

LES of Turbulent Flows: Lecture 23

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Fall 2016



① Lagrangian Particle Dispersion Modeling in LES



Lagrangian Particle Dispersion Modeling in LES

- This is a special lecture on Lagrangian particle dispersion in LES created by Brian Bailey





Lagrangian Particle Dispersion Modeling in LES

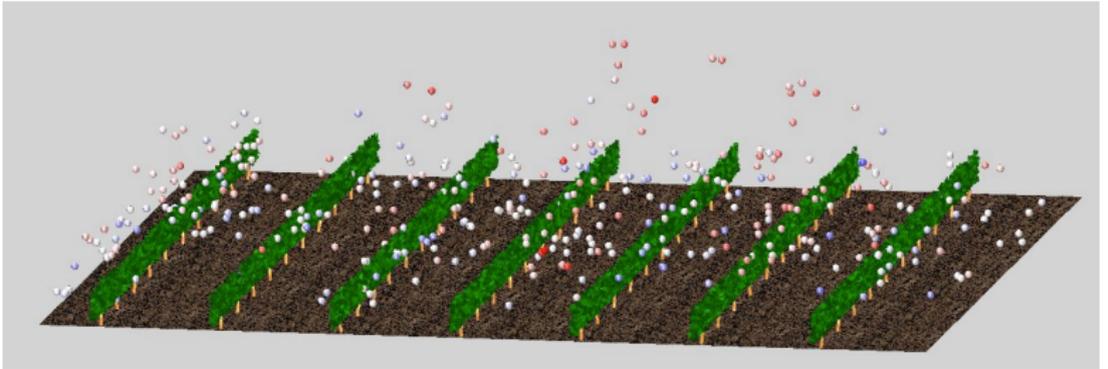
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November 18, 2014



Visualizations





Lagrangian vs Eulerian Reference Frames

Eulerian



Lagrangian



Best for smoothly varying
scalar fields (i.e., continuum)

Governing Equation

$$\frac{\partial C}{\partial t} + \frac{\partial u_j C}{\partial x_j} = D \frac{\partial^2 C}{\partial x_j \partial x_j}$$



Lagrangian vs Eulerian Reference Frames

Eulerian



Best for smoothly varying scalar fields (i.e., continuum)

Governing Equation

$$\frac{\partial C}{\partial t} + \frac{\partial u_j C}{\partial x_j} = D \frac{\partial^2 C}{\partial x_j \partial x_j}$$

Lagrangian



Best for discrete sources, or when details of individual particles are of interest

Governing Equation

$$\frac{dx_i}{dt} = u_i$$



Numerical solution

$$\frac{dx_i}{dt} = u_i$$

$$\frac{x_i(t + \Delta t) - x_i(t)}{\Delta t} = u_i(t)$$

$$x_i(t + \Delta t) = x_i(t) + u_i(t)\Delta t$$



Note

Side Note:

This form assumes particles are massless.

Could add generic velocity (say u_i^*) to account for gravitational settling, inertia, etc.

$$\frac{dx_i}{dt} = u_i + u_i^*$$



Numerical solution example

$$x_i(t + \Delta t) = x_i(t) + u_i(t)\Delta t$$

Consider $x(0) = 0$

$u(x = 0) = 1$, $u(x = 0.5) = 2$, $u(x = 1) = 1.5$

$\Delta t = 0.1$



Numerical solution example

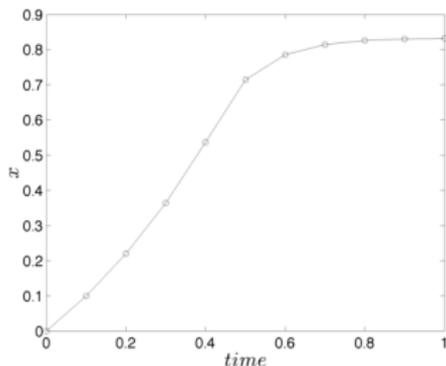
$$x_i(t + \Delta t) = x_i(t) + u_i(t)\Delta t$$

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$\Delta t = 0.1$

t	x	u
0	0	1
0.1	0.1	1.2
0.2	0.22	1.44
0.3	0.36	1.73
0.4	0.54	0.71





Application to LES

What's the problem if we want to apply this to LES?



