Outline

- Motivation:
- Simulation methodologies
- Governing equations
- **Boundary conditions**
- Subfilter-scale modelling
- Validation of an LES
- Applications
- Challenges
- Conclusions

Boundary and Initial Conditions

- Initial conditions.
- Boundary conditions
  - *Periodic.*
  - *Inflow.*
  - *Outflow.*
  - *Wall.*

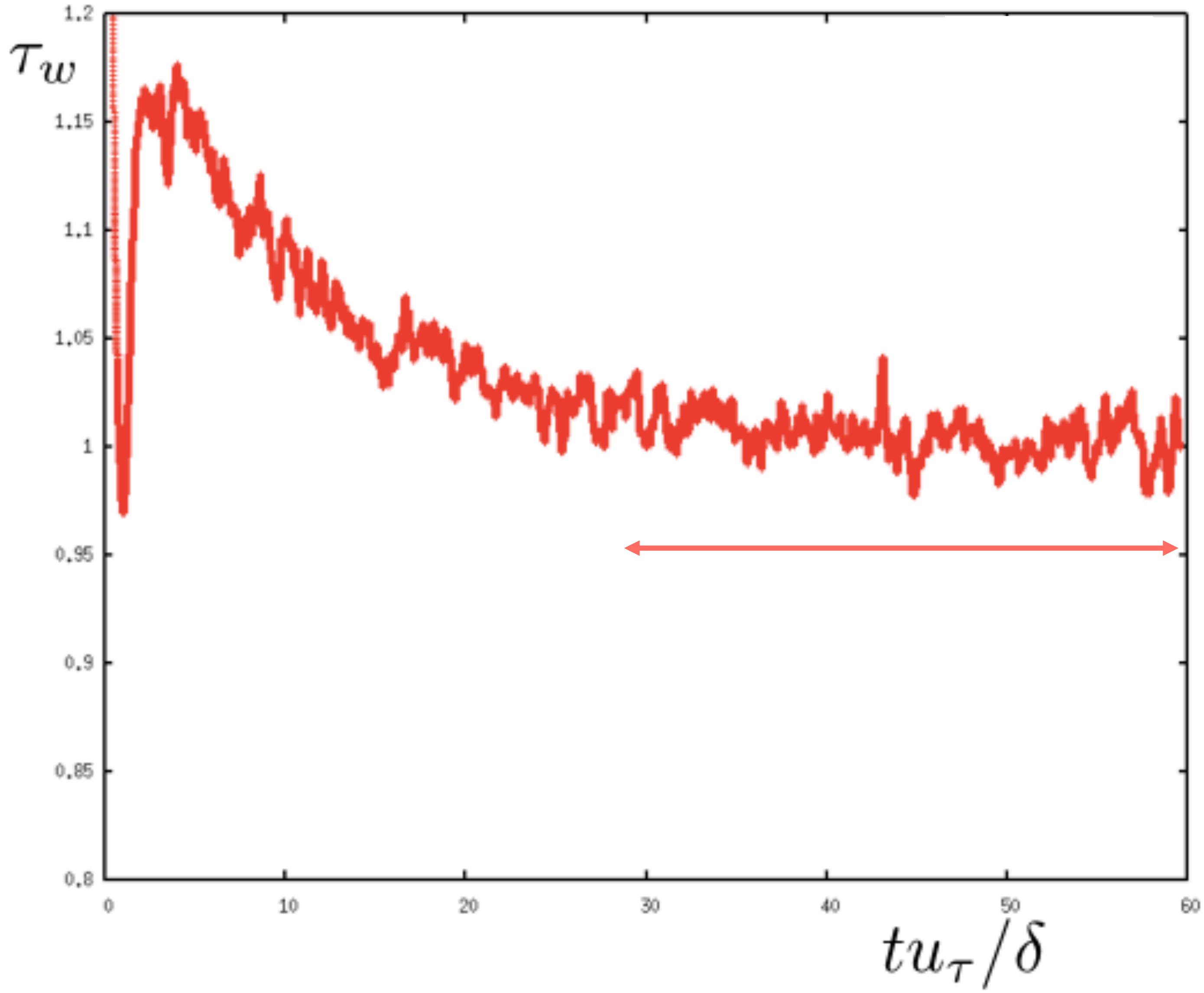
Initial conditions

- For statistically steady flows the initial conditions are relatively unimportant.
  - *Large-amplitude perturbations superposed on a realistic mean flow.*
  - *Steady state realization in similar configuration*
  - *The flow is allowed to develop until a steady state is reached, then statistics can be accumulated.*
- If the transient is important, realistic initial conditions must be used.
  - *Controlled or random perturbations in transitional flows.*

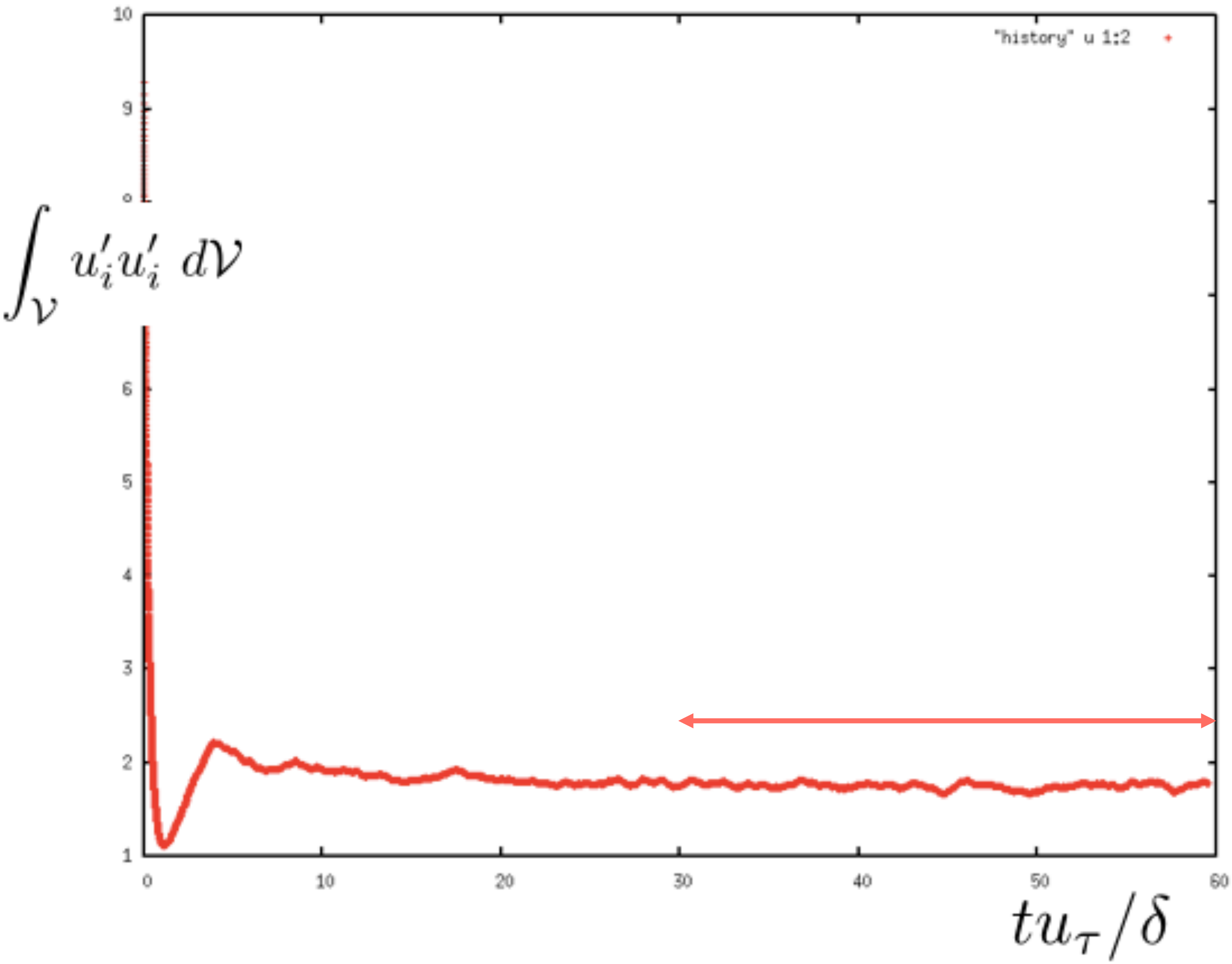
Initial conditions

- Plane channel flow
- Initial condition:
  - *Uniform flow*
  - *Random noise, 30% amplitude*
- Monitor:
  - *Wall stress*
  - $\int_{\mathcal{V}} (u^2 + v^2 + w^2) d\mathcal{V}$
  - *Velocity and Reynolds stress profiles.*

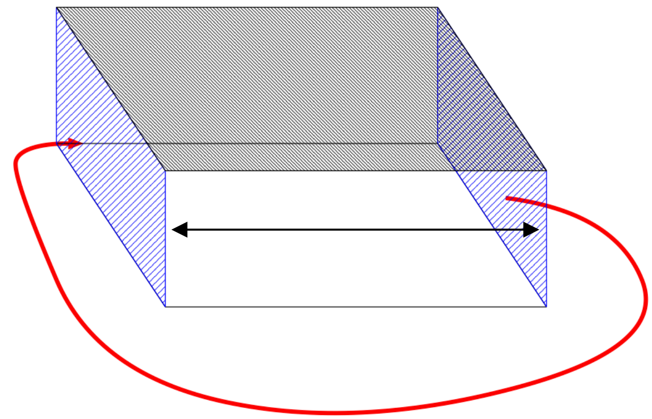
Initial conditions



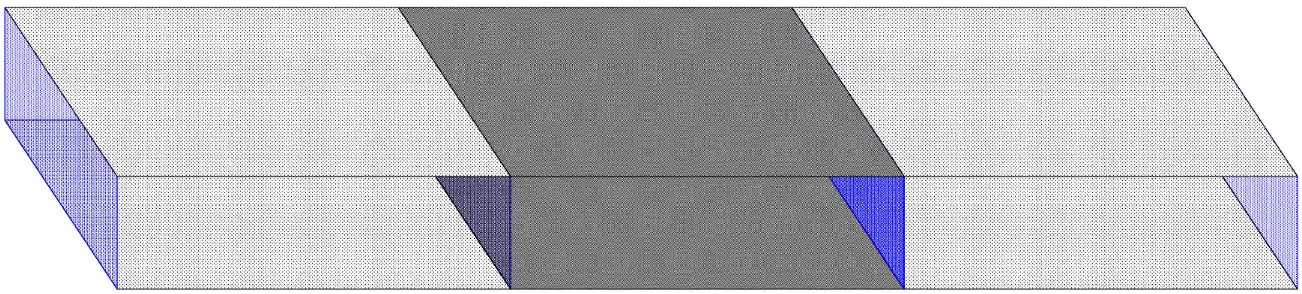
Initial conditions



Periodic B.C.s



- Require that $f(x) = f(x+L)$
- Equivalent to having an infinite sequence (in the periodic direction) of the basic box

