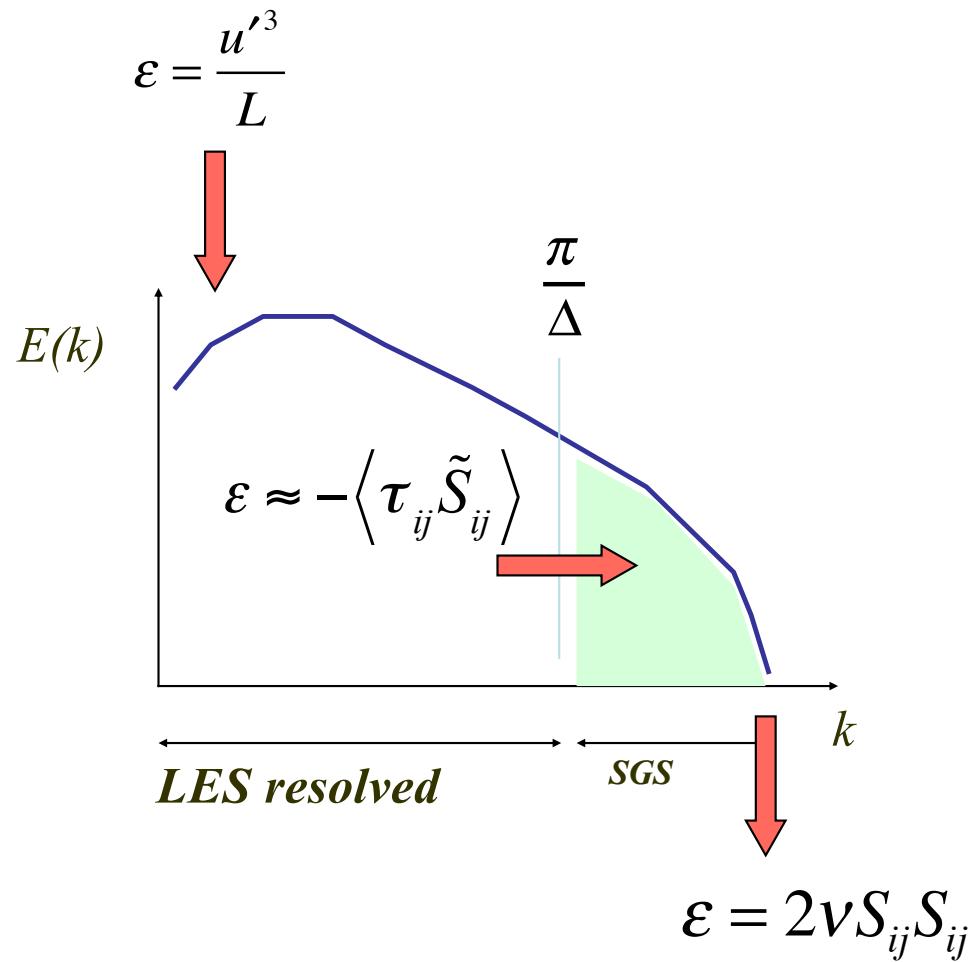
$$\frac{\partial \tilde{u}_j}{\partial t} + \tilde{u}_k \frac{\partial \tilde{u}_j}{\partial x_k} = -\frac{\partial \tilde{p}}{\partial x_j} + \nu \nabla^2 \tilde{u}_j - \frac{\partial}{\partial x_k} \tau_{jk}$$

SGS stress tensor: $\tau_{ij} = \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j$

10^5
d.o.f.



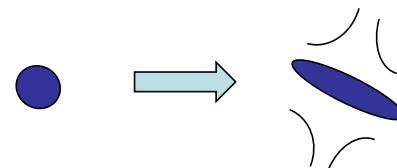
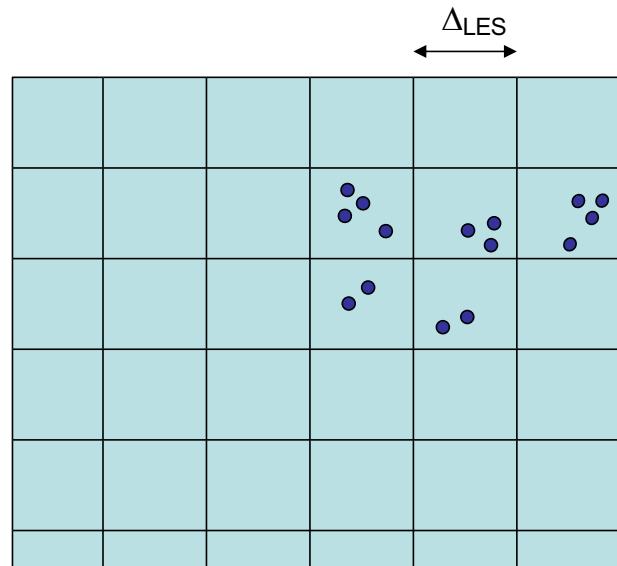
Dissipation of kinetic energy in LES



$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + \Omega_{ij}$$

What about LES dealing with “small-scale dominated physics” ?

