Large- and Small-Scale Dynamics of Variable-Density Rayleigh-Taylor Instability-Induced Turbulent Mixing

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The dynamical effects of 'small' (unresolved) scales on 'large' (resolved) scales cannot be neglected in a turbulent mixing layer

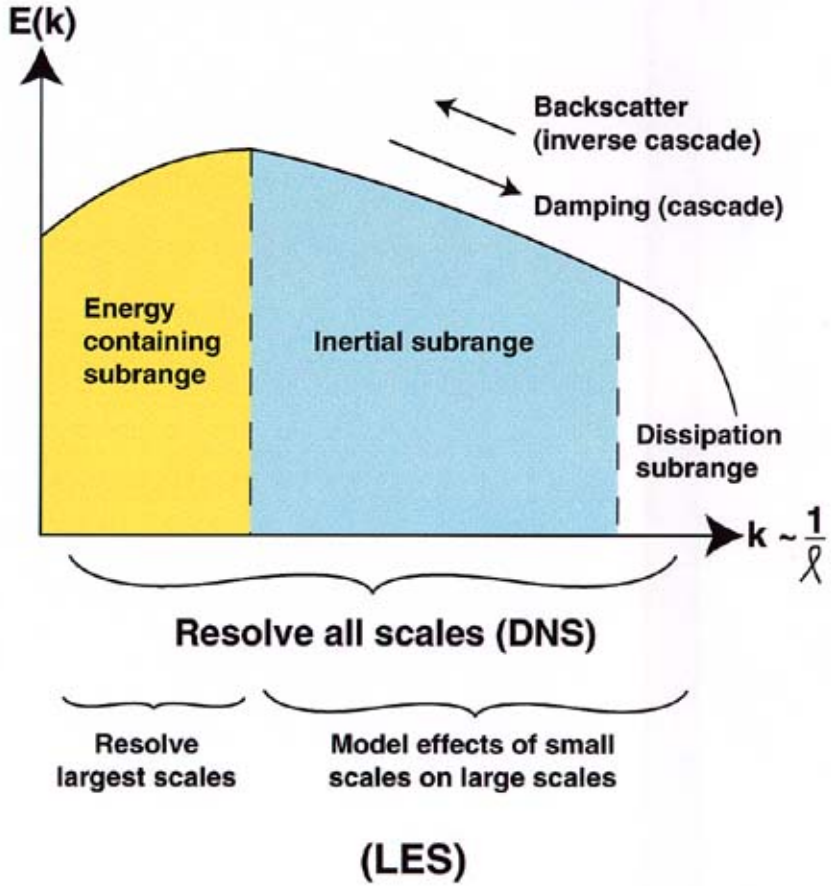
- The dynamical effect of small scales on large scales is a bi-directional, competing process
  - Energy transferred up and down scale through 'backscatter' and a cascade, respectively, over a wide range of eddies
  - As *Re* increases, contribution from the small scales increases
- *Rate of scalar mixing* is proportional to dissipation rate of the squared scalar ($\langle \cdot \rangle$ is an average and *D* is the scalar diffusion coefficient)

$$\langle \epsilon_\phi \rangle \equiv -\frac{\partial}{\partial t}\left\langle \frac{\phi^2}{2} \right\rangle = D\langle \phi \nabla^2 \phi \rangle$$

  - *Contribution to this quantity is dominated by the small scales*, where gradients are large
- Turbulent quantities (e.g., the kinetic energy) are contributed by all scales, not only by large-scale, integral quantities
- Simulation of Rayleigh-Taylor mixing requires capability to simulate smaller scales as well as the largest scales

Schematic of direct numerical simulation (DNS) and large-eddy simulation (LES) for turbulent mixing

- Turbulence enhances mass, momentum, energy transport
  - Coherent bubble/spike structures associated with energy containing subrange
- Energy *transferred* among eddies at all scales
  - Inertial subrange 'mediates' between largest and smallest scales
- Molecular (atomic) mixing associated with dissipation subrange, in which structures are too small to be resolved



The approaches used thus far to simulate Rayleigh-Taylor mixing have important physical and computational limitations