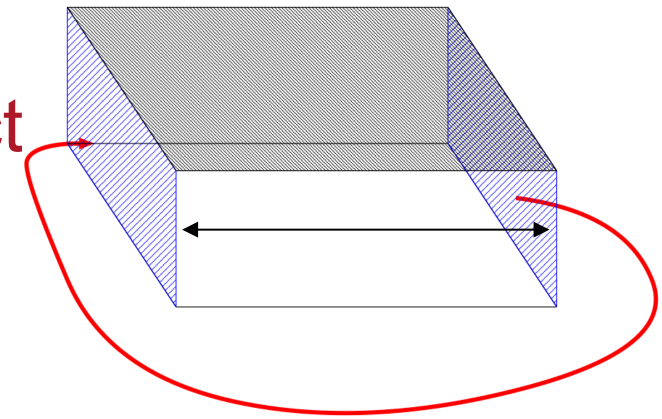


- Valid for fully-developed flows (pipe, plane channel….)
- If applied to spatially-developing flows result in temporal (instead of spatial) development.

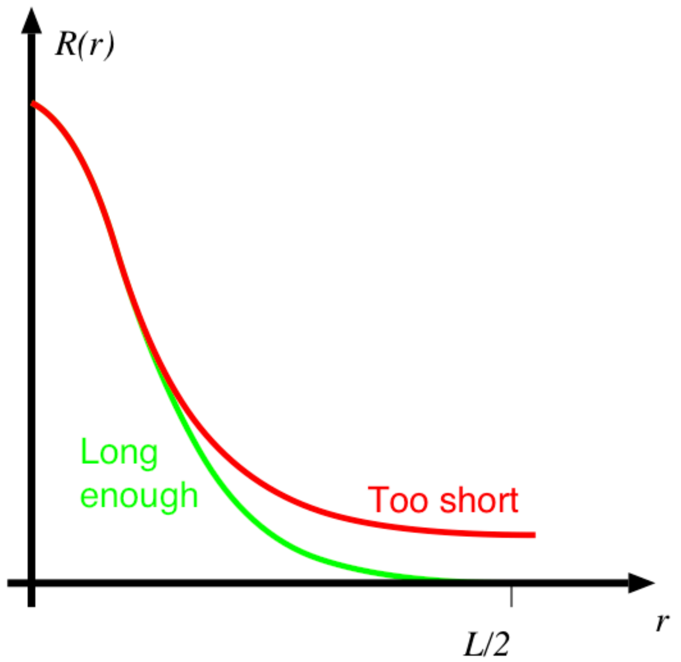
Periodic B.C.s

- Domain length must be large enough to accommodate longest struct flow:

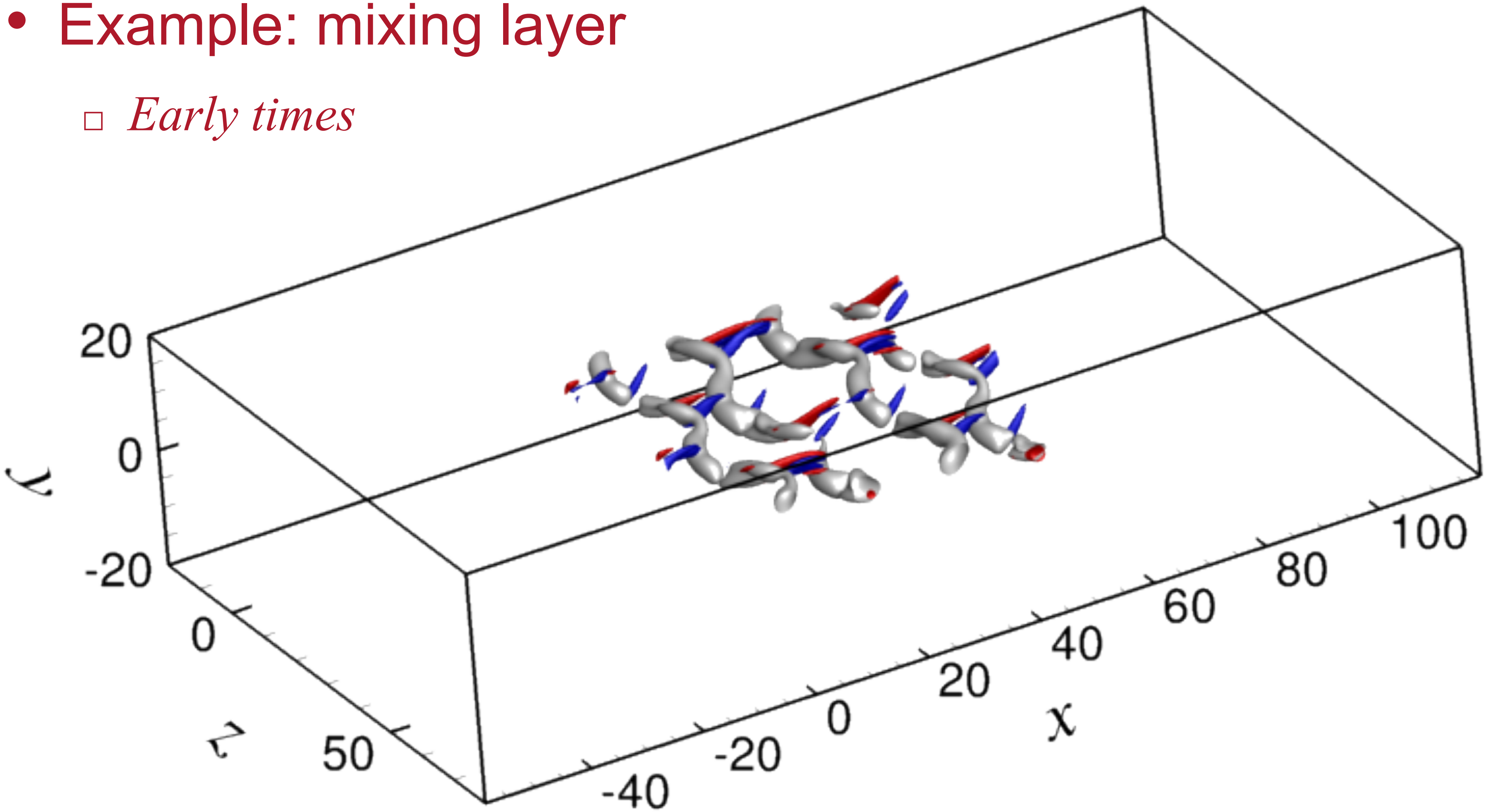
$$L > 2\lambda_{\max}$$



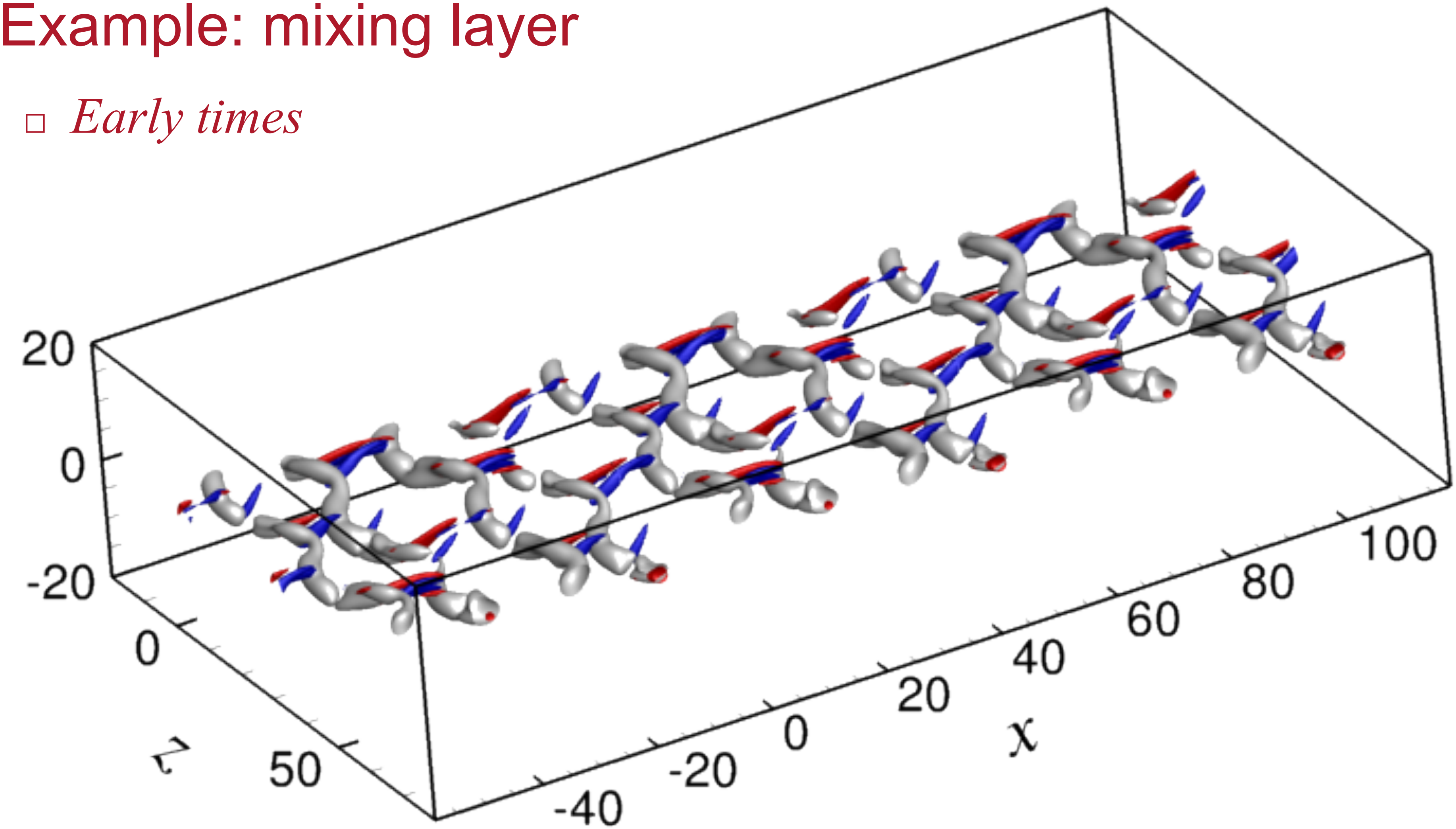
- Can be checked after the fact through the two-point correlation:
  - *If it does not reach zero at L/2 the domain is too short.*
- Must be checked for each variable.