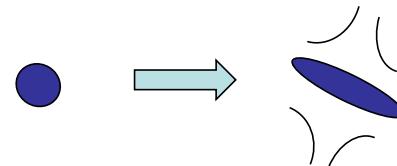
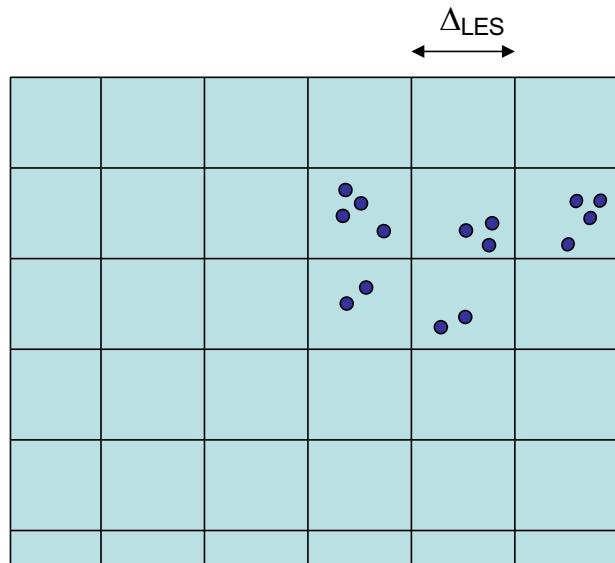
Large Eddy Simulation (LES) including predictions of small droplet deformation statistics & geometry (consider only $d_p < \eta_K$)



$$\left| \frac{\partial u_i}{\partial x_j} \right| \sim \frac{1}{\tau_K} \sim \sqrt{\frac{\varepsilon}{\nu}}$$

What about LES dealing with “small-scale dominated physics” ?

Large Eddy Simulation (LES) including predictions of small droplet deformation statistics & geometry (consider only $d_p < \eta_K$)



$$\left| \frac{\partial u_i}{\partial x_j} \right| \sim \frac{1}{\tau_K} \sim \sqrt{\frac{\varepsilon}{\nu}}$$

Traditional approach to model strain-rates responsible for droplet deformations:

$$\varepsilon \sim \langle \varepsilon \rangle_{LES} \sim \nu_{sgs} |S|^3 (\mathbf{x}, t)$$

Lacks intermittency and “directional information” (geometry)

Applications in LES:

Small scale intermittency of turbulence generates extreme events, difficult to characterize based on local averages

Small scale intermittency affects:

Johnson & CM (JFM, 2018)

- **droplet deformations in turbulence**
 - flame structure (quenching) in combustion
 - micro-organism motility and nutrient uptake
 - polymer stretching–relaxation dynamics

Here, focus on small (sub-Kolmogorov) droplets

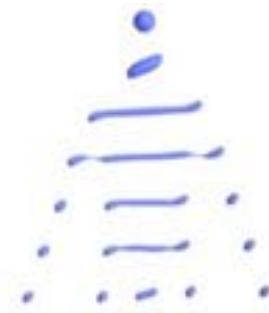
- The sub-Kolmogorov size of the droplets implies that: only viscous drag induced by the shear can distort the droplet shape (no inertial forces)
- The distortion is resisted by the surface tension that tends to restore the spherical shape
- Initial study by Taylor (1932) with drops in a laminar flow

Frijters et al. (2012)



Equilibrium configuration

or



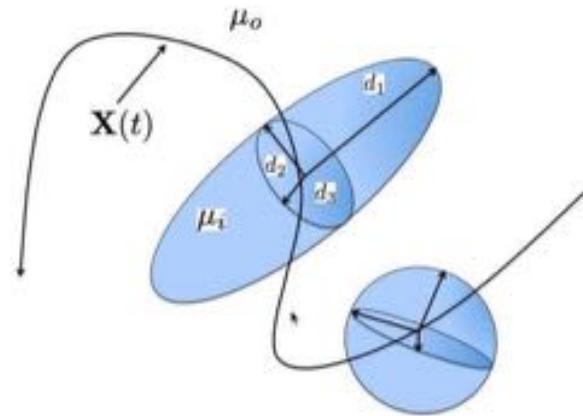
Kemnáková et al. (2012)

droplet break-up

See Kolmogorov (1949) and Hinze (1955), Lasheras et al. (2002),

Lagrangian model for sub-Kolmogorov droplets

- We model fluid with small but finite viscosity using standard DNS and LES
- Droplets of immiscible viscous fluid
- Surface tension at the interface
- Droplet shape approximated as triaxial ellipsoids (OK for initial, small, deformation)



The Maffettone Minale model:

Maffettone, Minale, J. Non-Newtonian Fluid Mech., 78 (1998) 227–241

ELLIPSOIDAL DROP DETERMINED BY A SYMMETRIC POSITIVE DEFINED SECOND RANK TENSOR

M 's eigenvalues: squared semiaxis of the ellipsoid $M_{ij}(X(t), t) = \rho_d \int_V (r_i - X_i(t))(r_j - X_j(t)) dV,$

$$G_i = \left\langle \left(\frac{\partial u_i}{\partial x_i} \right)^2 \right\rangle^{1/2}.$$



$$Ca = \frac{\mu_o R G_t}{A} = \tau G_t.$$

$$\frac{dM_{ij}}{dt} = \Omega_{ik} M_{kj} - M_{ik} \Omega_{kj} + f_2(S_{ik} M_{kj} + M_{ik} S_{kj}) - \frac{f_1}{\tau_e} (M_{ij} - g(II_M, III_M) \delta_{ij}),$$

$$\frac{dM_{ij}}{dr'} = [f_2(S'_{ik} M_{kj} + M_{ik} S'_{kj}) + \Omega'_{ik} M_{kj} - M_{ik} \Omega'_{kj}] - \frac{f_1}{Ca} \left(M_{ij} - 3 \frac{III_M}{II_M} \delta_{ij} \right).$$

$$A_{ij} = \frac{\partial u_i}{\partial x_j} \quad S_{ij} = \frac{1}{2} (A_{ij} + A_{ji}) \quad \Omega_{ij} = \frac{1}{2} (A_{ij} - A_{ji})$$

Consider for now

$$\lambda = 1 \rightarrow$$

$$f_1 = 0.457, \quad f_2 = 1$$

$$f_1 = \frac{40(\lambda + 1)}{(2\lambda + 3)(19\lambda + 16)}, \quad \lambda = \mu_1/\mu_2$$

$$f_2 = \frac{5}{2\lambda + 3}.$$

G.I. Taylor,
Proc. R. Soc. A 138 (1932) 41–48.