Application to LES

What's the problem if we want to apply this to LES?

$$\frac{dx_i}{dt} = u_i = \underbrace{\tilde{u}_i}_{\text{resolved}} + \underbrace{u_{s,i}}_{\text{subgrid}}$$



Application to LES

What's the problem if we want to apply this to LES?

$$\frac{dx_i}{dt} = u_i = \underbrace{\tilde{u}_i}_{\text{resolved}} + \underbrace{u_{s,i}}_{\text{subgrid}}$$

We don't know $u_{s,i}$!



Framework for modeling $u_{s,i}$

Could neglect it ($u_{s,i} = 0$)

e.g.,

Pure Convection:

Gopalakrishnan, S. G., and R. Avissar, 2000: An LES study of the impacts of land surface heterogeneity on dispersion in the convective boundary layer. *J. Atmos. Sci.*, **57**, 352–371.

Near-Canopy Flow:

Bailey, B. N., R. Stoll, E. R. Pardyjak, and W. F. Mahaffee, 2014: The effect of canopy architecture and the structure of turbulence on particle dispersion. *Atmos. Env.*, **95**, 480–489.



Framework for modeling $u_{s,i}$

Modeling $u_{s,i}$:
where should we start?



Framework for modeling $u_{s,i}$

Modeling $u_{s,i}$:

where should we start?

Let's copy the RANS people.

Why? RANS is essentially LES with the grid scale equal to the domain size....so this *should* be easier.



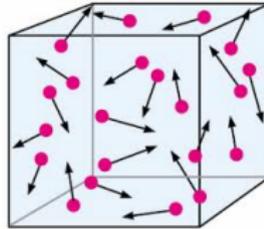
Framework for modeling $u_{s,i}$

Lagrangian dispersion in RANS:

$$\frac{dx_i}{dt} = \underbrace{\bar{u}_i}_{\text{mean}} + \underbrace{u_i}_{\text{fluctuations}}$$



RANS models



Analogy to molecular motion (Brownian motion):
Langevin Equation

$$du_i = \underbrace{-\mathbf{a}u_i}_{\text{memory}}dt + \underbrace{\mathbf{b}d\xi_i}_{\text{diffusion}}$$

u_i - molecule velocity

$d\xi_i$ - random Gaussian process with mean zero and variance dt



Langevin Equation

Application to isotropic turbulence:

$u_i \rightarrow$ Lagrangian particle velocity

$$du_i = -\mathbf{a}u_i dt + \mathbf{b}d\xi_i$$

How do we get \mathbf{a} and \mathbf{b} ?



Langevin Equation: finding b

$$du_i = -au_i dt + b d\xi_i \quad (1)$$

b comes directly from Kolmogorov's second hypothesis

Lagrangian structure function:

$$D(\Delta t) = \langle (\Delta w)^2 \rangle = C_0 \varepsilon \Delta t$$

Provided Δt is in the internal subrange (i.e., $\tau_\eta \ll \Delta t \ll \tau_L$)



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Provided Δt is in the internal subrange (i.e., $\tau_\eta \ll \Delta t \ll \tau_L$)

Square Eq.1 and take ensemble average:

$$\langle (\Delta w)^2 \rangle = -\langle a w^2 (\Delta t)^2 \rangle \overset{\approx 0}{\rightarrow} -\langle a w^2 \rangle \Delta t^2 - \langle a b w \Delta \xi \rangle \Delta t \overset{0}{\rightarrow} + b^2 \langle (\Delta \xi)^2 \rangle \Delta t$$

$$\langle (\Delta w)^2 \rangle = b^2 \Delta t = C_0 \varepsilon \Delta t \rightarrow \boxed{b = (C_0 \varepsilon)^{-1/2}}$$