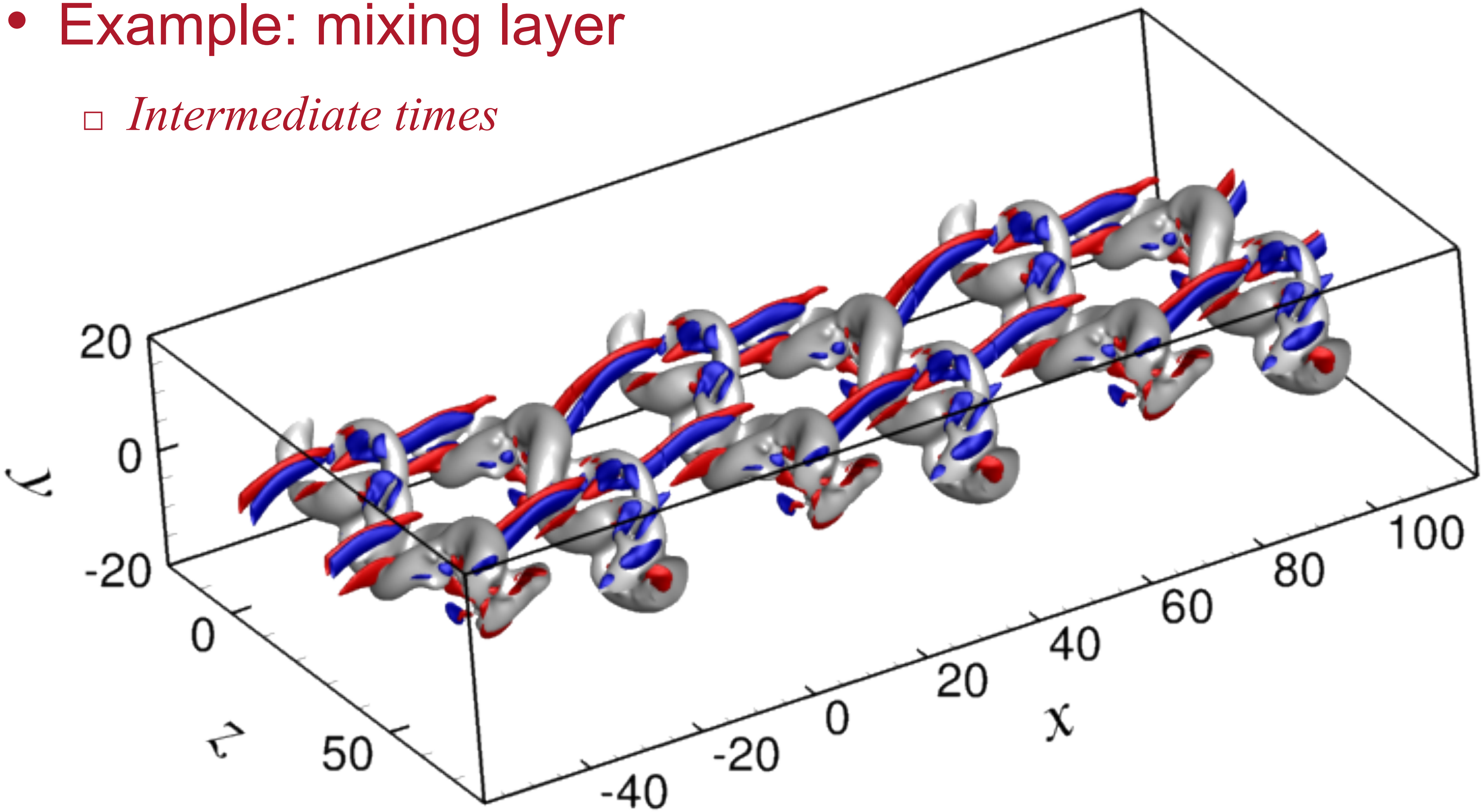
- Example: mixing layer
    - *Early times*



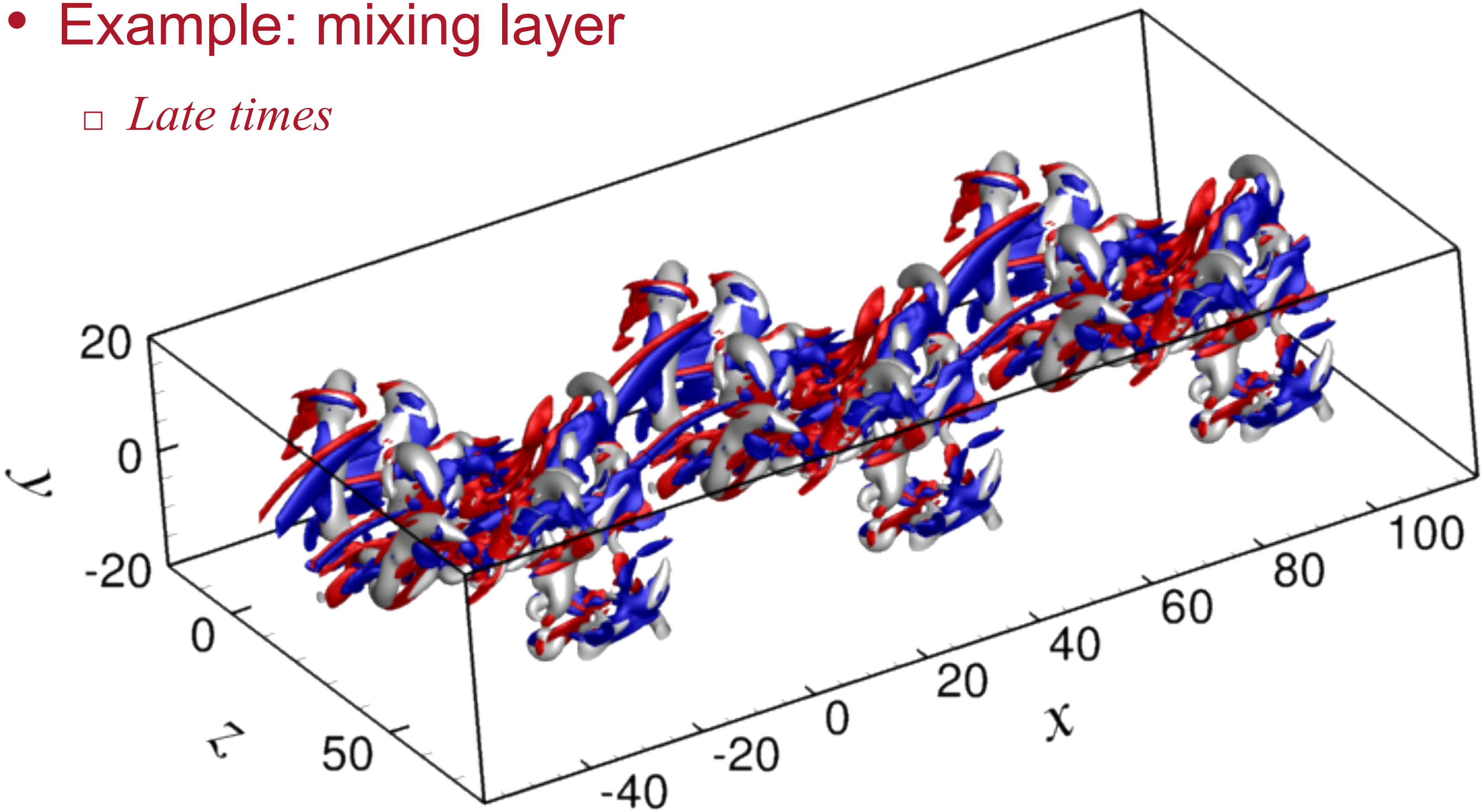
- Example: mixing layer
  - *Early times*