Evolution of small droplets, small deformation (ellipsoidal):

We require time evolution of unfiltered turbulent velocity gradient tensor along particle trajectories

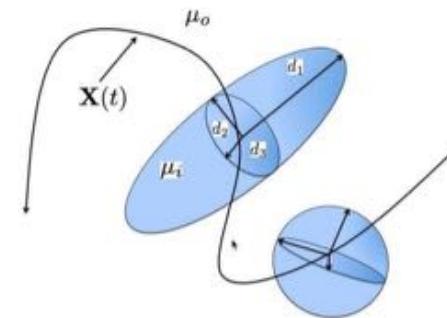
$$A_{ij} = \frac{\partial u_i}{\partial x_j}$$

$$S_{ij} = \frac{1}{2} (A_{ij} + A_{ji})$$

$$\Omega_{ij} = \frac{1}{2} (A_{ij} - A_{ji})$$



$$M_{ij}(t)$$



for “representative particle method” (RPM)
in a mixed Lagrangian Eulerian LES method

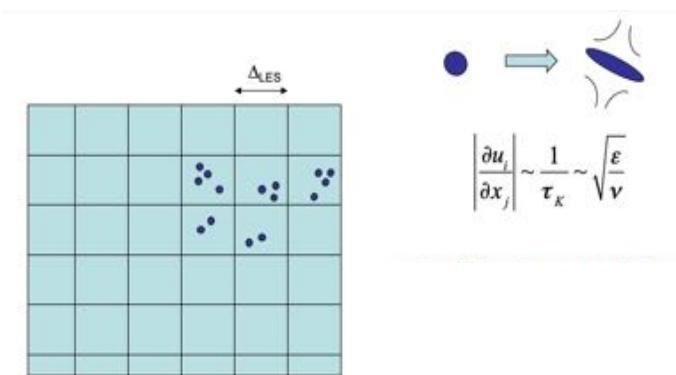
- We want to do LES of turbulent flow at high Re
- We want to keep track of deformation and orientation of “droplet microstructure”, even if unresolved in LES
- We will use hybrid Euler-Lagrangian approach
- We will follow droplets (Lagrangian) using M&M equation

$$\frac{dM_{ij}}{dt} = \Omega_{ik}M_{kj} - M_{ik}\Omega_{kj} + f_2(S_{ik}M_{kj} + M_{ik}S_{kj}) - \frac{f_1}{\tau_e}(M_{ij} - g(II_M, III_M)\delta_{ij}),$$

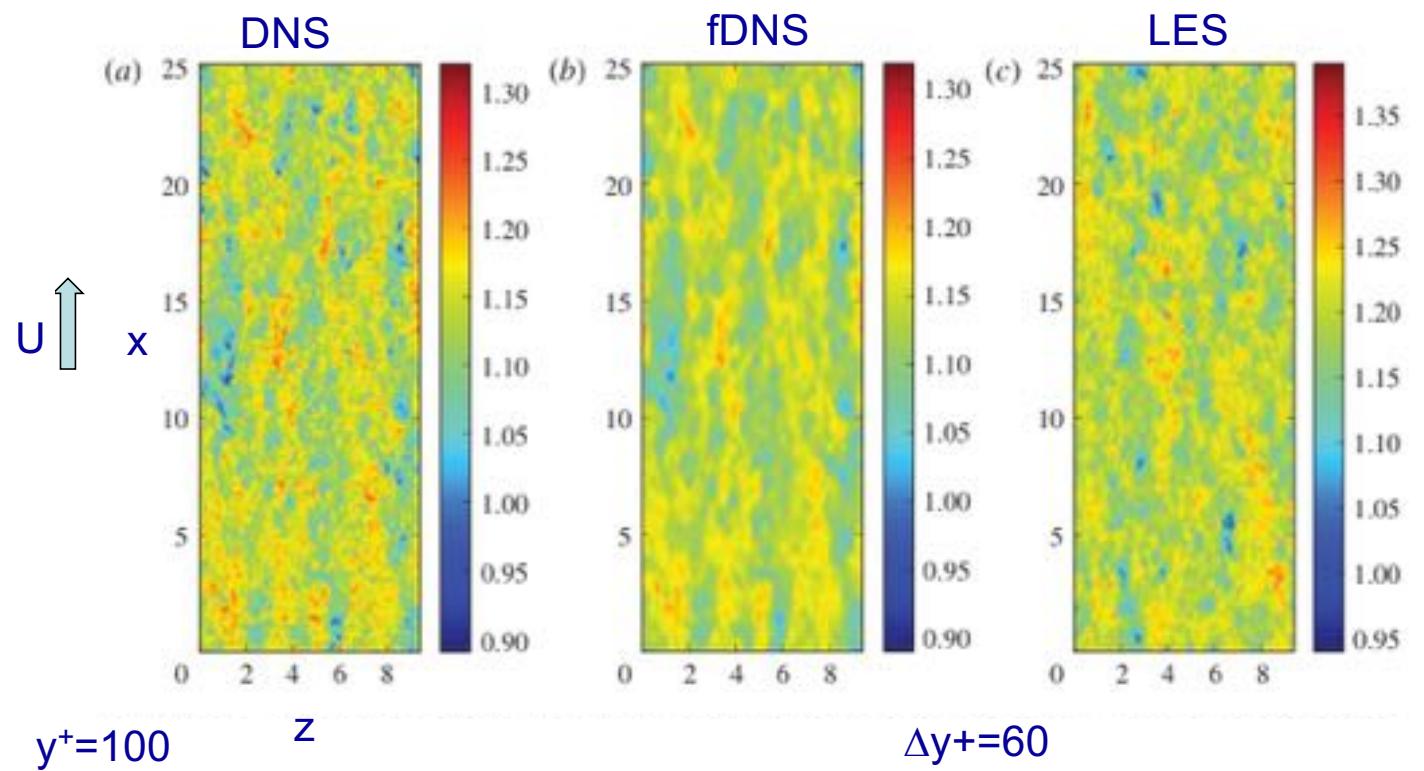
- But for this we need “unfiltered” velocity gradient tensor history along droplet trajectories, unavailable from LES

$$A_{ij} = \frac{\partial u_i}{\partial x_j} = S_{ij} + \Omega_{ij}$$

- We use our SGS modeling of Largangian history of gradients
- **application to LES of channel flow**