Langevin Equation: finding a

$$du_i = -au_i dt + b d\xi_i$$

Using stochastic calculus, we can solve this equation analytically

$$w(t) = w(0)e^{-at} + be^{-at} \int_0^t e^{as} \xi(s) ds$$



Langevin Equation: finding a

$$du_i = -au_i dt + b d\xi_i$$

Using stochastic calculus, we can solve this equation analytically

$$w(t) = w(0)e^{-at} + be^{-at} \int_0^t e^{as} \xi(s) ds$$

Square this equation and take ensemble average:

$$\langle w^2(t) \rangle = \langle w^2(0) \rangle e^{-2at} + \cancel{\langle w(0) \rangle} e^{-2at} \int_0^t e^{as} \xi(s) ds + \langle b^2 e^{-2at} \left[\int_0^t e^{as} \xi(s) ds \right]^2 \rangle$$

$$\langle w^2(t) \rangle = \langle w^2(0) \rangle e^{-2at} + \frac{b^2}{2a} [1 - e^{-2at}]$$



Langevin Equation: finding a

$$\langle w^2(t) \rangle = \langle w^2(0) \rangle e^{-2at} + \frac{b^2}{2a} [1 - e^{-2at}] \quad (2)$$

For homogeneous and isotropic turbulence,

$$\langle w^2(t) \rangle = \langle w^2(0) \rangle = \sigma_w^2 \text{ (const.)}$$

Make this substitution and evaluate Eq. 2 at $t \rightarrow \infty$

$$\sigma_w^2 = \frac{b^2}{2a}$$

$$a = \frac{b^2}{2\sigma_w^2} = \frac{C_0 \varepsilon}{2\sigma_w^2}$$



Langevin Equation

Application to homogeneous isotropic turbulence

$$du_i = -\frac{C_0\varepsilon}{2\sigma^2}u_i dt + (C_0\varepsilon)^{1/2} d\xi_i$$

for homogeneous isotropic turbulence,

$\frac{2\sigma^2}{C_0\varepsilon} = \tau_L$ is the integral timescale

$$du_i = -\frac{u_i}{\tau_L} dt + (C_0\varepsilon)^{1/2} d\xi_i$$

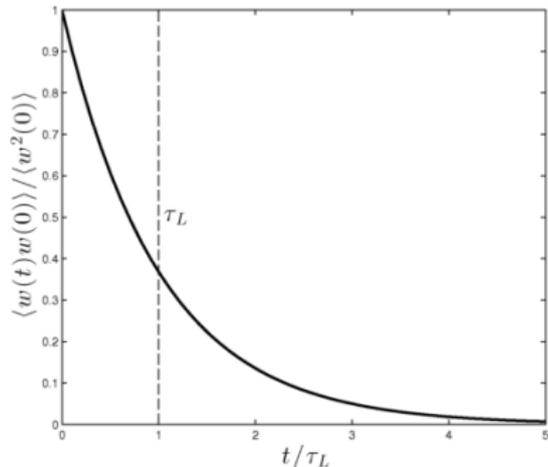


Langevin Equation

$$dw = \underbrace{-\frac{w}{\tau_L} dt}_I + \underbrace{(C_0 \varepsilon)^{1/2} d\xi_i}_{II}$$

- I Gives correct integral timescale of τ_L (long-time behavior)