- Example: mixing layer
  - *Intermediate times*

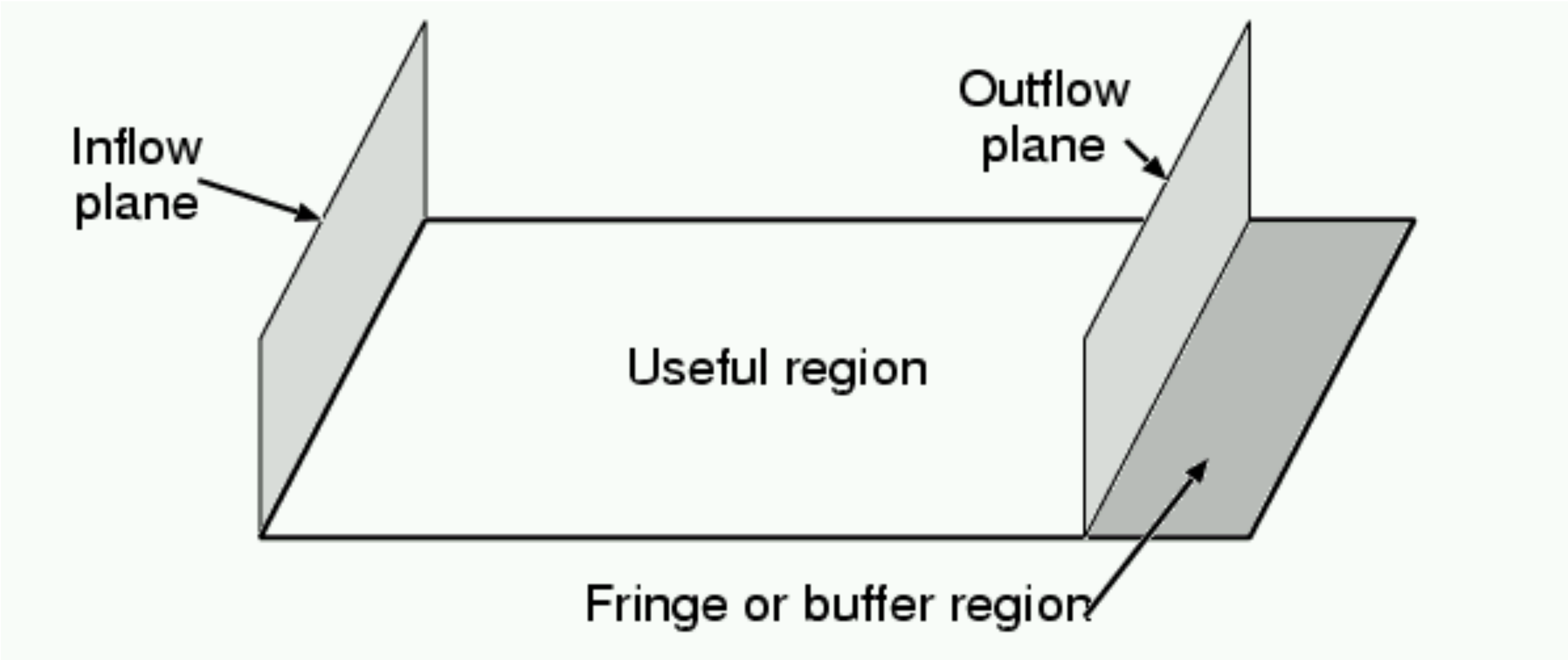


- Example: mixing layer
  - *Late times*



Outflow B.C.s

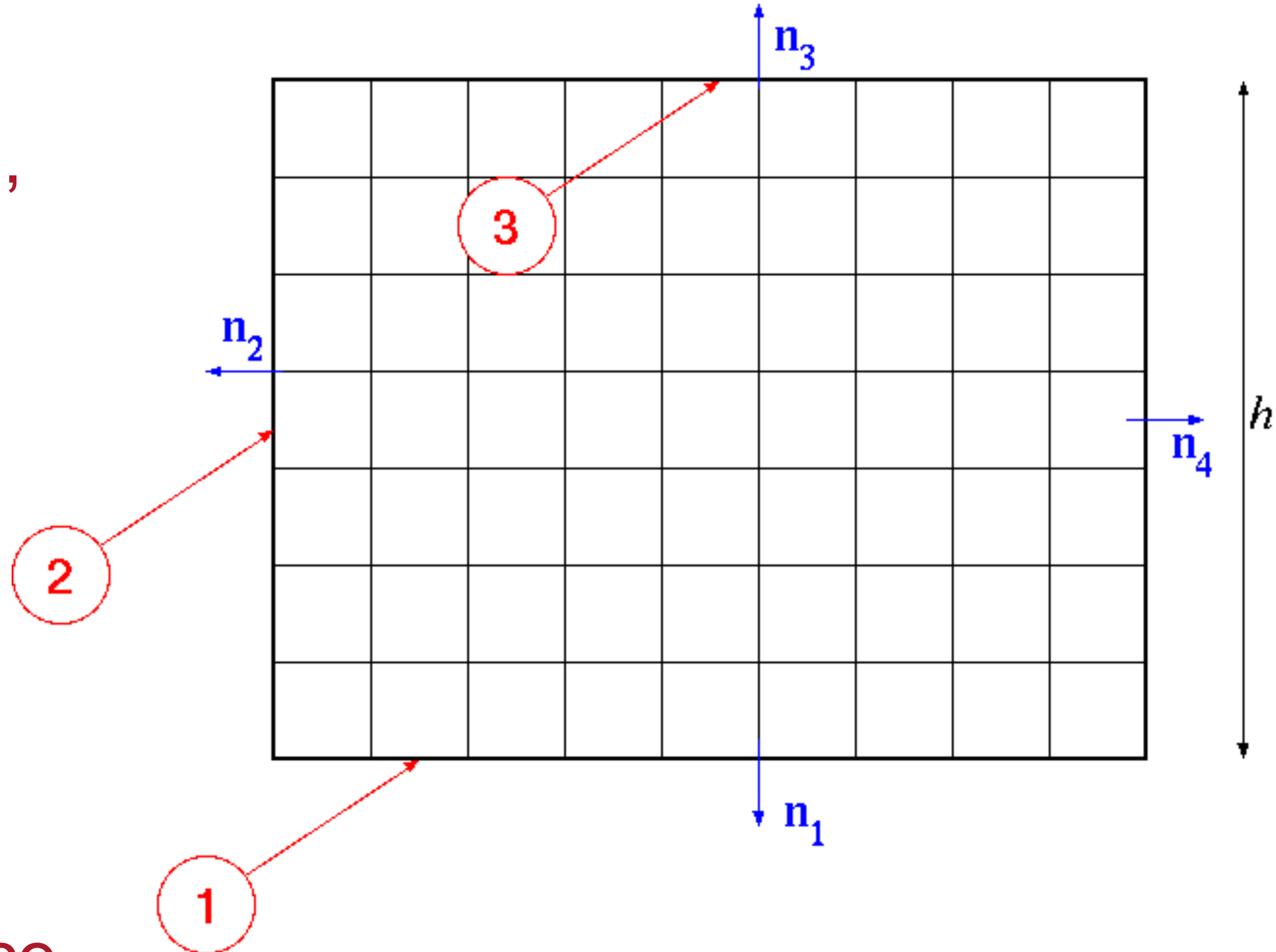
- Equations are parabolized in a “buffer region”.
- Often coupled with Orlanski outflow conditions.



Outflow B.C.s

- I. Orlanski
  J. Comput. Phys. **21**, 251 (1976).

$$\frac{\partial \phi}{\partial t} + U_c \frac{\partial \phi}{\partial n} = 0$$



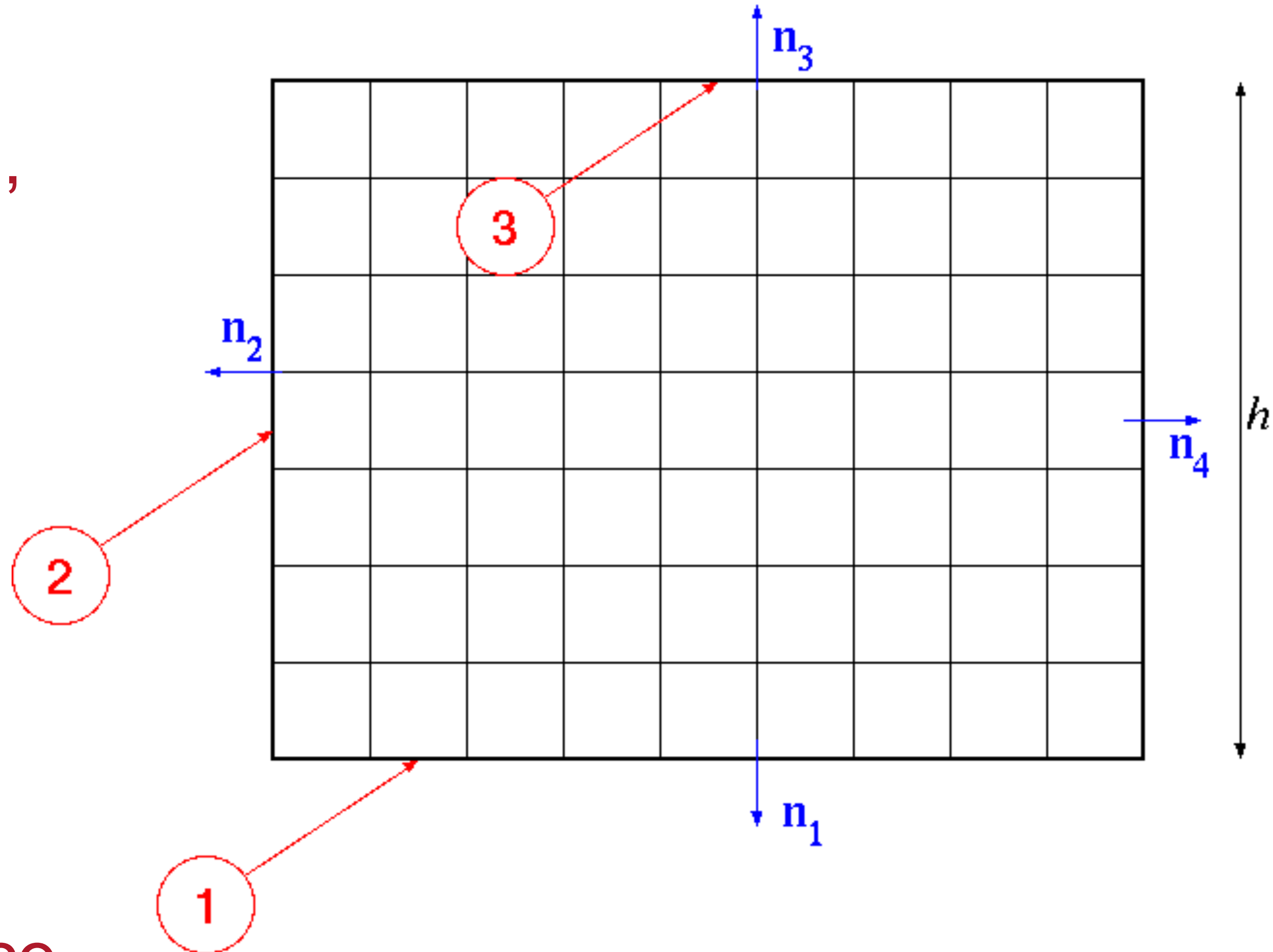
- U_c = component ⊥ to boundary or
- U_c from mass balance

$$U_c \mathcal{S}_4 + \int_1 \mathbf{V} \cdot \mathbf{n} d\mathcal{S} + \int_2 \mathbf{V} \cdot \mathbf{n} d\mathcal{S} + \int_3 \mathbf{V} \cdot \mathbf{n} d\mathcal{S} = 0$$

Outflow B.C.s

- I. Orlanski
  J. Comput. Phys. **21**,
  251 (1976).

$$\frac{\partial \phi}{\partial t} + U_c \frac{\partial \phi}{\partial n} = 0$$



- U_c = component ⊥ to boundary or
- U_c from mass balance
- Add “sponge layer” at the end of the domain to remove reflections

Wall boundary conditions

- To apply the no-slip conditions, the wall layer must be fully resolved:
  - *First grid point at* $y^+<1$.
  - *Reynolds-stress producing events are resolved by the grid (streaks, near-wall eddies…):*