Application to drops in channel (1-way coupling):



Case	$\Delta_x/dx = \Delta_z/dz$	$N_x \times N_y \times N_z$	dx^+, dy_c^+, dz^+	N_t	dt_{sim}	dt_{DG}	U_{bulk}	$\tau_{\eta,bulk}$
DNS	1	$2048 \times 512 \times 1536$	12.3, 6.2, 6.1	4000	0.0013	0.0065	1.00	0.141
fDNS	32	$128 \times 32 \times 96$	196, 98.5, 98.2	250	(N/A)	0.104	1.00	(N/A)
LES	16	$128 \times 32 \times 96$	196, 98.5, 98.2	250	0.0104	0.104	1.04	0.139

Applications: channel flow, DNS & LES

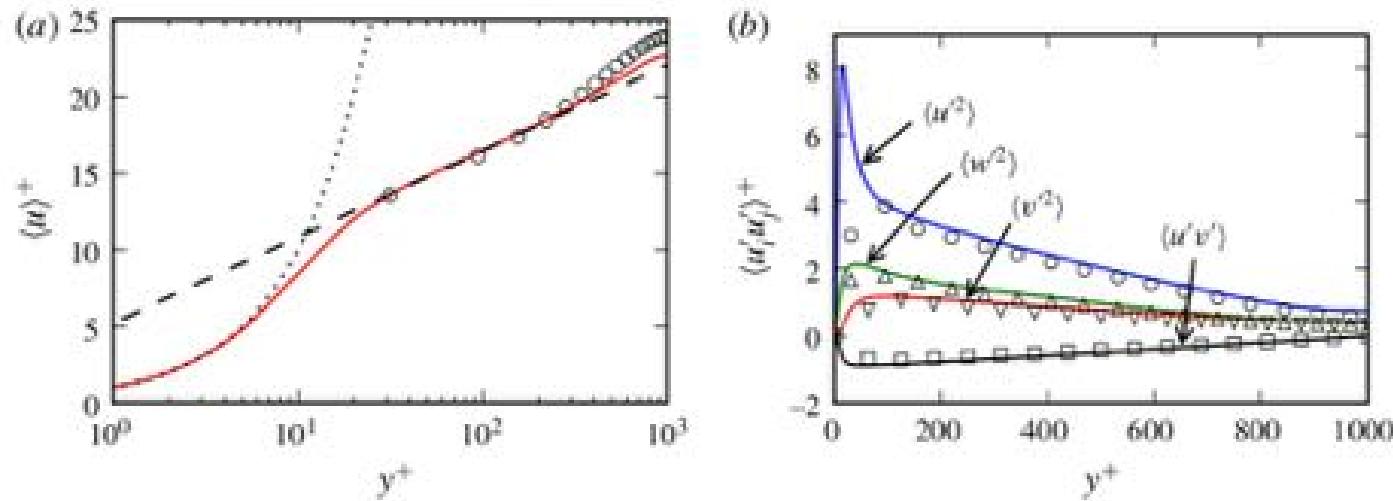


FIGURE 3. (Colour online) Mean velocity (a) and Reynolds stress tensor components (b) profiles for DNS (continuous lines) and LES (symbols). In (a), the well-established linear, $\langle u^+ \rangle = y^+$ (dotted line), and log-law, $\langle u^+ \rangle = \ln y^+ / 0.41 + 5.2$ (dashed line), profiles are also shown for reference. For the Reynolds stress components in (b): $\langle u'^2 \rangle$ (\circ), $\langle v'^2 \rangle$ (∇), $\langle w'^2 \rangle$ (Δ), and $\langle u' v' \rangle$ (\square).

**LES: Lagrangian scale dependent dynamic SGS model
Algebraic equilibrium wall model**

LES + “representative particles”:

- Langevin equation, $dA_{ij} =$

$$\left[- \left((\mathbf{A}^2)_{ij} - \frac{C_{ij}^{-1}}{C_{kk}^{-1}} \text{tr}(\mathbf{A}^2) \right) - \left(G_{ij} - \frac{C_{ij}^{-1}}{C_{kk}^{-1}} \text{tr}(\mathbf{G}) \right) + V_{ij} \right] dt + dF_{ij}$$

so far: 1 level RDGF model

- 9 ODEs for droplet conformation tensor

$$\frac{d\mathcal{D}_{ij}}{dt} = \Omega_{ik}\mathcal{D}_{kj} + f_2(\hat{\mu})S_{ik}\mathcal{D}_{kj} - \frac{f_1(\hat{\mu})}{2\tau_d} \left(\mathcal{D}_{ij} - \frac{3\text{III}}{\text{II}}\mathcal{D}_{ji}^{-1} \right)$$

Better conditioned matrix ODE

Equivalent to Maffetone – Minale model for $\mathbf{M} = \mathcal{D}\mathcal{D}^T$

information

about the semi-axes can be extracted from the deformation using a singular value decomposition, $\mathcal{D} = \mathbf{U}\Sigma\mathbf{V}^T$, where \mathbf{U} is a unitary matrix comprised of the singular vectors indicating the semi-axis directions and Σ is a diagonal matrix whose elements are the associate singular values $\sigma_1 \geq \sigma_2 \geq \sigma_3$, i.e., the length of the semi-axes (Greene & Kim 1987). The total extent of deformation away from a spherical droplet is commonly measured using a deformation parameter, $D = (\sigma_1 - \sigma_3)/(\sigma_1 + \sigma_3)$.