- Monotone integrated LES (MILES)
  - Implicit numerical dissipation (finite-volume simulations of the non-dissipative equations)
  - Advantage: modest computational requirements
  - Disadvantage: small-scale structures and statistics not estimated well, while large-scale structures and lowest-order integral properties are

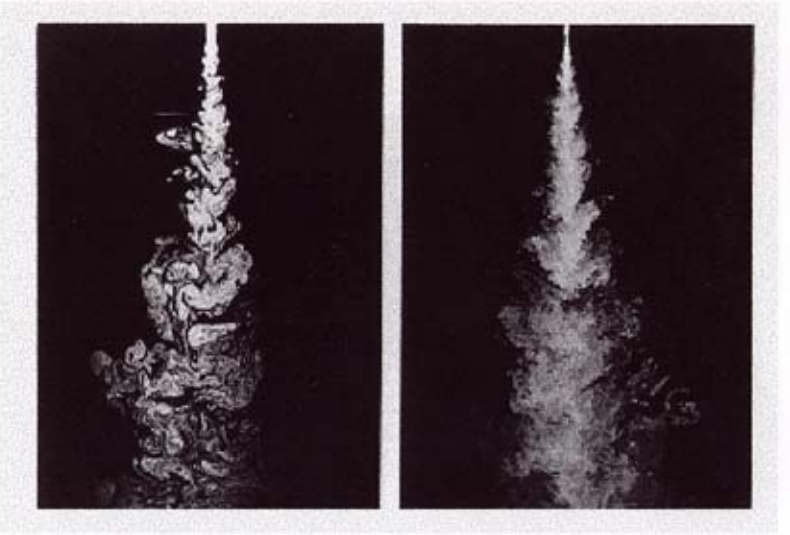
- DNS
  - Physical dissipation (spectral and finite-difference simulations of the dissipative equations)
  - Advantage: all structures and statistics estimated well
  - Disadvantage: very high computational and data storage/processing requirements

High-resolution DNS is too computationally expensive to simulate Rayleigh-Taylor mixing: an LES capability is needed

- DNS is too expensive to simulate a mixing layer that exceeds the *mixing transition Reynolds number* $Re \sim 10^4$
  - Issue is more acute for miscible, reacting flows in which all scales are below any possible grid resolution

- Therefore, development of a true LES capability to predict mean hydrodynamic fields and lowest-order transport and mixing statistics is essential

$Re \sim 2.5 \times 10^3$ $Re \sim 1 \times 10^4$



Liquid-jet concentration in a round turbulent jet (Dimotakis 1983)

To develop an LES capability, an examination of interaction between unresolved and resolved scales in Rayleigh-Taylor mixing layers is needed

- Study transfer (exchange) of $\rho^2/2$ and $v^2/2$ among different wavenumber regions (corresponding to spatial scales or eddies)
  - ρ and v_i fields obtained from high-resolution DNS data
  - An artificial cutoff scale is used to partition scales into computationally resolved and unresolved scales
- Fourier space representation determines magnitude and other properties of transfer process as a function of scale k and height in the domain
  - Wavelet transforms can also be used to add information *as a function of position*
- Data obtained from this study will be used to develop and assess subgrid-scale and backscatter models for LES
  - Work will improve the classical Smagorinsky eddy viscosity and scale-similarity subgrid-scale models

A high-resolution ($512^2 \times 2040$) DNS was performed for miscible, variable-density, Rayleigh-Taylor unstable fluids with $At = 1/2$

Density isosurface at times 1, 2, 3, 4, 5, 6
red: $\rho = 3$; green: $\rho = 2$; blue: $\rho = 1$

- Spectral/8th-order compact finite-difference method with 3rd-order, Adams-Bashforth time-evolution
- Small-scale initial perturbations on fluid interface
- Turbulence attains late-time Reynolds number based on mixing layer width

$$Re_h(t) = \frac{(\rho_1 + \rho_2)}{2\mu} h(t) \frac{dh(t)}{dt}$$

$$\approx 5.5 \times 10^3$$

Similarly, the analysis of kinetic energy transfer dynamics begins with a 2-dimensional Fourier transform of the momentum equation