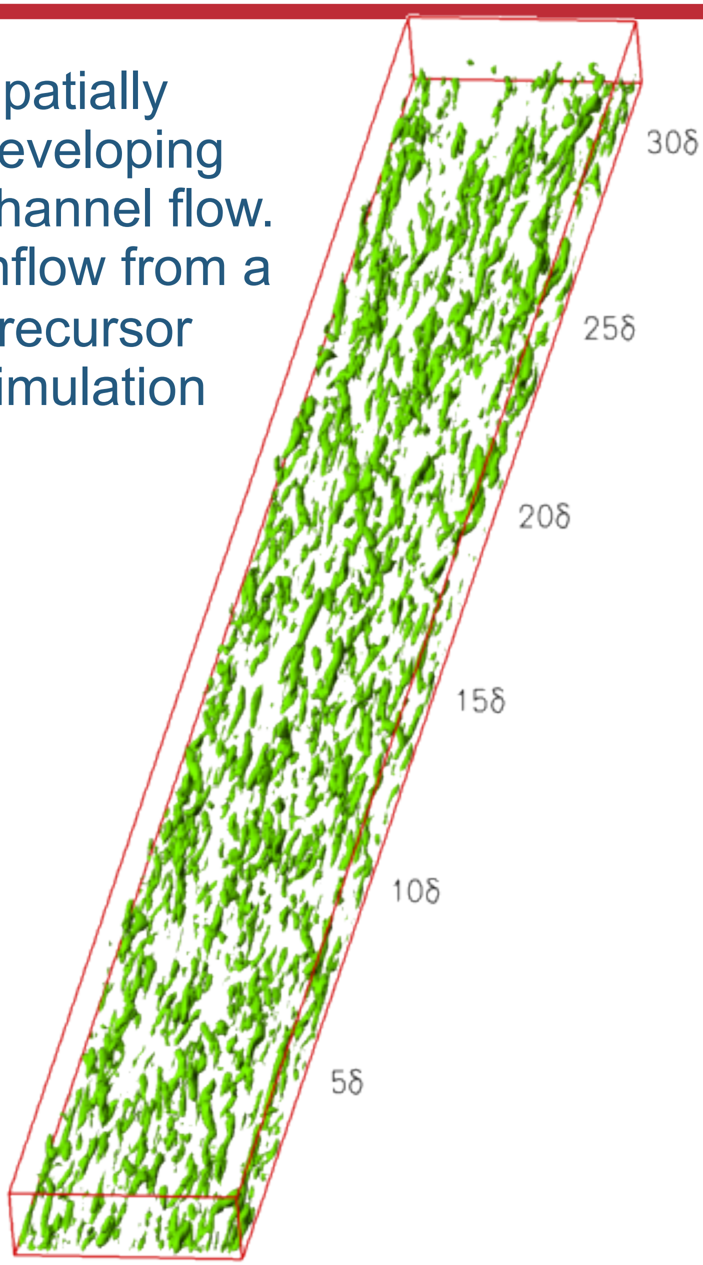
    $$\Delta x^+ \approx 5\text{-}20. \ \Delta z^+ \approx 2\text{-}5.$$
  - *High aspect-ratio grid cells near the wall.*
  - *As* $Re \rightarrow \infty$ *the percentage of points required to resolve the near-wall layer* $\rightarrow$ 100%.

Inflow conditions

- DNS and LES requires an unsteady, three-dimensional velocity field at the inflow plane.
  - *Experiments only yield mean values → Matching DNS to exp. is difficult.*

Inflow conditions

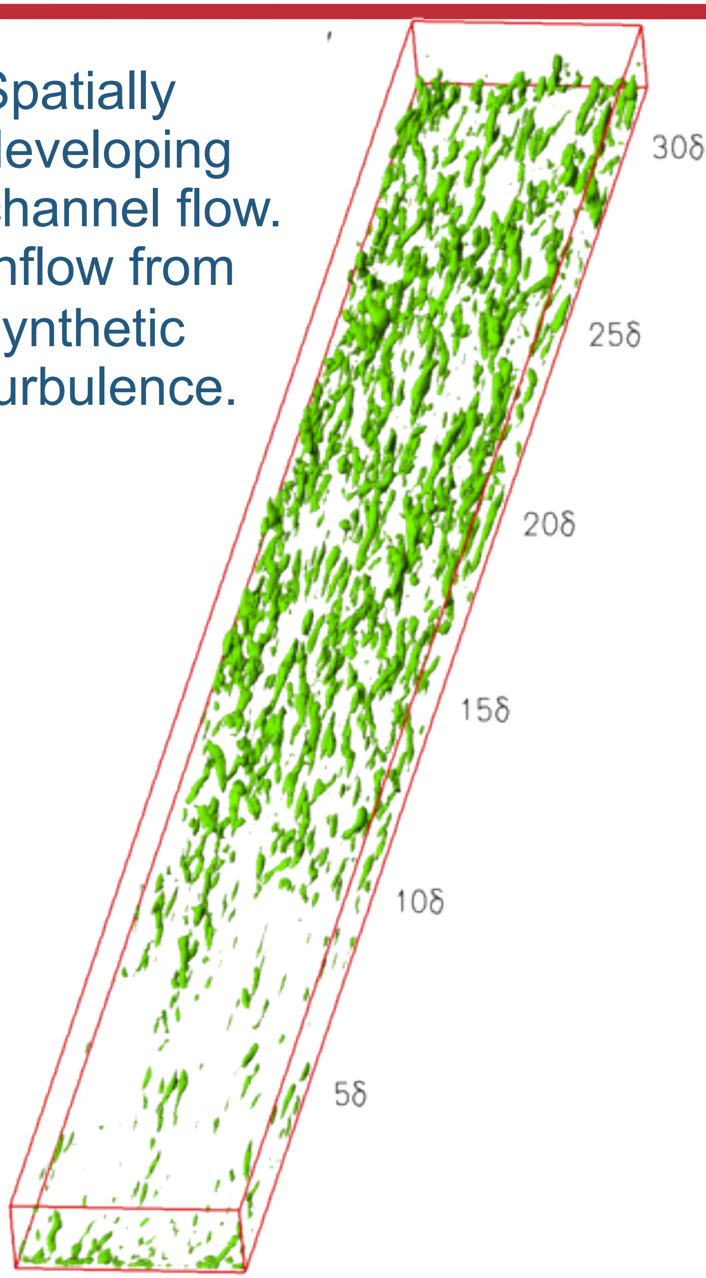
Spatially developing channel flow. Inflow from a precursor simulation



- Existing methods:
  - *Inflow from a separate calculation (w/ or w/o rescaling)*
    - Requires that the inlet be in an "equilibrium region".
    - Increases the computational cost and storage requirement.

Inflow conditions

Spatially developing channel flow. Inflow from synthetic turbulence.



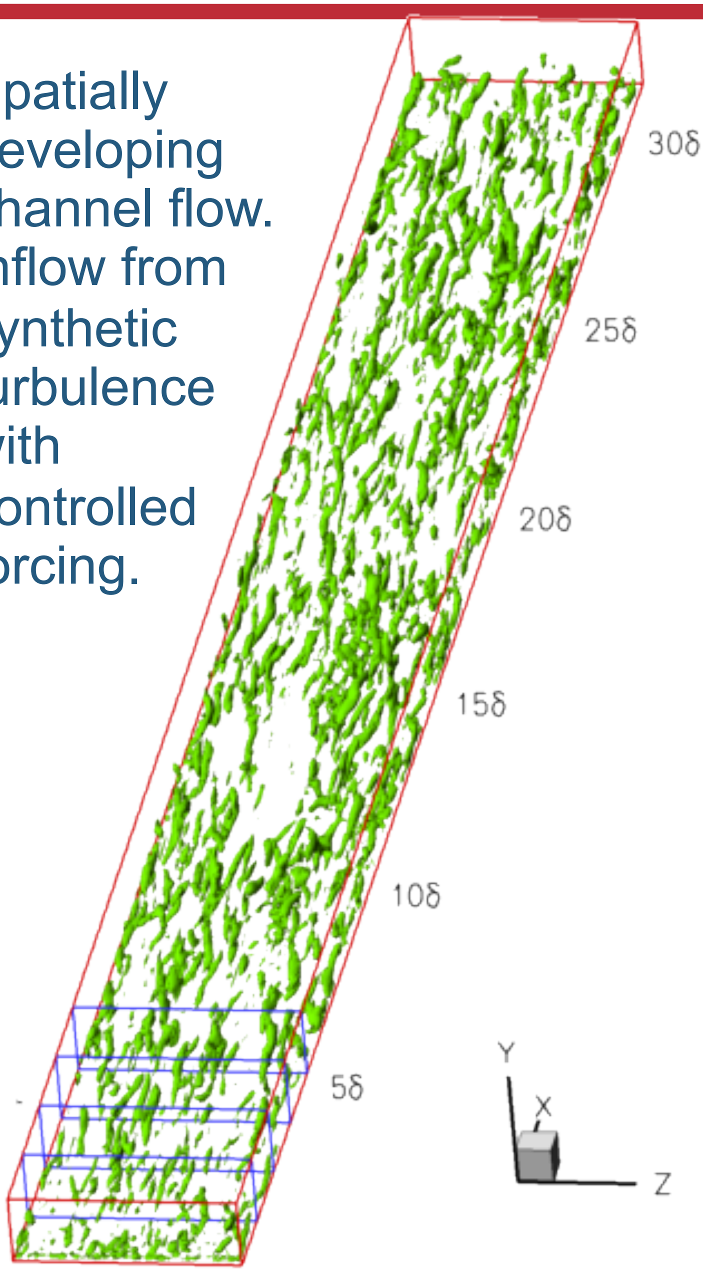
- Existing methods:
  - *Inflow from a separate calculation (w/ or w/o rescaling)*
  - *Superposition of mean profiles with random fluctuations.*
    - Requires long transition distances for the flow to redevelop.

Inflow conditions

- Existing methods:
  - *Inflow from a separate calculation (w/ or w/o rescaling)*
  - *Superposition of mean profiles with random fluctuations.*
  - *Recycling-Rescaling*
    - Requires that the inlet be in an "equilibrium region" and known scaling laws.
    - Increases the computational cost and memory requirement.

Inflow conditions

Spatially developing channel flow. Inflow from synthetic turbulence with controlled forcing.



- Existing methods:
  - *Inflow from a separate calculation (w/ or w/o rescaling)*
  - *Superposition of mean profiles with random fluctuations.*
  - *Recycling-Rescaling*
  - *Controlled forcing*
    - Speeds up the development of realistic turbulence from random fluctuations.