LES and initial conditions: sprinkle droplets on channel center-plane



Stochastic Dispersion Model: (Fede et al. 2006)

Tracer particle tracking:

$$\frac{dX_i}{dt} = u_i(X_i(t), t) = \tilde{u}_i + u'_i.$$

$$du'_i = \frac{\partial \tau_{ij}}{\partial x_j} dt - u'_j \frac{\partial \tilde{u}_i}{\partial x_j} dt - \left(\frac{1}{2} + \frac{3}{4} C_0 \right) \frac{\Pi}{k_r} u'_i dt + \sqrt{C_0 \Pi} dW_i,$$

where

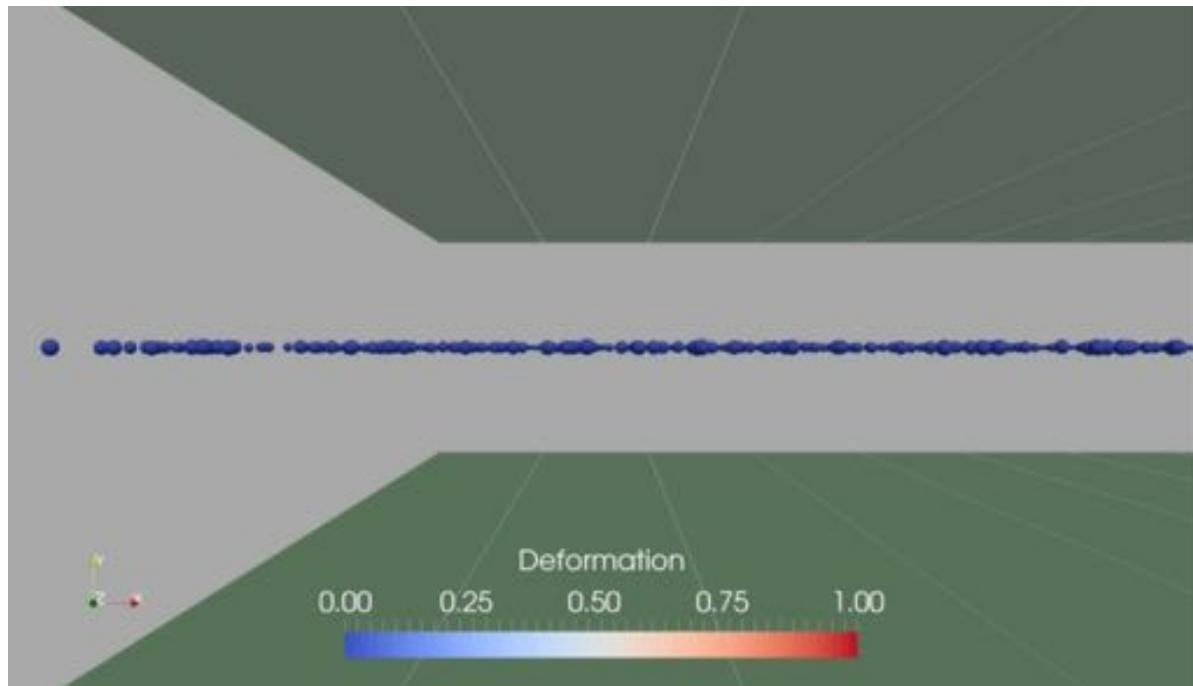
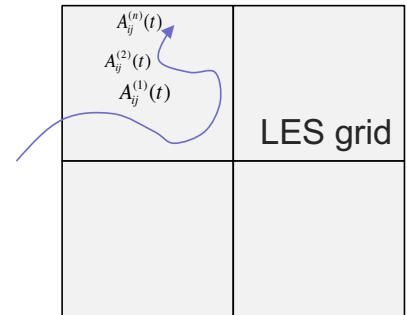
$$\Pi = (C_s \Delta)^2 |\tilde{S}|^3, \quad k_r = 2C_y \Delta^2 |\tilde{S}|^2,$$

$$\frac{\Pi}{k_r} = C' |\tilde{S}|, \quad C' = \frac{C_s^2}{2C_y} = \frac{1}{S_s} \left(\frac{2}{3C_k} \right)^{3/2} \approx 0.21,$$