- Applying the Fourier transform to the momentum equation in homogeneous directions gives ($V = 1/\rho$ is the specific volume)

$$\frac{\partial v_i(\mathbf{k}_\perp,z,t)}{\partial t} \equiv \underbrace{F_i(\mathbf{k}_\perp,z,t)}_{\text{forcing term}} + \underbrace{N_i(\mathbf{k}_\perp,z,t)}_{\text{advection term}} + \underbrace{D_i(\mathbf{k}_\perp,z,t)}_{\text{dissipation terms}}$$

$$= -g(t)\,\delta_{i3}$$

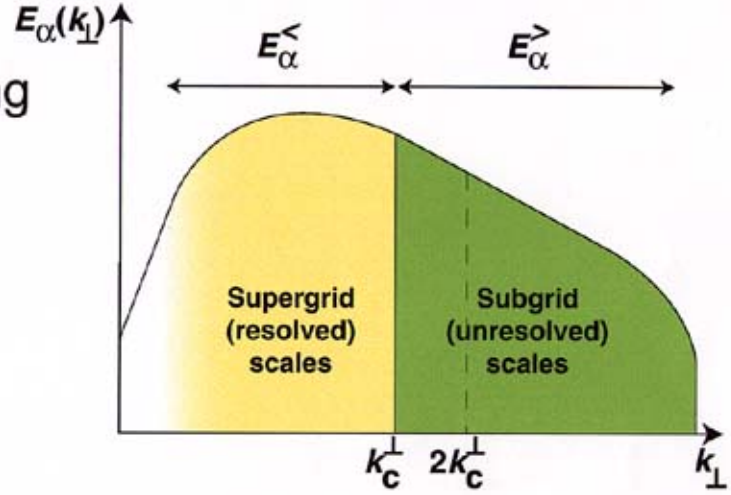
$$-\iint V(\mathbf{p}_\perp,z,t)\left(iq_\perp^i + \delta^{i3}\frac{\partial}{\partial z}\right)p(\mathbf{q}_\perp,z,t)\,\delta^2(\mathbf{k}_\perp-\mathbf{p}_\perp-\mathbf{q}_\perp)\,d^2p_\perp\,d^2q_\perp$$

$$-\iint v_j(\mathbf{p}_\perp,z,t)\left(iq_\perp^j + \delta^{j3}\frac{\partial}{\partial z}\right)v_i(\mathbf{q}_\perp,z,t)\,\delta^2(\mathbf{k}_\perp-\mathbf{p}_\perp-\mathbf{q}_\perp)\,d^2p_\perp\,d^2q_\perp$$

$$-\nu\left(k_\perp^2 - \frac{\partial^2}{\partial z^2}\right)v_i(\mathbf{k}_\perp,z,t) - \frac{4}{3}\nu\,k_\perp^i\,k_\perp^j\,v_j(\mathbf{k}_\perp,z,t)$$

For a given $k_\perp$, N_ρ and N_i describe the integrated nonlinear interactions of *all other scales* with $k_\perp$

- Decompose nonlinear terms into partial sum N_ρ^A and N_i^A corresponding to different disjoint regions A э $k_\perp$
  - Each term represents nonlinear interactions contributed by any 2 such regions
- Define regions