Effect of inflow conditions

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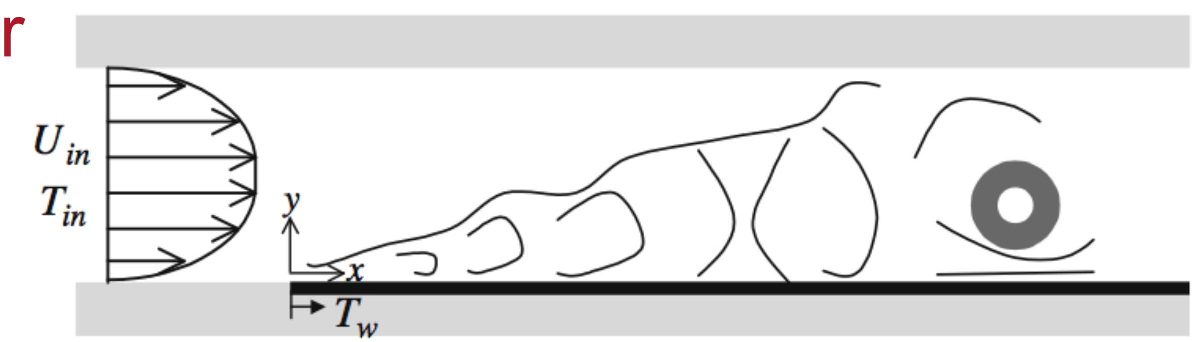
DNS of buoyancy-dominated turbulent flows on a bluff body using the immersed boundary method

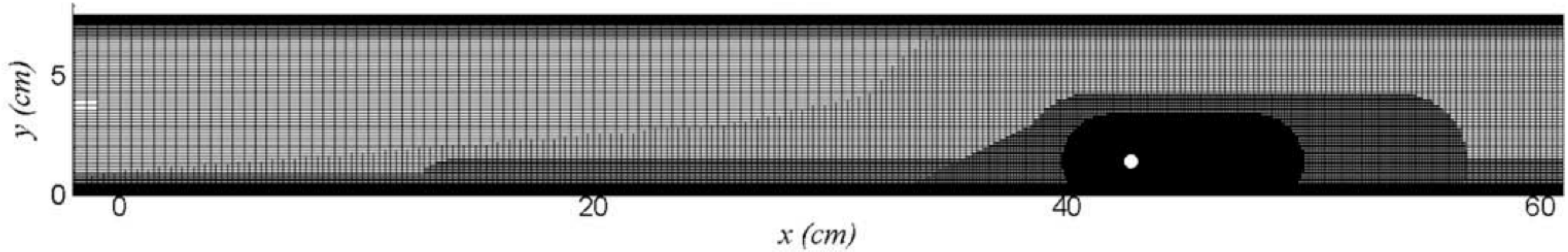
Seongwon Kang *, Gianluca Iaccarino, Frank Ham

Center for Turbulence Research, Stanford University, 488 Escondido Mall, Building 500, Room 501N3, Stanford, CA 94305, USA

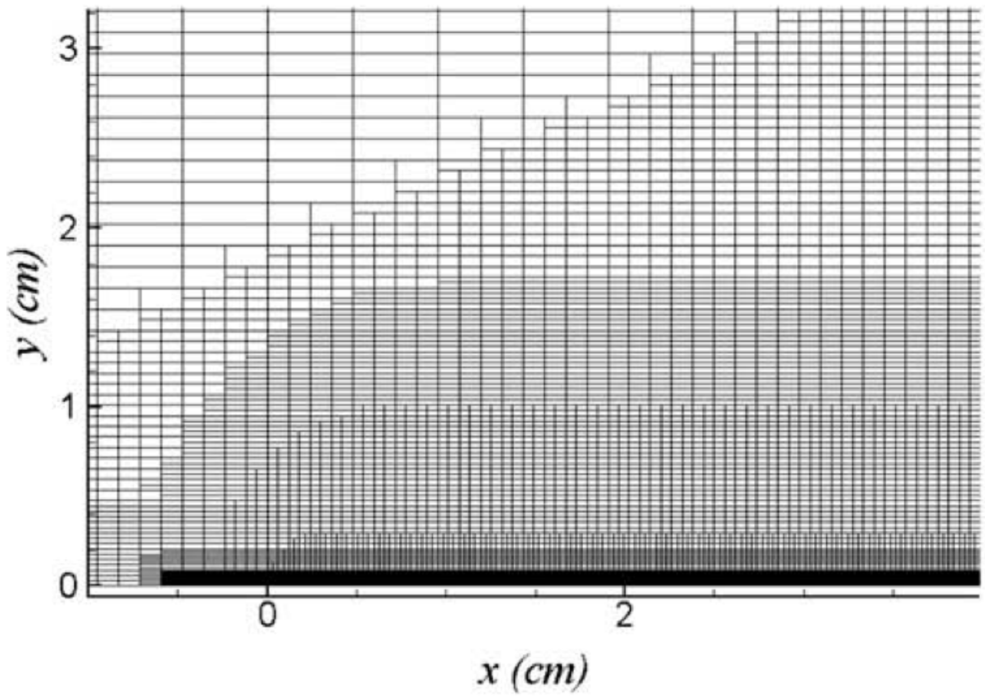
- Finite volume unstructured code (2nd-order).
- Locally refined mesh.
- Immersed-boundary method.
- Problem: heated cylinder inside a channel.