$$\frac{\langle w(t)w(0) \rangle}{\langle w^2(0) \rangle} = e^{-t/\tau_L}$$





Langevin Equation

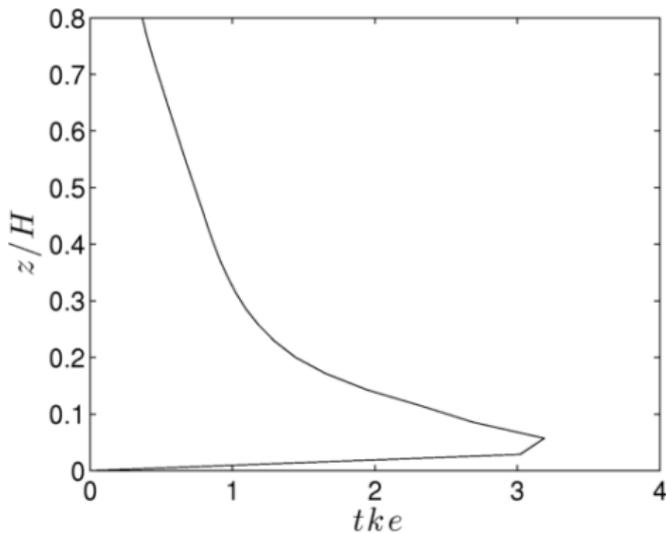
$$dw = - \underbrace{\frac{w}{\tau_L}}_I dt + \underbrace{(C_0 \varepsilon)^{1/2} d\xi_i}_{II}$$

- I Gives correct integral timescale of τ_L (long-time behavior)
- II Makes velocity consistent with Kolmogorov's second hypothesis (short-time behavior)



Langevin Equation

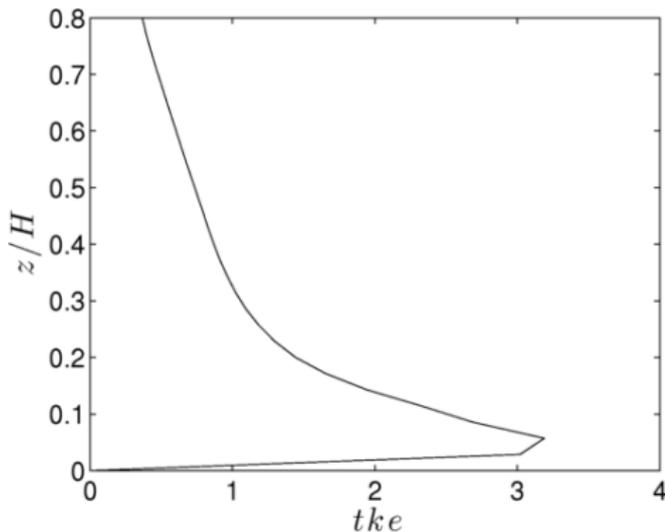
Inhomogeneous Turbulence (in 1D)





Langevin Equation

Inhomogeneous Turbulence (in 1D)



$\frac{\partial k}{\partial z} \neq 0$ implies a
mean flux!



Well-Mixed Condition

Well-Mixed Condition¹ or Thermodynamic Constraint²

An initially well-mixed (uniform) particle distribution must remain well-mixed for all time in the absence of sources or sinks (second law of thermodynamics).

¹Thomson, D. J., 1987: Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid Mech.*, **180**, 529–556.

²Pope, S. B., 1987: Consistency conditions for random walk models of turbulent dispersion. *Phys. Fluids*, **30**, 2374–2379.



Langevin Equation: Inhomogeneous Turbulence

$$du_i = \underbrace{\mathbf{a}_0 dt}_{\substack{\text{drift} \\ \text{correction}}} + \underbrace{\mathbf{a}_1 u_i dt}_{\text{memory}} + \underbrace{b d\xi_i}_{\text{diffusion}}$$



Langevin Equation: Inhomogeneous Turbulence

How to determine unknown coefficients?

Fokker-Planck Equation

$$\frac{\partial P_E}{\partial t} + \frac{\partial u_i P_E}{\partial x_i} = - \frac{\partial (a P_E)}{\partial u_i} + \frac{1}{2} \frac{\partial^2 (b^2 P_E)}{\partial u_i^2}$$

Advection-diffusion for Eulerian velocity PDF – Eulerian equivalent of Langevin equation.

For derivation see:

van Kampen, N.G.; 2nd ed., 1981. *Stochastic Processes in Physics and Chemistry*. North-Holland Pub. Co., 465 pp.