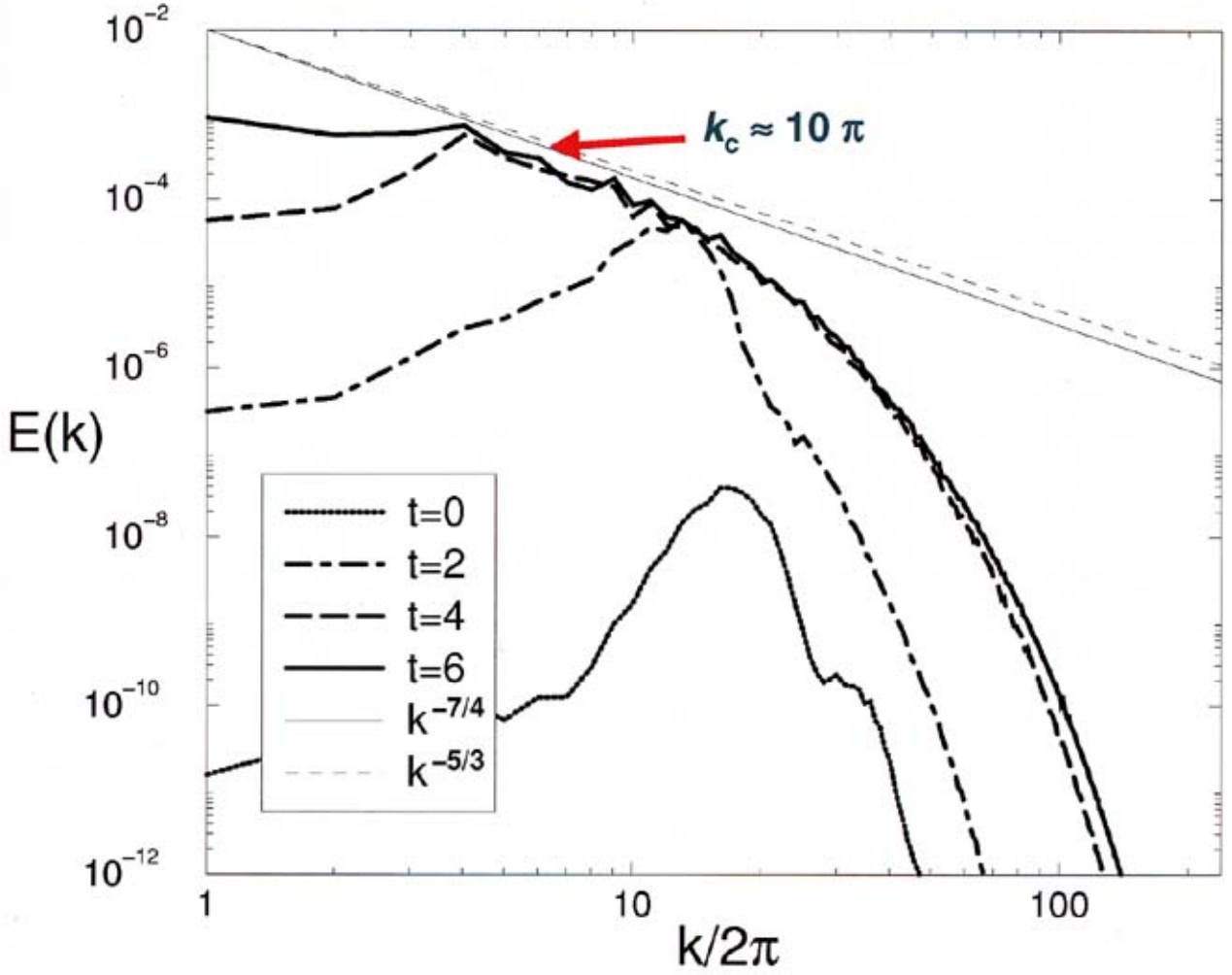
$$k_0^\perp = 0 < k_1^\perp = k_c^\perp < k_2^\perp = 2k_c^\perp < k_3^\perp = k_{max}^\perp$$

where $k_c^\perp$ and $k_{max}^\perp$ are cutoff and maximum wavenumbers

- Partial nonlinear terms computed by truncating v_i and ρ to region A,

$$\phi_\alpha^{\mathcal{A}}(\mathbf{k}_\perp, z, t) \equiv \begin{cases} \phi_\alpha(\mathbf{k}_\perp, z, t) & \mathbf{k}_\perp \in \mathcal{A} \\ 0 & \text{otherwise} \end{cases}$$

The kinetic energy spectrum at the midplane ($z = 0$) evolves to a state with a very short inertial subrange



Previous decomposition of nonlinear terms can be used to derive expressions for supergrid and subgrid nonlinear terms

- The nonlinear term describing interactions of modes $k_\perp \in K$ with modes in regions P and Q can be expressed as a sum

$$N_\alpha(\mathbf{k}_\perp, z, t) = \sum_{\mathcal{K}=1}^{3} \sum_{\mathcal{P}=1}^{3} \sum_{\mathcal{Q}\geq\mathcal{P}=1}^{3} N_\alpha^{\mathcal{K}\mathcal{P}\mathcal{Q}}(\mathbf{k}_\perp, z, t)$$