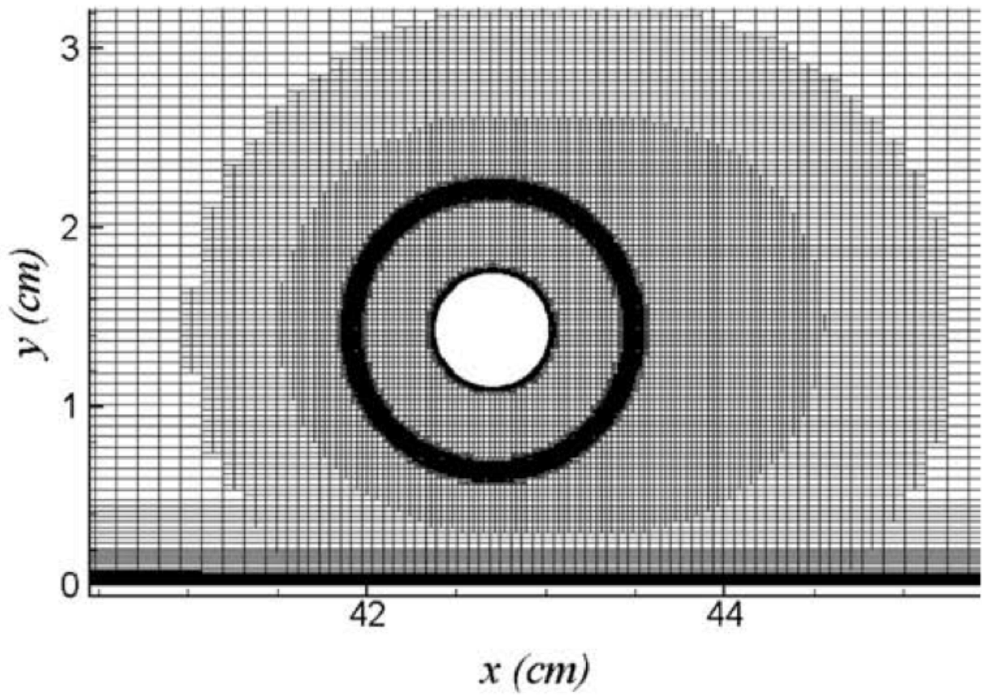
Effect of inflow conditions



(a) Whole domain

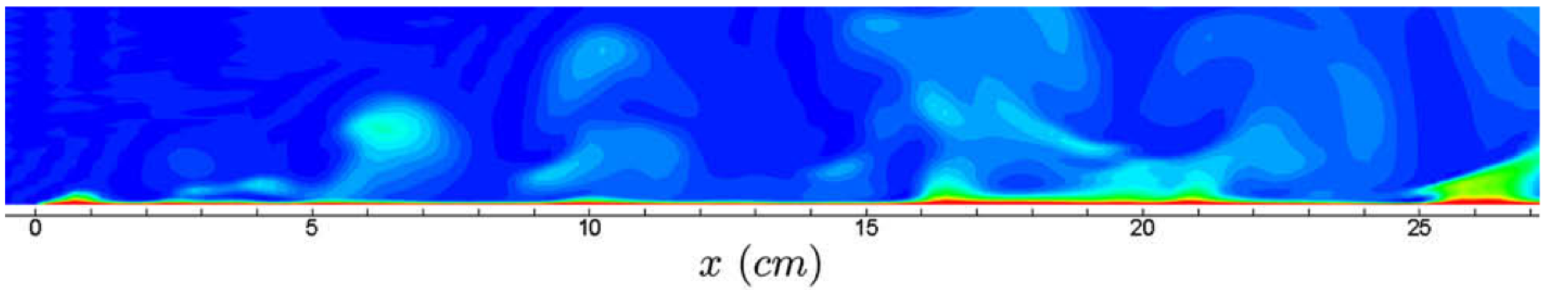


(b) Entry region

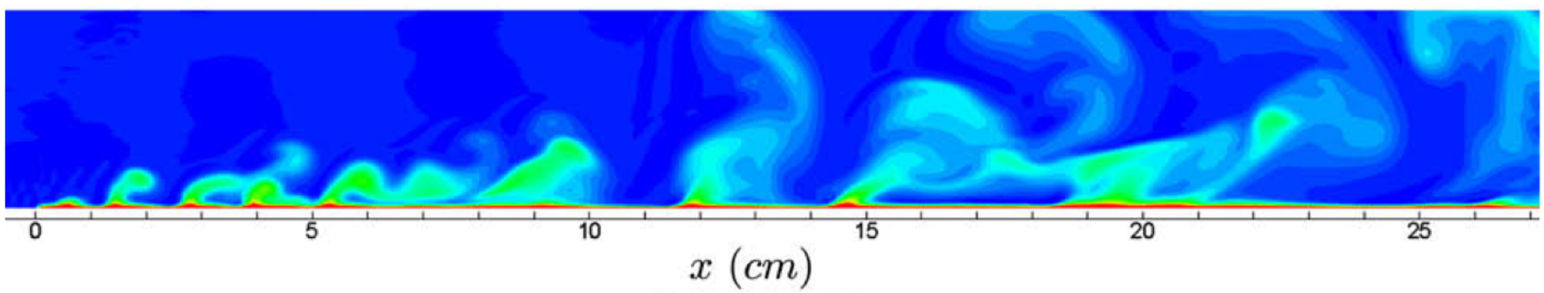


(c) Cylinder region

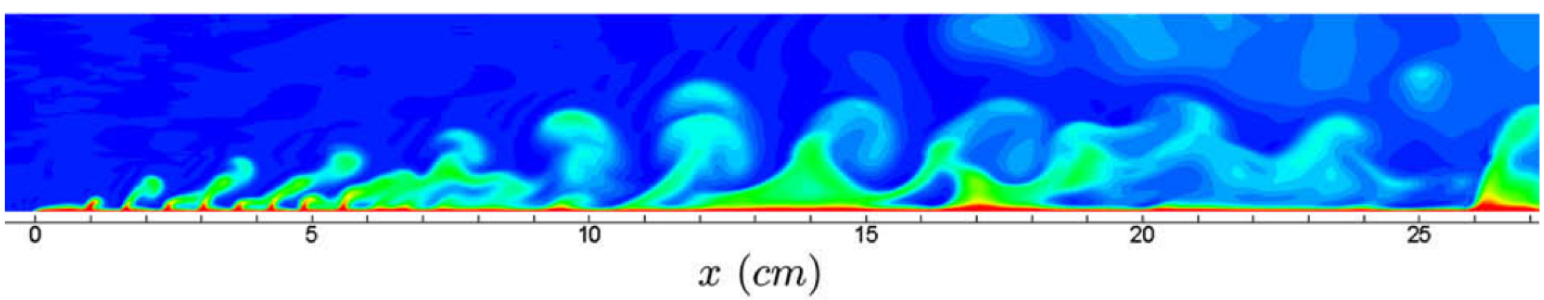
Effect of inflow conditions



(a) Grid #1

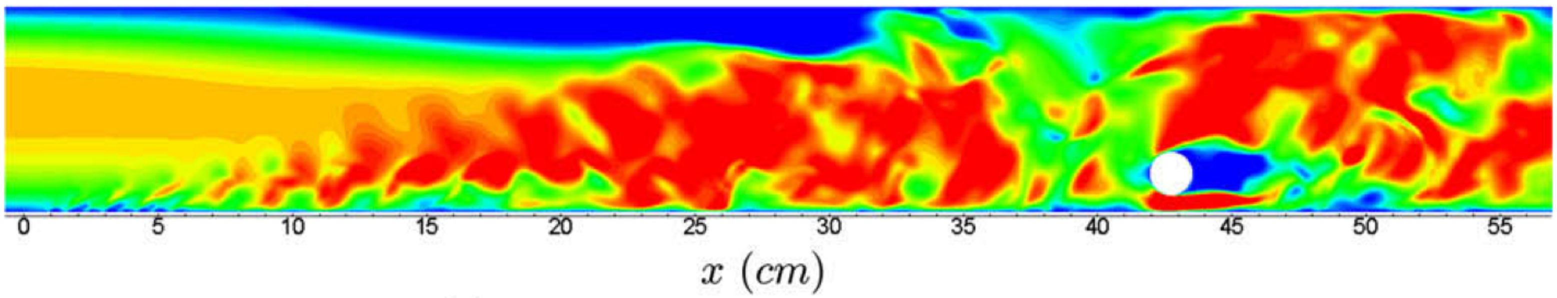


(b) Grid #2

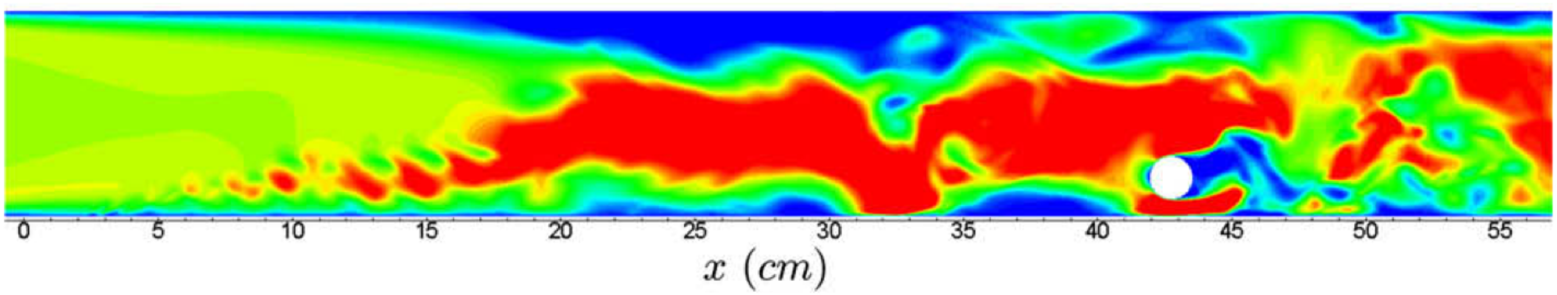


(c) Grid #3

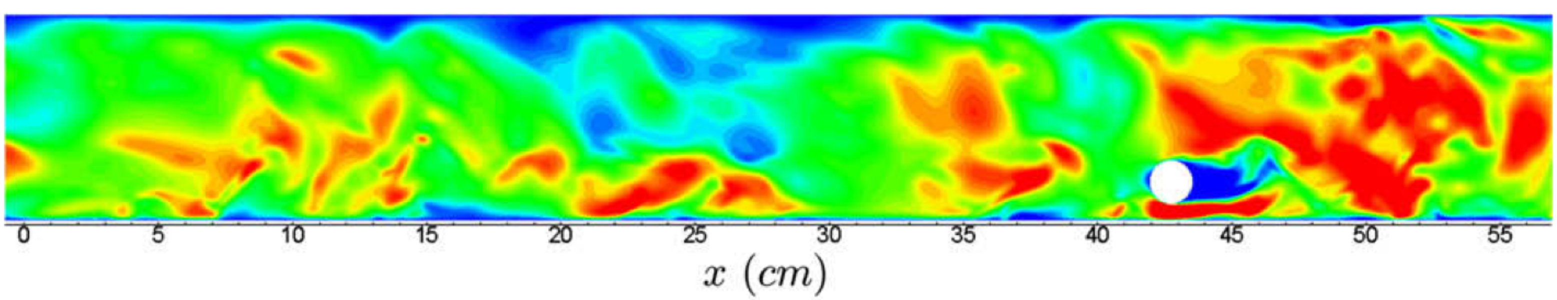
Effect of inflow conditions



(a) Interpolated from the experiment

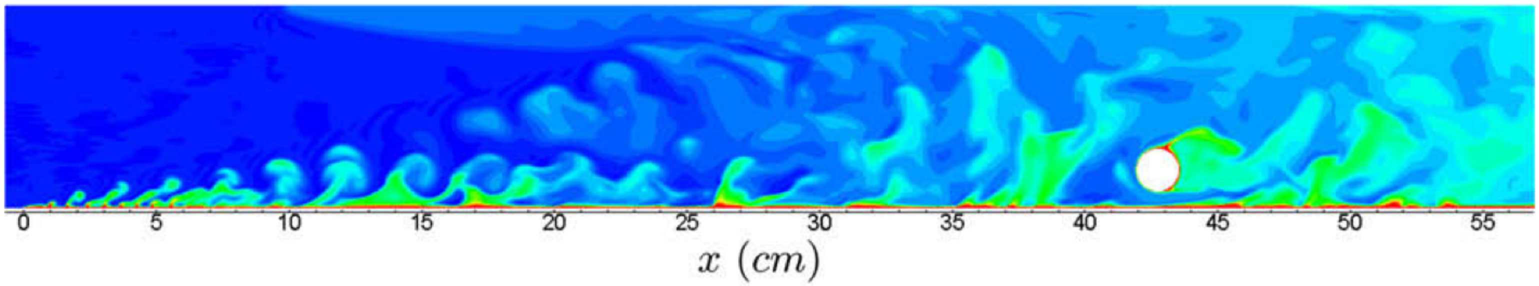


(b) Uniform

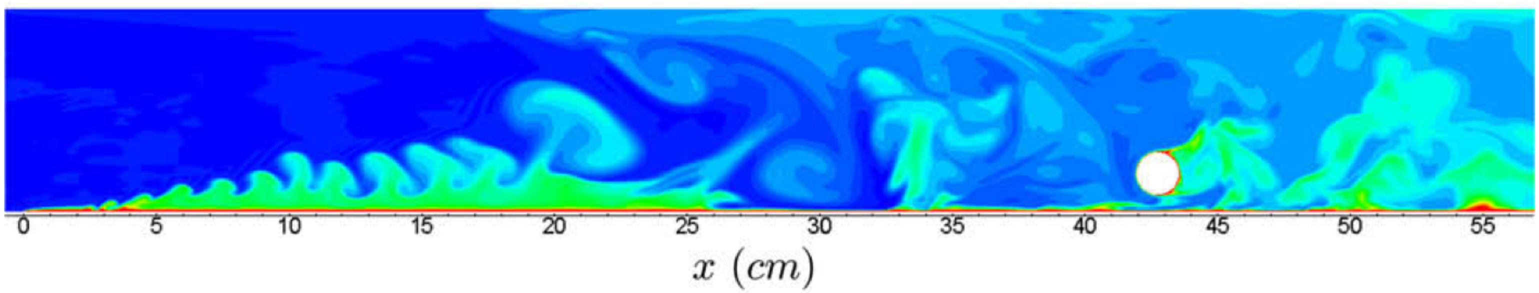


(c) Recycled from x=36cm

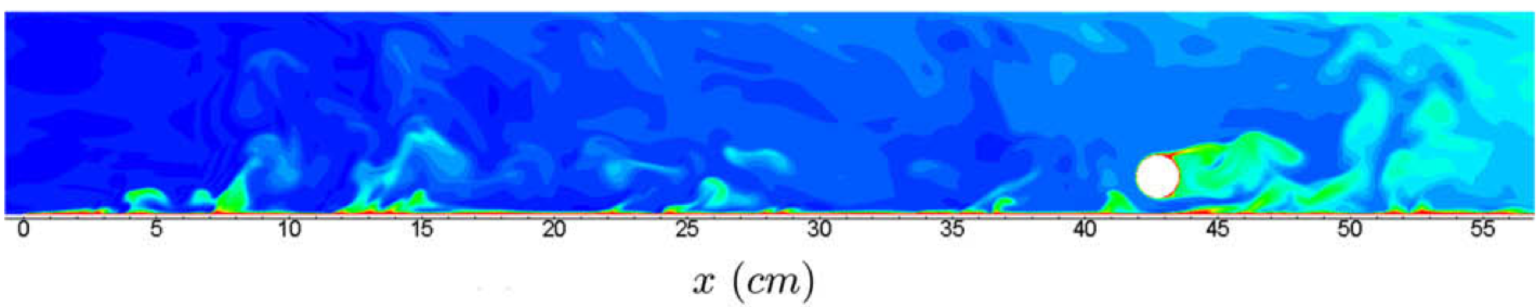
Effect of inflow conditions



(a) Interpolated from the experiment



(b) Uniform



(c) Recycled from x=36cm

Outline

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- Simulation methodologies
- Governing equations
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- **Subfilter-scale modelling**
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OUTLINE

