Lagrangian Particle Dispersion Modeling in LES

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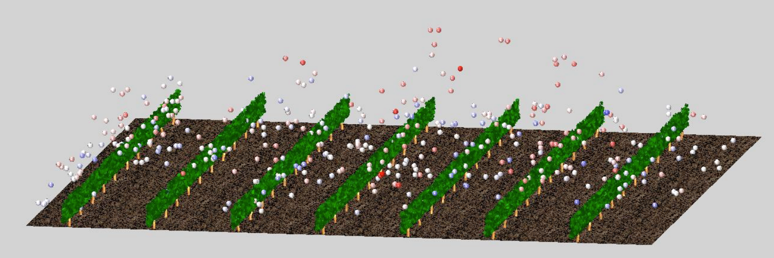
Visualizations



Lagrangian vs Eulerian Reference Frames

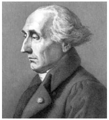
Eulerian

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

Governing Equation

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

Lagrangian



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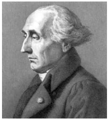


Best for discrete sources, or when details of individual particles are of interest

Governing Equation

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = u_i$$

Numerical solution

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = u_i$$

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

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

Note

Side Note:

This form assumes particles are massless.

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

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = u_i + u_i^*$$

Numerical solution example

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

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

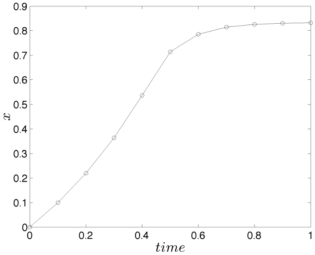
$$\boxed{x_i(t+\Delta t) = x_i(t) + u_i(t)\Delta t}$$

Consider $x(0) = 0$

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

$\Delta t = 0.1$

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?

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$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = u_i = \underbrace{\tilde{u}_i}_{\text{resolved}} + \underbrace{u_{s,i}}_{\text{subgrid}}$$

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Application to LES

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$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = u_i = \underbrace{\tilde{u}_i}_{\text{resolved}} + \underbrace{u_{s,i}}_{\text{subgrid}}$$

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.

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

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where should we start?

Let's copy the RANS people.

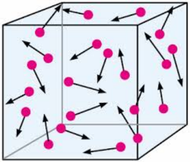
Why? RANS is essentially LES with the grid scale equal to the domain size....so this *should* be easier.

Framework for modeling $u_{s,i}$

Lagrangian dispersion in RANS:

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \underbrace{\overline{u}_i}_{\text{mean}} + \underbrace{u_i}_{\text{fluctuations}}$$

RANS models



Analogy to molecular motion (Brownian motion):
Langevin Equation

$$\mathrm{d}u_i = \underbrace{-\boldsymbol{a}u_i\mathrm{d}t}_{\text{memory}} + \underbrace{\boldsymbol{b}\mathrm{d}\xi_i}_{\text{diffusion}}$$

u_i - molecule velocity
$\mathrm{d}\xi_i$ - random Gaussian process with mean zero and variance $\mathrm{d}t$

Langevin Equation

Application to isotropic turbulence:
$u_i \rightarrow$ Lagrangian particle velocity

$$\mathrm{d}u_i = -\boldsymbol{a} u_i \mathrm{d}t + \boldsymbol{b} \mathrm{d}\xi_i$$

How do we get $\boldsymbol{a}$ and $\boldsymbol{b}$?

Langevin Equation: finding b

$$\mathrm{d}u_i = -\boldsymbol{a}u_i\mathrm{d}t + \boldsymbol{b}\mathrm{d}\xi_i \tag{1}$$

$\boldsymbol{b}$ comes directly from Kolmogorov's second hypothesis

Lagrangian structure function:

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

Provided $\boldsymbol{\Delta}t$ is in the internal subrange (i.e., $\boldsymbol{\tau}_\eta \ll \Delta t \ll \tau_L$)

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Lagrangian structure function:

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Provided $\boldsymbol{\Delta} t$ is in the internal subrange (i.e., $\boldsymbol{\tau}_\eta \ll \Delta t \ll \tau_L$)

Square Eq.1 and take ensemble average:

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

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

Langevin Equation: finding a

$$\mathrm{d}u_i = -\boldsymbol{a} u_i \mathrm{d}t + \boldsymbol{b} \mathrm{d}\xi_i$$

Using stochastic calculus, we can solve this equation analytically

$$w(t) = w(0) e^{-\boldsymbol{a}t} + \boldsymbol{b} e^{-\boldsymbol{a}t} \int_0^t e^{\boldsymbol{a}s} \xi(s) \mathrm{d}s$$

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Langevin Equation: finding a