Rodean, H. C., 1996: *Stochastic Lagrangian Models of Turbulent Diffusion*. Amer. Meteor. Soc., Boston, MA, 84 pp.



Langevin Equation: Inhomogeneous Turbulence

Solution in one dimension (unique):

$$dw = \underbrace{\frac{1}{2} \frac{\partial \sigma_w^2}{\partial z} dt}_I - \underbrace{\left[\frac{C_0 \varepsilon}{2\sigma_w^2} - \frac{w}{2\sigma_w^2} \frac{\partial \sigma_w^2}{\partial z} \right] w dt}_{II} + \underbrace{(C_0 \varepsilon)^{1/2} d\xi_i}_{III}$$

- I Drift correction term
- II Memory term
- III Diffusion term



Langevin Equation: Non-Uniqueness Problem

Solution in three dimensions: method for determining Langevin coefficients is non-unique!

Thomson's (1987) 'simplest solution' (weak solution):

$$du_i = \frac{1}{2} \frac{\partial R_{il}}{\partial x_l} dt - \frac{C_0 \varepsilon}{2} R_{ik}^{-1} u_k + \frac{1}{2} \frac{dR_{il}}{dt} R_{lj}^{-1} u_j dt + (C_0 \varepsilon)^{1/2} d\xi_i$$

R_{ij} is the Reynolds stress tensor and R_{ij}^{-1} is its inverse

We can add any arbitrary rotation vector to the drift term and we'll still satisfy the well-mixed condition.



Langevin Equation: Rogue Trajectory Problem

$$dw = \frac{1}{2} \frac{\partial \sigma_w^2}{\partial z} dt - \left[\frac{C_0 \varepsilon}{2\sigma_w^2} - \frac{w}{2\sigma_w^2} \frac{\partial \sigma_w^2}{\partial z} \right] w dt + (C_0 \varepsilon)^{1/2} d\xi_i$$

It is possible for our Langevin equation to become unstable and get cases where $u_i \rightarrow \infty$



Langevin Equation: Rogue Trajectory Problem

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It is possible for our Langevin equation to become unstable and get cases where $u_i \rightarrow \infty$

ROGUE TRAJECTORY!

SSSSH! This is our dirty little secret.



Rogue Trajectories

What can we do about rogue trajectories?

- *ad hoc* constraints (violates well-mixed condition)
- Yee and Wilson (2007): semi-analytical scheme
- Postma et al. (2012): refine timestep
- Bailey et al. (2014): semi-implicit scheme



Langevin Equation: LES

Application to LES

$$dw_s = \frac{1}{2} \frac{\partial \sigma_s^2}{\partial z} dt - \left[\frac{C_0 \varepsilon_s}{2\sigma_s^2} - \frac{w_s}{2\sigma_s^2} \frac{\partial \sigma_s^2}{\partial z} \right] w_s dt + (C_0 \varepsilon_s)^{1/2} d\xi_i^*$$

Replace 'fluctuating' quantities with subgrid quantities

- $w \rightarrow w_s$
- $\sigma^2 \rightarrow \sigma_s^2$
- $\varepsilon \rightarrow \varepsilon_s$ (for Δ in inertial subrange, $\bar{\varepsilon} \approx \bar{\varepsilon}_s = -\tilde{S}_{ij}\tau_{ij}$)

*NOTE: this form assumes horizontal homogeneity and that τ_{ij} is isotropic. See Weil et al. (2004) for fully general version.