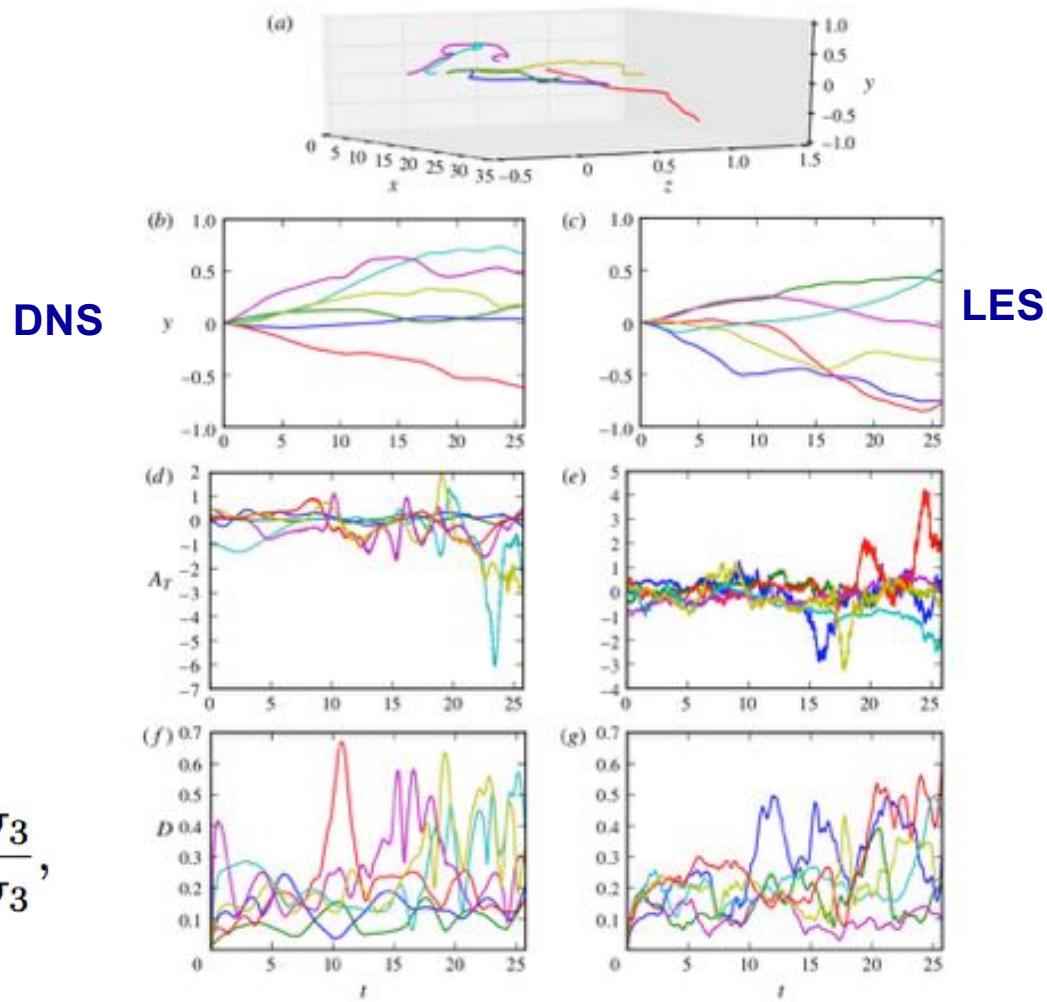
derived using spectral cutoff theory (following Lilly 1967).

LES of deforming droplets in channel flow:

- DNS + $(9+3) \times N \times$ Lagr. SDE for M&M model
- LES + $(18+3) \times N \times$ Lagr. SDEs)
- Ensemble of $N=172,000$
- See Johnson & CM (JFM 2018)



Sample signals:



$$D = \frac{\sigma_1 - \sigma_3}{\sigma_1 + \sigma_3},$$

FIGURE 5. (Colour online) Sample time histories of particle locations in three dimensions (a), the wall-normal location (b,c), the transverse velocity gradient (d,e) and deformation magnitude parameter D (f,g) from the DNS (b,d,f) and LES-RDGF (c,e,g) results for 6 independent Lagrangian trajectories. The droplets shown have $Ca = 1.0$ and $\hat{\mu} = 1.0$.

Time evolution of concentration of particles:

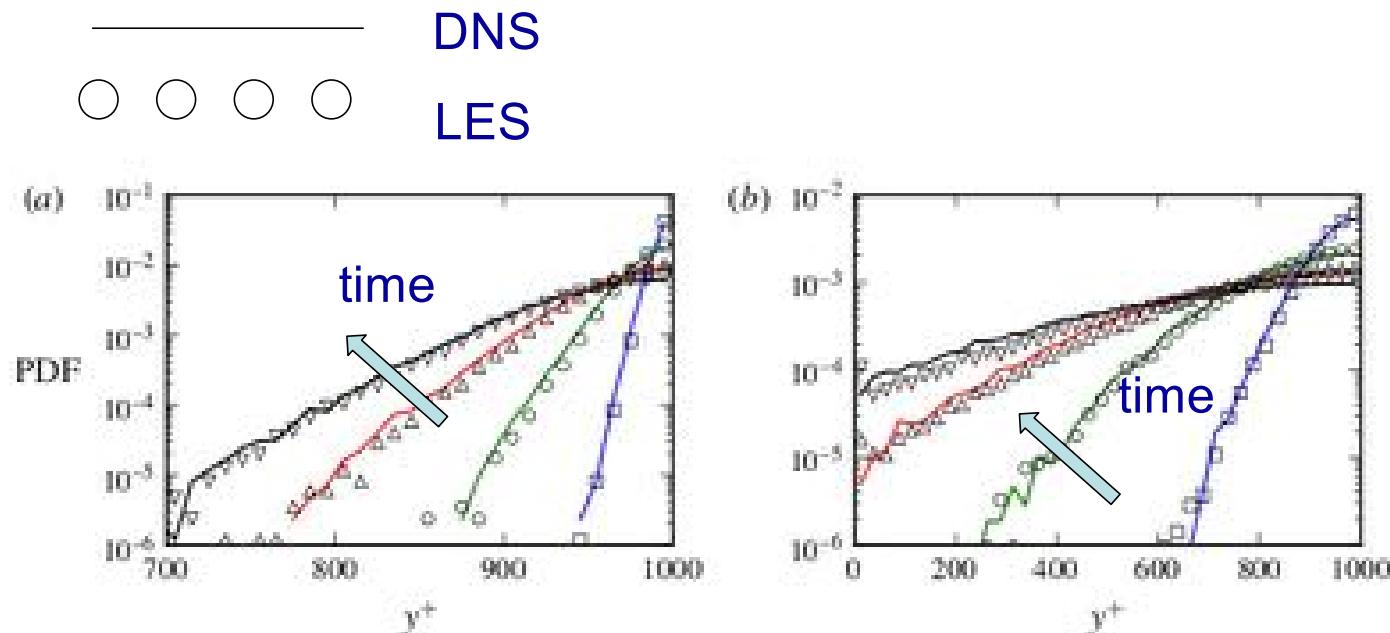
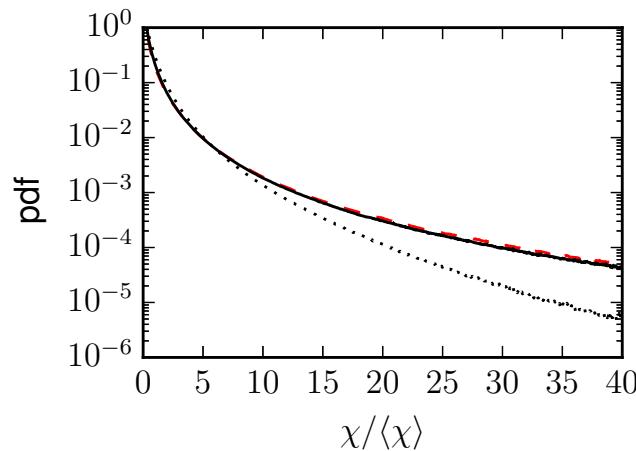
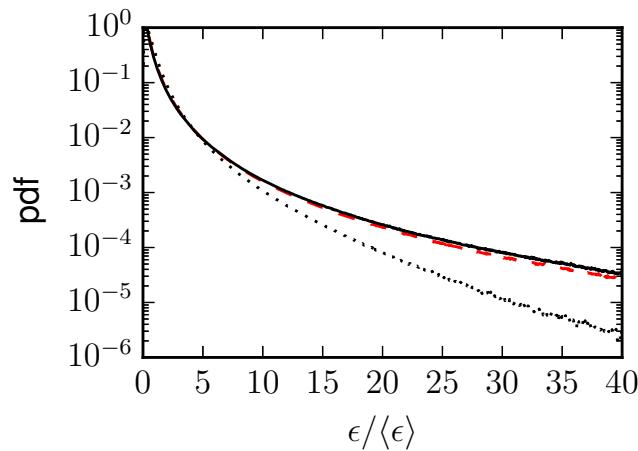