- Supergrid (resolved) nonlinear terms corresponding to modes $k_\perp < k_c^\perp$ and to modes $k_\perp < k_2^\perp = 2\, k_c^\perp$:

$$N_\alpha^{<}(\mathbf{k}_\perp | \mathbf{k}_\perp^c, z, t) = N_\alpha^{111}$$

$$N_\alpha^{<}(\mathbf{k}_\perp | 2\mathbf{k}_\perp^c, z, t) = N_\alpha^{111} + N_\alpha^{121} + N_\alpha^{221} + N_\alpha^{112} + N_\alpha^{122} + N_\alpha^{222}$$

- Subgrid (unresolved) nonlinear terms corresponding to modes $k_\perp > k_c^\perp$ and to modes $k_c^\perp > k_2^\perp = 2\, k_c^\perp$:

$$N_\alpha^{>}(\mathbf{k}_\perp | \mathbf{k}_\perp^c, z, t) = N_\alpha^{121} + N_\alpha^{131} + N_\alpha^{221} + N_\alpha^{231} + N_\alpha^{331}$$

$$N_\alpha^{>}(\mathbf{k}_\perp | 2\mathbf{k}_\perp^c, z, t) = N_\alpha^{131} + N_\alpha^{231} + N_\alpha^{331} + N_\alpha^{132} + N_\alpha^{232} + N_\alpha^{332}$$

The supergrid and subgrid energy density evolution equations can be formed in terms of the nonlinear terms

- Partial transfer spectra describe rate of $\rho^2/2$ and $v^2/2$ change in modes $k_\perp \in K$ due to nonlinear interactions between modes $p_\perp \in P$ and $q_\perp \in Q$:

$$T_\alpha^{KPQ}(\mathbf{k}_\perp, z, t) = \mathrm{Re}\left[\phi_\alpha(\mathbf{k}_\perp, z, t)^* N_\alpha^{KPQ}(\mathbf{k}_\perp, z, t)\right]$$

- Introducing large-scale density and velocity truncated at $k_2^\perp = 2\, k_c^\perp$,

$$\rho^< = \rho^1 + \rho^2 \quad , \quad v_i^< = v_i^1 + v_i^2$$

the supergrid (resolved) density squared and kinetic energy are

$$E_\rho^<(\mathbf{x}, t) = \frac{\rho^<(\mathbf{x},t)^2}{2} \quad , \quad E^<(\mathbf{x}, t) = \frac{v^<(\mathbf{x},t)^2}{2}$$

- The equations for these quantities contain the supergrid and subgrid transfers

The subgrid-scale energy transfer spectra $T_\alpha(k_\perp|k_\perp^c;z,t)$ provide information on *magnitude* and *direction* of the energy transfer

- Computation of subgrid-scale energy transfers requires summation over all $k_\perp$ in a spherical shell centered around $k_\perp$:

$$T_\alpha^{>}(k_\perp|k_c^\perp;z,t) = \sum_{k_\perp-\frac{\Delta k_\perp}{2}<|\mathbf{k}_\perp|<k_\perp+\frac{\Delta k_\perp}{2}} T_\alpha^{>PQ}(k_\perp|k_c^\perp;z,t)$$

  where P and Q are spherical wavenumber bands centered around $p_\perp$ and $q_\perp$

- Computation involves interactions in which components of the sum can be either positive or negative
  - Positive component (forward energy cascade):

$$T_\alpha^{(+)>}(k_\perp|k_c^\perp;z,t) \equiv \frac{T_\alpha^{>}(k_\perp|k_c^\perp;z,t)+|T_\alpha^{>}(k_\perp|k_c^\perp;z,t)|}{2}$$

  - Negative component (backward energy cascade):

$$T_\alpha^{(-)>}(k_\perp|k_c^\perp;z,t) \equiv \frac{T_\alpha^{>}(k_\perp|k_c^\perp;z,t)-|T_\alpha^{>}(k_\perp|k_c^\perp;z,t)|}{2}$$