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$$w(t) = w(0)e^{-\boldsymbol{a}t} + \boldsymbol{b}e^{-\boldsymbol{a}t}\int_0^t e^{\boldsymbol{a}s}\xi(s)\mathrm{d}s$$

Square this equation and take ensemble average:

$$\langle w^2(t)\rangle = \langle w^2(0)\rangle e^{-2\boldsymbol{a}t} + \cancelto{0}{\langle w(0)\rangle} e^{-2\boldsymbol{a}t}\int_0^t e^{\boldsymbol{a}s}\xi(s)\mathrm{d}s + \langle \boldsymbol{b}^2 e^{-2\boldsymbol{a}t}\left[\int_0^t e^{\boldsymbol{a}s}\xi(s)\mathrm{d}s\right]^2\rangle$$

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

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Langevin Equation: finding a

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

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 $t \to \infty$

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

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

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Langevin Equation

Application to homogeneous isotropic turbulence

$$\mathrm{d}u_i = -\frac{C_0\varepsilon}{2\sigma^2}u_i\mathrm{d}t + \left(C_0\varepsilon\right)^{1/2}\mathrm{d}\xi_i$$

for homogeneous isotropic turbulence,
$\dfrac{2\sigma^2}{C_0\varepsilon} = \tau_L$ is the integral timescale

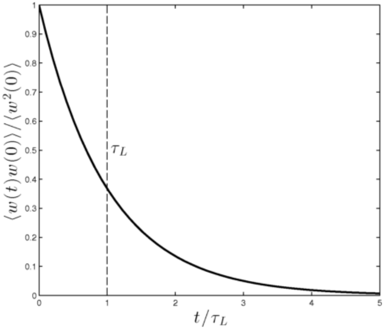
$$\mathrm{d}u_i = -\frac{u_i}{\tau_L}\mathrm{d}t + \left(C_0\varepsilon\right)^{1/2}\mathrm{d}\xi_i$$

Langevin Equation

$$\mathrm{d}w = -\underbrace{\frac{w}{\tau_L}\mathrm{d}t}_{\mathrm{I}} + \underbrace{(C_0\varepsilon)^{1/2}\,\mathrm{d}\xi_i}_{\mathrm{II}}$$

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

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

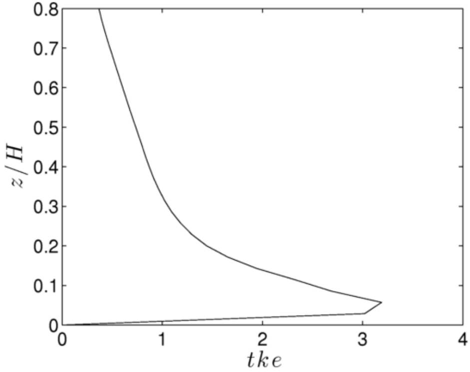


Langevin Equation

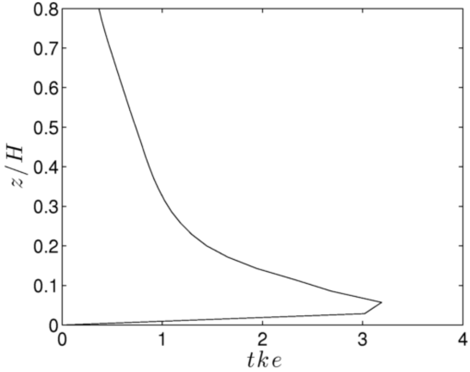
$$\mathrm{d}w = -\underbrace{\frac{w}{\tau_L}\mathrm{d}t}_{\mathrm{I}} + \underbrace{(C_0\varepsilon)^{1/2}\,\mathrm{d}\xi_i}_{\mathrm{II}}$$

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

Inhomogeneous Turbulence (in 1D)



Inhomogeneous Turbulence (in 1D)



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

Well-Mixed Condition

Well-Mixed Condition[1] or Thermodynamic Constraint[2]

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).

[1] Thomson, D. J., 1987: Criteria for the selection of stochastic models of particle trajectories in turbulent flows. *J. Fluid Mech.*, **180**, 529–556.
[2] Pope, S. B., 1987: Consistency conditions for random walk models of turbulent dispersion. *Phys. Fluids*, **30**, 2374–2379.