Langevin Equation: LES

e.g.,

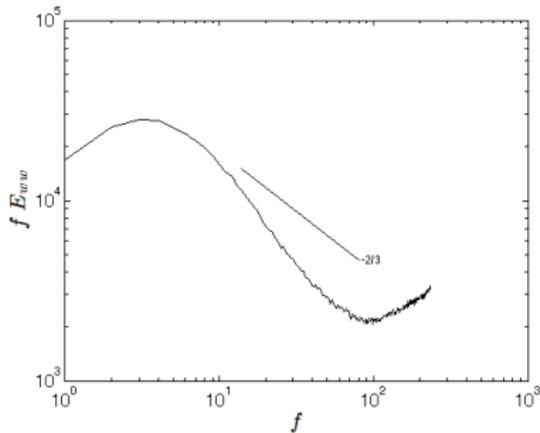
- Kemp, J. R. and Thomson, D. J. (1996). Dispersion in stable boundary layers using large-eddy simulation. *Atmos. Env.* 30:2911-2923.
- Weil, J. C. and Sullivan, P. P. and Patton, E. G. (2004). The use of large-eddy simulations in Lagrangian particle dispersion models. *J. Atmos. Sci.* 61:2877-2997.
- Vinkovic, I., Aguirre, C., and Simoëns, S. (2006). Large-eddy simulation and Lagrangian stochastic modeling of passive scalar dispersion in a turbulent boundary layer. *J. Turb.* 7:N30.

End Current Literature
(this is state-of-the-art)



LES Lagrangian Energy Spectra

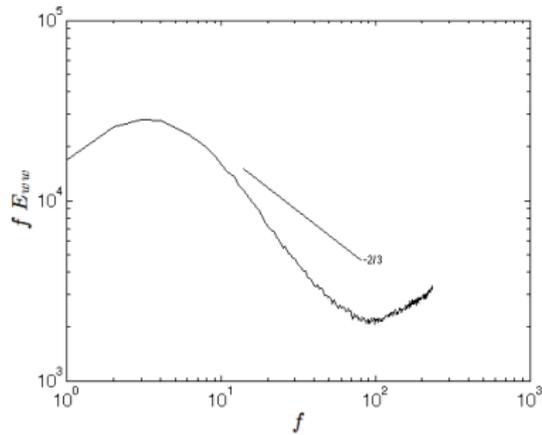
No SGS model ($u_{si} = 0$)



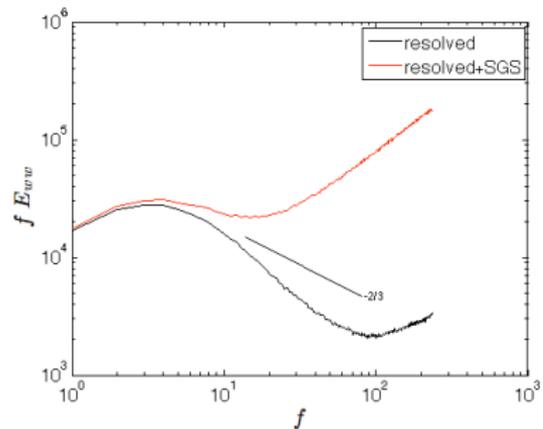


LES Lagrangian Energy Spectra

No SGS model ($u_{si} = 0$)



SGS model





LES Lagrangian Energy Spectra

Where might all this energy be coming from?

- ① Langevin equation is inappropriate?
- ② Langevin coefficients are incorrect?
- ③ Rogue trajectories?



Rogue Trajectories

Where do ROGUE TRAJECTORIES come from?

Homogeneous version (1D RANS):

$$dw = - \underbrace{\frac{C_0 \varepsilon}{2\sigma^2}}_{1/\tau_L} w dt + (C_0 \varepsilon)^{1/2} d\xi$$



Rogue Trajectories

Where do ROGUE TRAJECTORIES come from?

Homogeneous version (1D RANS):

$$dw = - \underbrace{\frac{C_0 \varepsilon}{2\sigma^2}}_{1/\tau_L} w dt + (C_0 \varepsilon)^{1/2} d\xi$$

Inhomogeneous version (1D RANS):

$$dw = \underbrace{\frac{1}{2} \frac{\partial \sigma^2}{\partial z}}_{\text{drift correction}} - \underbrace{\left[\frac{C_0 \varepsilon}{2\sigma^2} - \frac{w}{2\sigma^2} \frac{\partial \sigma^2}{\partial z} \right]}_{1/\tau_L} w dt + (C_0 \varepsilon)^{1/2} d\xi$$



Rogue Trajectories

Where do ROGUE TRAJECTORIES come from?