FIGURE 6. (Colour online) Distribution of particles at different times after being released from the centreline at $t = 0$. Continuous lines show the distributions from DNS while symbols show the results from LES with stochastic model for subgrid velocity. (a) $t = 0.26$ (\square), $t = 0.78$ (\circ), $t = 1.56$ (\triangle), $t = 2.34$ (∇). (b) $t = 2.6$ (\square), $t = 7.8$ (\circ), $t = 15.6$ (\triangle), $t = 23.4$ (∇).

Dissipation and Enstrophy Statistics

- ensemble histogram from all data $t \in [0, L_t]$
- includes $\hat{\epsilon}$ fluctuations from LES and internal fluctuations from RDGF

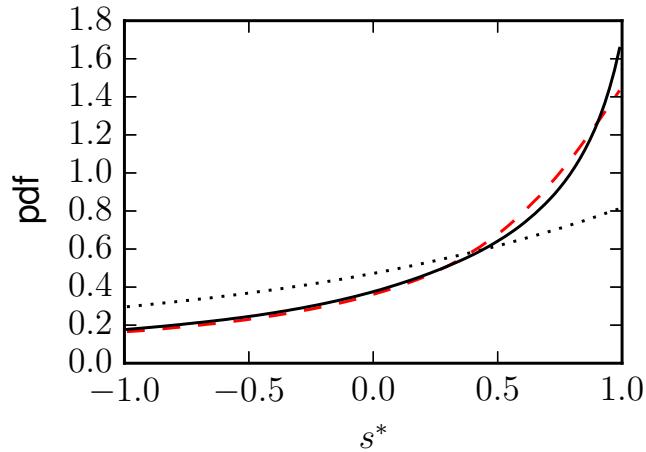
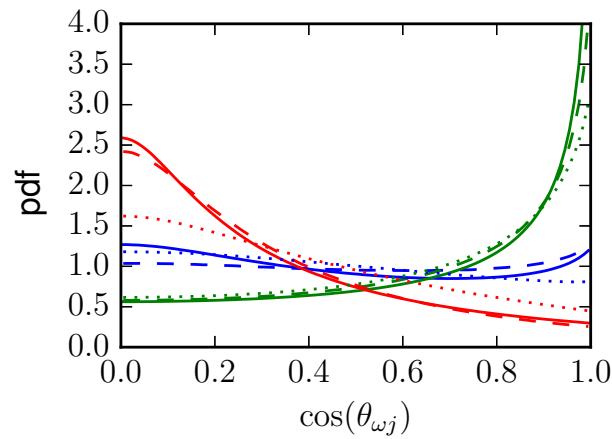


Dashed line: DNS

Solid line: LES-RDGF

Dotted line: LES, no model

Velocity Gradient Geometry Statistics



$$\cos(\theta_{\omega j}) = \hat{\omega} \cdot \hat{\mathbf{e}}_j,$$

Dashed line: DNS

Solid line: LES-RDGF

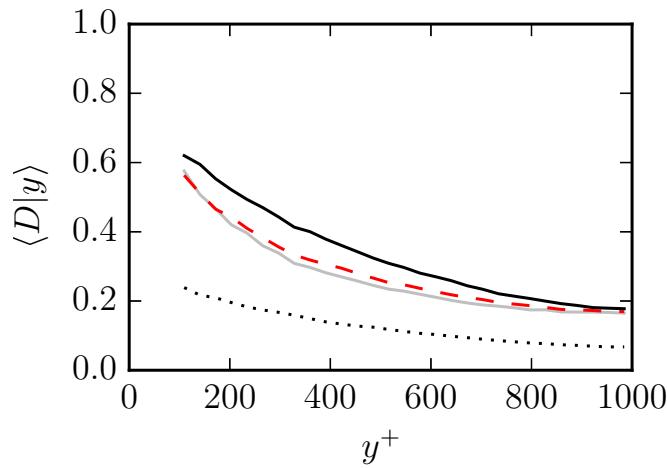
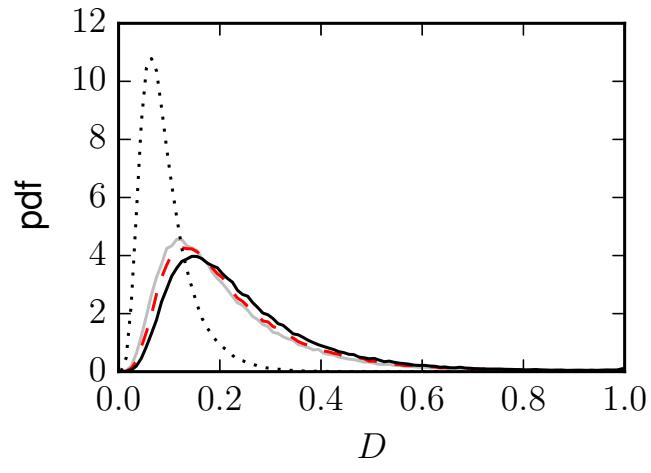
Dotted line: LES, no model