Langevin Equation: Inhomogeneous Turbulence

$$\mathrm{d}u_i = \underbrace{\boldsymbol{a}_0\mathrm{d}t}_{\text{drift correction}} + \underbrace{\boldsymbol{a}_1 u_i \mathrm{d}t}_{\text{memory}} + \underbrace{\boldsymbol{b}\mathrm{d}\xi_i}_{\text{diffusion}}$$

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):

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

- 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):

$$\mathrm{d}u_i = \frac{1}{2}\frac{\partial R_{il}}{\partial x_l}\mathrm{d}t - \frac{C_0\varepsilon}{2}R^{-1}_{ik}u_k + \frac{1}{2}\frac{\mathrm{d}R_{il}}{\mathrm{d}t}R^{-1}_{lj}u_j\mathrm{d}t + (C_0\varepsilon)^{1/2}\,\mathrm{d}\xi_i$$

R_{ij} is the Reynolds stress tensor and R^{-1}_{ij} 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

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

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

Langevin Equation: Rogue Trajectory Problem

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

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

Application to LES

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

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, $\overline{\varepsilon} \approx \overline{\varepsilon_s} = -\tilde{S}_{ij}\tau_{ij}$)

*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.,

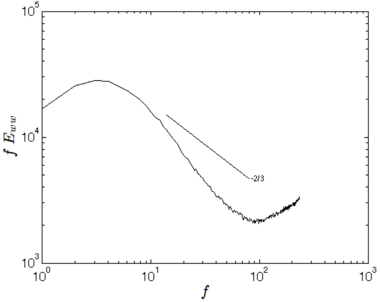
- Kemp, J. R. and Thomson, D. J. (1996). Dispersion in stable boundary layers using large-eddy simulation. Atmos. Env. 30:2911-2923.
- Weil, J. C. and Sullivan, P. P. and Patton, E. G. (2004). The use of large-eddy simulations in Lagrangian particle dispersion models. *J. Atmos. Sci.* 61:2877-2997.
- 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 ($u_{si} = 0$)



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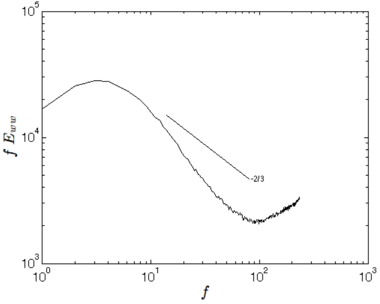
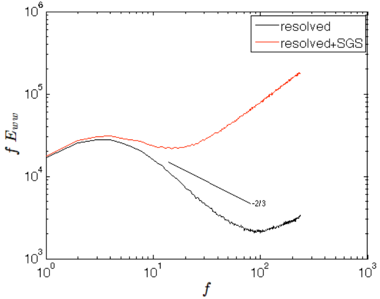


SGS model



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):

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

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Inhomogeneous version (1D RANS):

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

Rogue Trajectories

Where do ROGUE TRAJECTORIES come from?

Memory term:

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

- $\boldsymbol{\tau}_1$: Local decorrelation time scale (isotropic)
- $\boldsymbol{\tau}_2$: Heterogeneity decorrelation time scale

Rogue Trajectories

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

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

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

What could cause τ to be NEGATIVE?

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

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

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

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Rogue Trajectories

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

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

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Unstable if
$C_0\varepsilon_s < \dfrac{\mathrm{d}\sigma_s^2}{\mathrm{d}t}$ (this means τ is negative)

Rogue Trajectories

Generalizing to 3D (anisotropic τ_{ij})

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

Rogue Trajectories

Generalizing to 3D (anisotropic τ_{ij})

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

Unstable if

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

$\boxed{|\lambda_{\mathrm{max}}| > 1}$ (λ_{max} 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

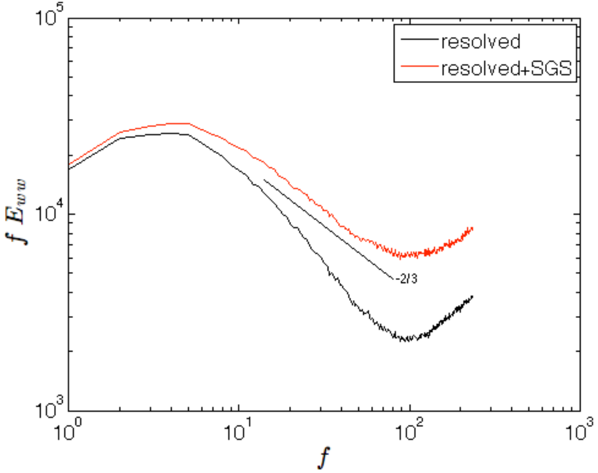
Violates well-mixed condition.

LES: Rogue Trajectory Problem

Possible Solution: Use mean quantities to calculate memory term

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

LES Energy Spectra



LES: Rogue Trajectory Problem

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

We use Lagrangian scale-dependent SGS momentum model, which gives τ_{Ls}

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.

$$\mathrm{d}u_{s,i} = \frac{1}{2}\frac{\partial \sigma_s^2}{\partial x_i}\mathrm{d}t - \frac{u_{s,i}}{\tau_{Ls}}\mathrm{d}t + \left(C_0 \varepsilon_s\right)^{1/2}\mathrm{d}\xi_i$$

this form is unconditionally stable!