Memory term:

$$- \underbrace{\left[\frac{C_0 \varepsilon}{2\sigma_s^2} - \frac{w}{2\sigma_w^2} \frac{\partial \sigma_w^2}{\partial z} \right]}_{\frac{1}{\tau} = \frac{1}{\tau_1} - \frac{1}{\tau_2}} w dt$$

- τ_1 : Local decorrelation time scale (isotropic)
- τ_2 : Heterogeneity decorrelation time scale



Rogue Trajectories

$$- \underbrace{\left[\frac{C_0 \varepsilon}{2\sigma_w^2} - \frac{w}{2\sigma_w^2} \frac{\partial \sigma_w^2}{\partial z} \right]}_{\frac{1}{\tau}} w dt$$

What if τ turns out to be NEGATIVE? Or

$$C_0 \varepsilon < w \frac{\partial \sigma_w^2}{\partial z}$$

Recall our autocorrelation function:

$$\frac{\langle w(t)w(0) \rangle}{\langle w^2(0) \rangle} = e^{-t/\tau}$$



Rogue Trajectories

$$- \underbrace{\left[\frac{C_0 \varepsilon}{2\sigma_w^2} - \frac{w}{2\sigma_w^2} \frac{\partial \sigma_w^2}{\partial z} \right]}_{\frac{1}{\tau}} w dt$$

What could cause τ to be NEGATIVE?

Δt not in the inertial subrange i.e., $\tau_L \lesssim \Delta t$

Thus $\frac{2\sigma_w^2}{C_0 \varepsilon}$ is not the proper decorrelation timescale!

In this case, it is the problem not the discretization scheme that is unstable!!!!



Rogue Trajectories

Generalizing to 3D (assume τ_{ij} is isotropic)

$$du_{s,i} = \frac{1}{2} \frac{\partial \sigma_s^2}{\partial x_i} dt - \underbrace{\left(\frac{C_0 \varepsilon_s}{2\sigma_s^2} - \frac{1}{2\sigma_s^2} \frac{d\sigma_s^2}{dt} \right)}_{1/\tau} u_{s,i} dt + (C_0 \varepsilon_s)^{1/2} d\xi_i$$



Rogue Trajectories

Generalizing to 3D (assume τ_{ij} is isotropic)

$$du_{s,i} = \frac{1}{2} \frac{\partial \sigma_s^2}{\partial x_i} dt - \underbrace{\left(\frac{C_0 \varepsilon_s}{2\sigma_s^2} - \frac{1}{2\sigma_s^2} \frac{d\sigma_s^2}{dt} \right)}_{1/\tau} u_{s,i} dt + (C_0 \varepsilon_s)^{1/2} d\xi_i$$

Unstable if

$$C_0 \varepsilon_s < \frac{d\sigma_s^2}{dt} \quad (\text{this means } \tau \text{ is negative})$$



Rogue Trajectories

Generalizing to 3D (anisotropic τ_{ij})

$$du_{s,i} = \frac{1}{2} \frac{\partial \tau_{il}}{\partial x_l} dt - \frac{C_0 \varepsilon_s}{2} \lambda_{ik} u_{s,k} + \frac{1}{2} \frac{d\tau_{il}}{dt} \lambda_{lj} u_{s,j} dt + (C_0 \varepsilon_s)^{1/2} d\xi_i$$



Rogue Trajectories

Generalizing to 3D (anisotropic τ_{ij})

$$du_{s,i} = \frac{1}{2} \frac{\partial \tau_{il}}{\partial x_l} dt - \frac{C_0 \varepsilon_s}{2} \lambda_{ik} u_{s,k} + \frac{1}{2} \frac{d\tau_{il}}{dt} \lambda_{lj} u_{s,j} dt + (C_0 \varepsilon_s)^{1/2} d\xi_i$$

Unstable if

$$G_{ij} = \delta_{ij} + \frac{\Delta t}{2} \left(-C_0 \varepsilon_s \lambda_{ij} + \frac{d\tau_{il}}{dt} \lambda_{lj} \right)$$

$$\boxed{|\lambda_{\max}| > 1} \quad (\lambda_{\max} \text{ is largest eigenvalue of } G_{ij})$$



LES: Rogue Trajectory Problem

Possible Solution: Reduce Δt

Sometimes not computationally feasible.