$$s^* = -\frac{3\sqrt{6}\Lambda_1\Lambda_2\Lambda_3}{(\Lambda_1 + \Lambda_2 + \Lambda_3)^{3/2}},$$

Droplet deformation results:

$$D = \frac{\sigma_1 - \sigma_3}{\sigma_1 + \sigma_3},$$

Droplet Deformation at $Ca = 1.0$ ($t = 23.4$)



Red: baseline DNS

Gray: *a priori* (fDNS-RDGF)

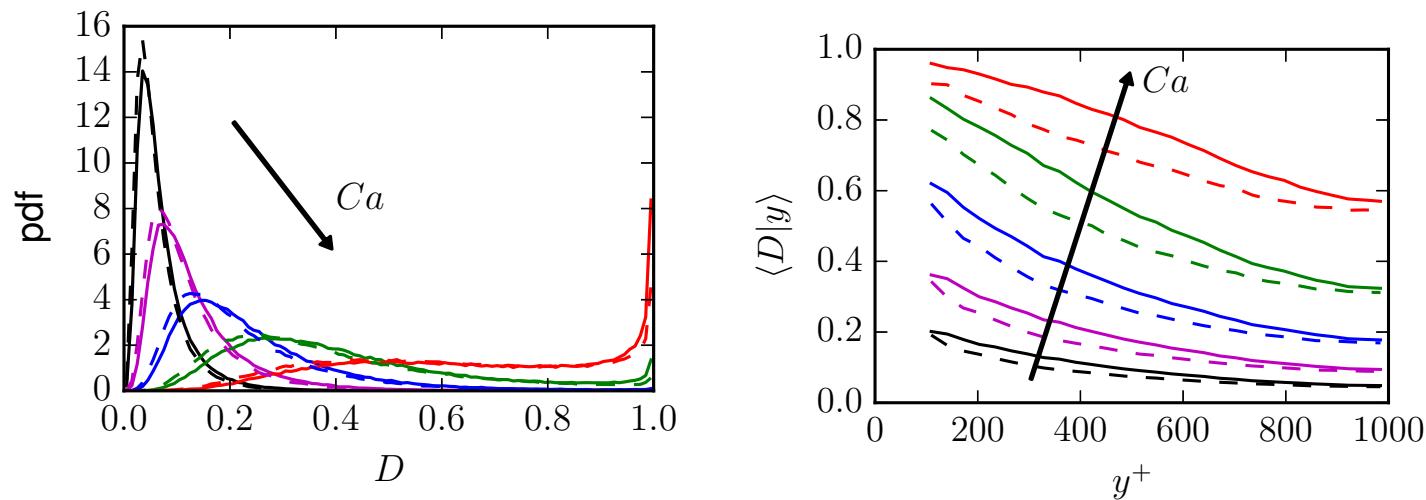
Black: *a posteriori* (LES-RDGF)

Dotted: LES, no model

Dependence on surface tension (Capillary number):

Effect of Ca Number on Droplet Deformation ($t = 23.4$)

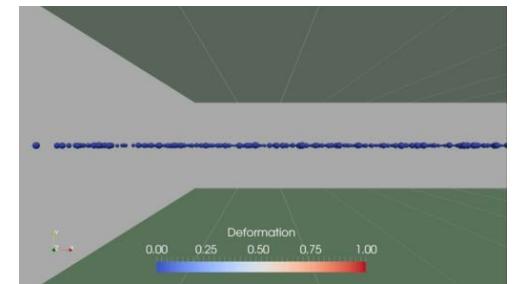
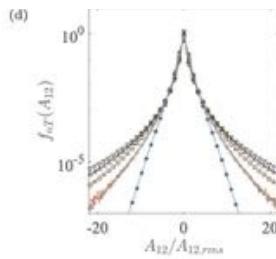
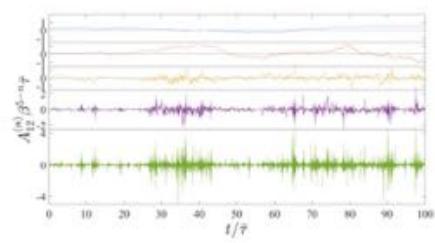
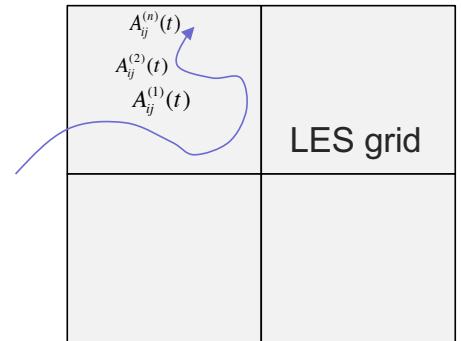
$$Ca = 0.25, 0.5, 1.0, 2.0, 4.0$$



Solid lines: LES-RDGF
Dashed lines: DNS

Conclusions:

- Enriching LES with small-scale models
- Lagrangian stochastic model for A_{ij}
- Applications to model droplet deformation statistics in turbulent channel flow
- Refs:
 - Johnson & CM (J Fluid Mech. 2016, 2017, 2018)
 - Luo, Shi & CM (Phys. Rev. Fluids 7, 2022)



Thank you!