Net eddy viscosities $\nu_\alpha^n(k_\perp|k_\perp^c;z,t)$ can be defined for $k_\perp < k_\perp^c$ in terms of eddy and backscatter viscosities

- *Net* eddy viscosities:

$$\nu_\alpha^n(k_\perp|k_c^\perp;z,t) \equiv -\frac{T_\alpha^{>}(k_\perp|k_c^\perp;z,t)}{2k_\perp^2 E_\alpha^{<}(k_\perp,z,t)}$$

- Eddy viscosities: (representing energy removal by small scales)

$$\nu_\alpha(k_\perp|k_c^\perp;z,t) \equiv -\frac{T_\alpha^{(+)>}(k_\perp|k_c^\perp;z,t)}{2k_\perp^2 E_\alpha^{<}(k_\perp,z,t)}$$

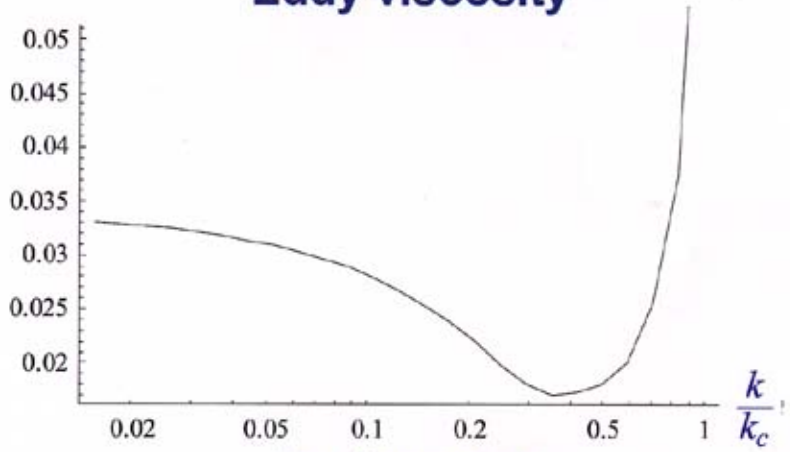
- Backscatter viscosities: (representing energy transfer from small to larger scales)

$$\nu_\alpha^b(k_\perp|k_c^\perp;z,t) \equiv \frac{T_\alpha^{(-)>}(k_\perp|k_c^\perp;z,t)}{2k_\perp^2 E_\alpha^{<}(k_\perp,z,t)}$$

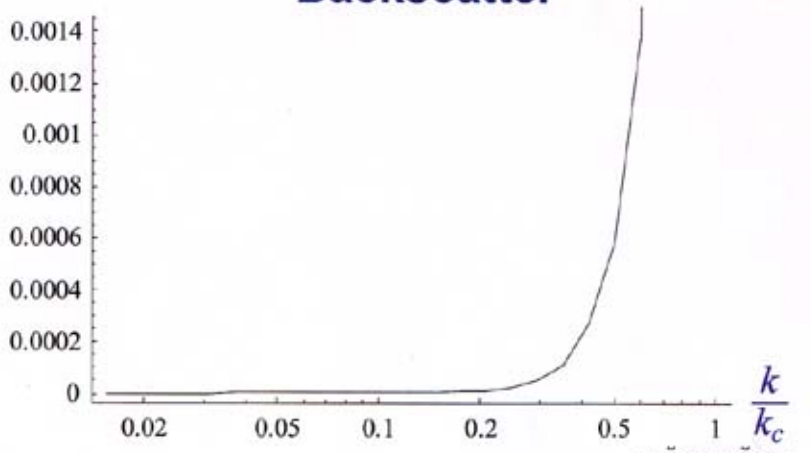
- Thus, net viscosities are

$$\nu_\alpha^n(k_\perp|k_c^\perp;z,t) = \nu_\alpha(k_\perp|k_c^\perp;z,t) - \nu_\alpha^b(k_\perp|k_c^\perp;z,t)$$