LES: Rogue Trajectory Problem

Possible Solution: *ad-hoc* intervention

Violates well-mixed condition.



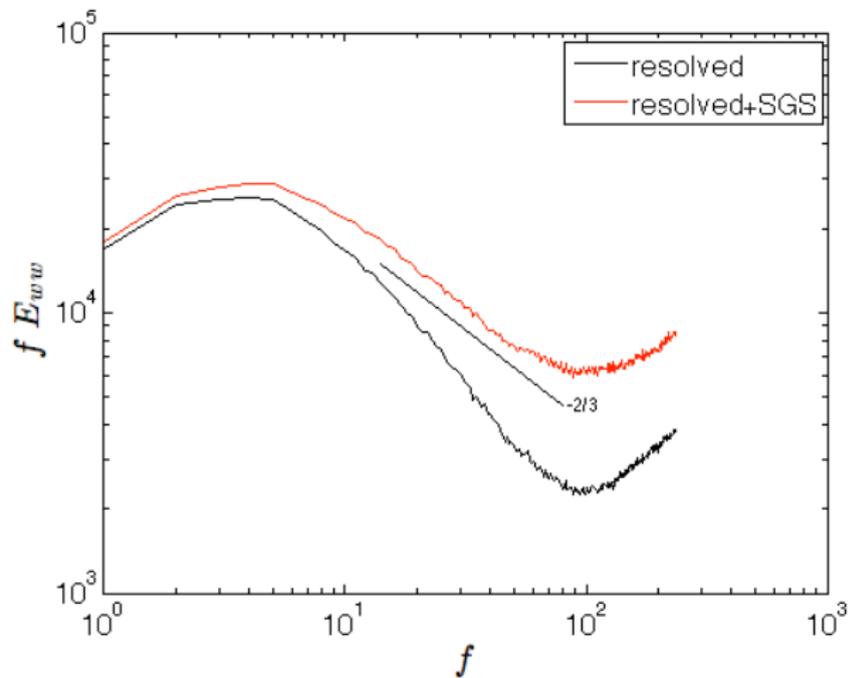
LES: Rogue Trajectory Problem

Possible Solution: Use mean quantities to calculate memory term

$$du_{s,i} = \frac{1}{2} \frac{\partial \sigma_s^2}{\partial x_i} dt - \left[\frac{C_0 \overline{\epsilon_s}}{2 \overline{\sigma_s^2}} - \frac{u_{s,j} \overline{\partial \sigma_s^2}}{2 \overline{\sigma_s^2} \partial x_j} \right] u_{s,i} dt + (C_0 \epsilon_s)^{1/2} d\xi_i$$



LES Energy Spectra





LES: Rogue Trajectory Problem

Possible Solution: Directly calculate $\tau_{L,s}$

We use Lagrangian scale-dependent SGS momentum model, which gives $\tau_{L,s}$

See:

Stoll, R., and Porté-Agel, F. (2006). Dynamic Subgrid-Scale Models for Momentum and Scalar Fluxes in Large-Eddy Simulations of Neutrally Stratified Atmospheric Boundary Layers Over Heterogeneous Terrain. *Water Resour. Res.* 42:W01409.

$$du_{s,i} = \frac{1}{2} \frac{\partial \sigma_s^2}{\partial x_i} dt - \frac{u_{s,i}}{\tau_{L,s}} dt + (C_0 \varepsilon_s)^{1/2} d\xi_i$$

this form is unconditionally stable!