Eddy viscosity



Backscatter



Given the eddy and backscatter viscosities, a subgrid-scale model can be defined

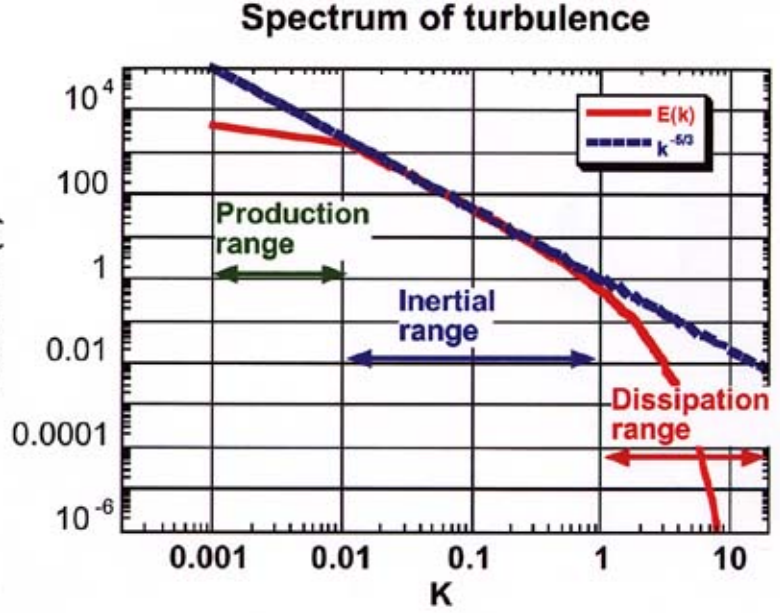
- Large-eddy equations have the form (only the Navier-Stokes equation is shown)

$$\frac{\partial}{\partial t}(\rho^{<} v_i^{<}) + \frac{\partial}{\partial x_j}\left(\rho^{<} v_i^{<} v_j^{<} + p\delta_{ij} - \sigma_{ij}\right) - \rho^{<} g_i = -\frac{\partial \tau_{ij}}{\partial x_j}$$

- Left side is computed explicitly
- Right side involves the Reynolds stress tensor τ_{ij}
  - The Smagorinsky model is

$$\tau_{ij} = \frac{\delta_{ij}}{3}(\nu^{<})^2 - \nu_t\left(\frac{\partial v_i^{<}}{\partial x_j} + \frac{\partial v_j^{<}}{\partial x_i}\right)$$

- A similar parameterization may be reasonable for resolved density equation



Turbulence dynamics of enstrophy (vorticity squared) transfer is particularly relevant to interfacial instability-induced turbulent mixing

- Dynamics of enstrophy $\rho\,\Omega = \rho\,\omega^2 / 2$ will also be examined (dissipation terms are not written)

$$\frac{\partial}{\partial t}(\rho\Omega) + \frac{\partial}{\partial x_j}(\rho\Omega v_j) = \underbrace{\epsilon_{ijk}\frac{\omega^i}{\rho}\frac{\partial\rho}{\partial x_j}\frac{\partial p}{\partial x_k}}_{\text{baroclinic production}} + \underbrace{\rho\,\omega_i S^{ij}\omega_j}_{\text{enstrophy stretching}} - \underbrace{2\rho\Omega\frac{\partial v_j}{\partial x_j}}_{\text{dilatation}}$$

  - Baroclinic production term is an instability source term, existing due to misalignment of $\nabla\rho$ and ∇p
  - Stretching term is related to development of turbulence
  - Dilatation term is small in a variable-density flow, but is important in a compressible (Richtmyer-Meshkov) flow
- Baroclinic production and stretching terms exist in 3D, but only the former exists in 2D
  - Nature of turbulent energy and enstrophy cascades is, therefore, very different in 2D and 3D

Conclusions and work in progress

- A subgrid-scale transfer analysis can be applied to Rayleigh-Taylor and Richtmyer-Meshkov mixing layers
  - Provides time- and scale-dependent measure of energy transfer process
  - Provides parameterizable eddy viscosities/backscatters for LES of Rayleigh-Taylor mixing at large *Re*
  - Also provides information for scale-similarity and more recent deconvolution subgrid-scale models
- Data processing at LLNL requires 256 IBM SP nodes (1,024 CPUs) and sufficient computer time
- Purpose of this research is to acquire physical insight into coupling of the large and small scales, in order to develop and assess subgrid-scale models for LES