- Motivation:
- Simulation methodologies
- Governing equations
- Boundary conditions
- **Subfilter-scale modelling**
  - *Modelling considerations*
  - *Overview of SFS models*
    - Eddy-viscosity models
    - Scale similar and mixed models
    - Dynamic models
    - Deconvolution models
    - Implicit LES
- Validation of an LES
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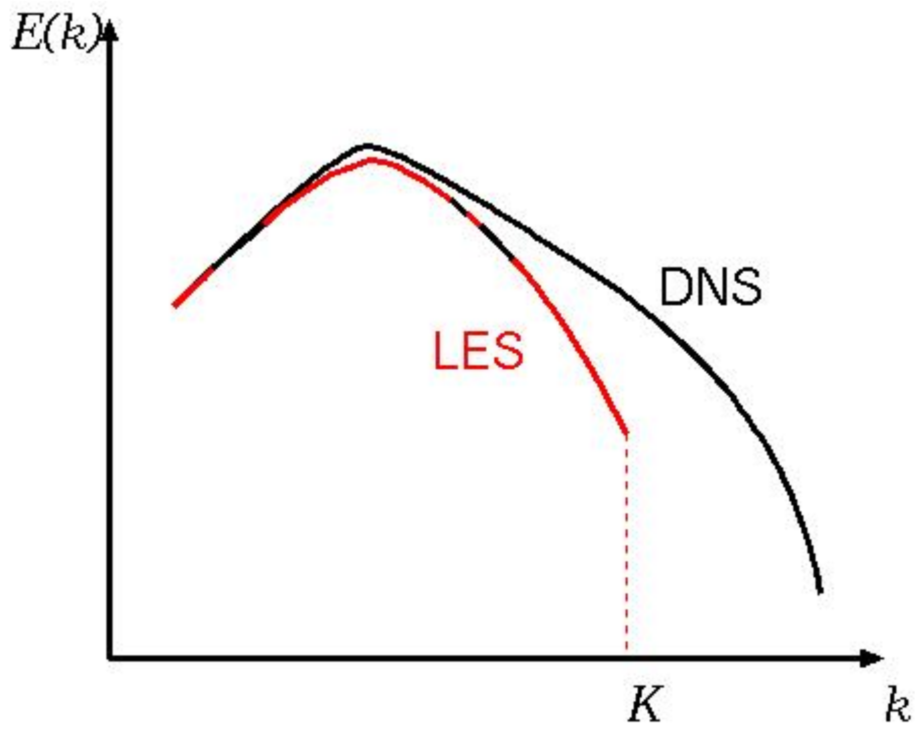
Modelling considerations

- LES velocity fields contain substantially more information than RANS solutions (frequency, wavenumber).
- This information can be used to improve SFS models.

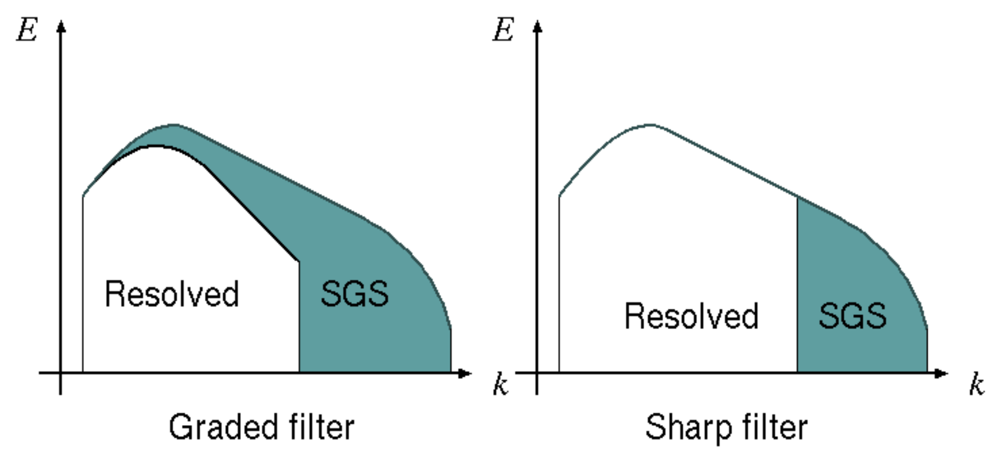


K = cutoff wavenumber ∝ 1/Δ (filter width)

Modelling considerations

$$
\begin{aligned}
\frac{\partial \overline{u}_i}{\partial x_i} &= 0 \\
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{u}_i \overline{u}_j\right) &= -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \nu \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_j}
\end{aligned}
$$

- $\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j$ are the SFS stresses that require closure.
- They are due mostly to the small scales, but may have some large-scale contribution as well.



Energy transfer mechanisms

$$\frac{D}{Dt}[\text{Resolved TKE}] = \cdots - \underbrace{\frac{\partial}{\partial x_j}(\tau_{ij}\overline{u}_i)}_{\text{SFS Diff.}} + \underbrace{\tau_{ij}\overline{S}_{ij}}_{\text{SFS Diss.}}$$

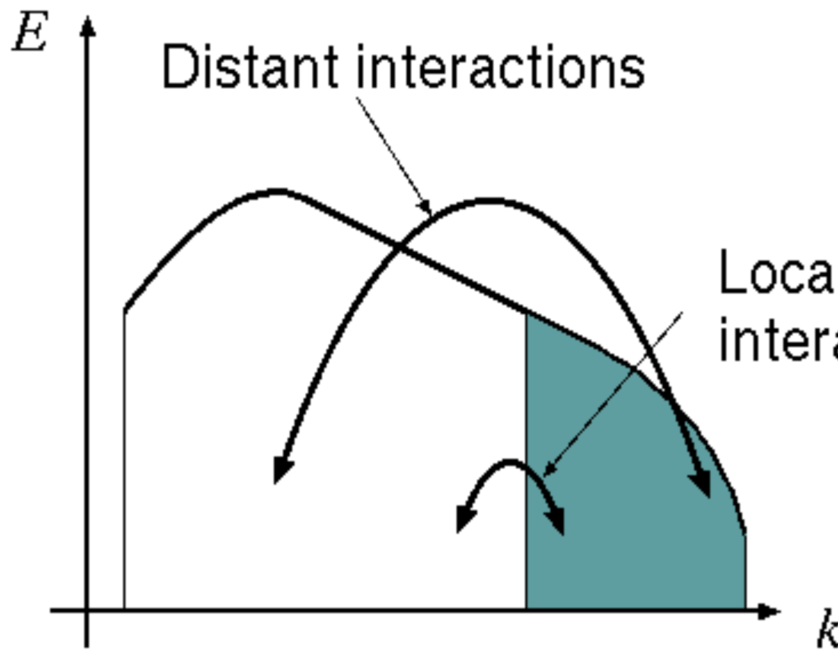
$$\frac{D}{Dt}[\text{SFS TKE}] = \cdots \underbrace{\frac{\partial}{\partial x_j}(\tau_{ij}\overline{u}_i)}_{\text{SFS Diff.}} - \underbrace{\tau_{ij}\overline{S}_{ij}}_{\text{SFS Diss.}} - \underbrace{\varepsilon}_{\text{Visc. Diss. of SFS TKE}}$$

Resolved scales → **Subfilter scales** → **Heat**

- Large scales set the dissipation level: $\varepsilon \sim \frac{(\overline{u}_i\overline{u}_i)^{3/2}}{L}$
- Energy is transferred from the large scales to the small ones by the SFS Diffusion + SFS Dissipation.
- The subfilter scales provide the dissipation into heat.

Subfilter-scale modelling

- Two types of energy-exchange mechanisms are important:
  - *Local (in wave-number) interactions.*
  - *Distant interactions*



Eddy-viscosity models

- Most common choice: eddy-viscosity model.

$$\tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk} = -2\nu_T \overline{S}_{ij}; \qquad \underbrace{\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right)}_{\text{Strain-rate tensor}}$$

- The eddy viscosity ν_T has dimensions

$$[\text{length}] \times [\text{velocity}] \Rightarrow= \ell \times q_{sfs}$$

- The most active SFS scales are those close to the cutoff (i.e., the filter-width)

$$\Rightarrow \quad \boxed{\ell \propto \overline{\Delta}}$$

Equilibrium assumption

$-\tau_{ij}\overline{S}_{ij}$ → **Subfilter scales** → $\varepsilon \sim q_{sfs}^3/\overline{\Delta}$

Production of SFS TKE

Viscous dissipation of SFS TKE

$$q_{sfs}^2 \sim \tau_{kk} \sim (\overline{\Delta}|\overline{S}|)^2 \Rightarrow \nu_T = (C_S\overline{\Delta})^2\overline{S}|$$

Smagorinsky (1963); Lilly (1967)

[Reprinted from Proceedings of the IBM Scientific Computing Symposium on Environmental Sciences, held on November 14–16, at the Thomas J Watson Research Center, Yorktown Heights, N Y]

14

The Representation of Small-Scale Turbulence in Numerical Simulation Experiments

D. K. Lilly
National Center for Atmospheric Research

Smagorinsky model

- $\nu_T = (C_S\overline{\Delta})^2\overline{S}|$
- Since the constant C_S (the Smagorinsky constant) is real, the model is absolutely dissipative:

$$\varepsilon_{sfs} = \tau_{ij}\overline{S}_{ij}(C_S\overline{\Delta})^2\overline{S}|^3 \leq 0$$

Smagorinsky model

- To evaluate C_S assume a spectrum with an inertial range:

$$E(\kappa) = C_K \varepsilon^{2/3} \kappa^{-5/3}$$

- Integrate the dissipation spectrum $k^2 E(k)$ over all resolved wave-numbers:

$$|\overline{S}|^2 \simeq 2 \int_0^{\pi/\overline{\Delta}} \kappa^2 E(\kappa) d\kappa = \frac{3}{2} C_K \varepsilon^{2/3} \left(\frac{\pi}{\overline{\Delta}} \right)^{4/3}$$

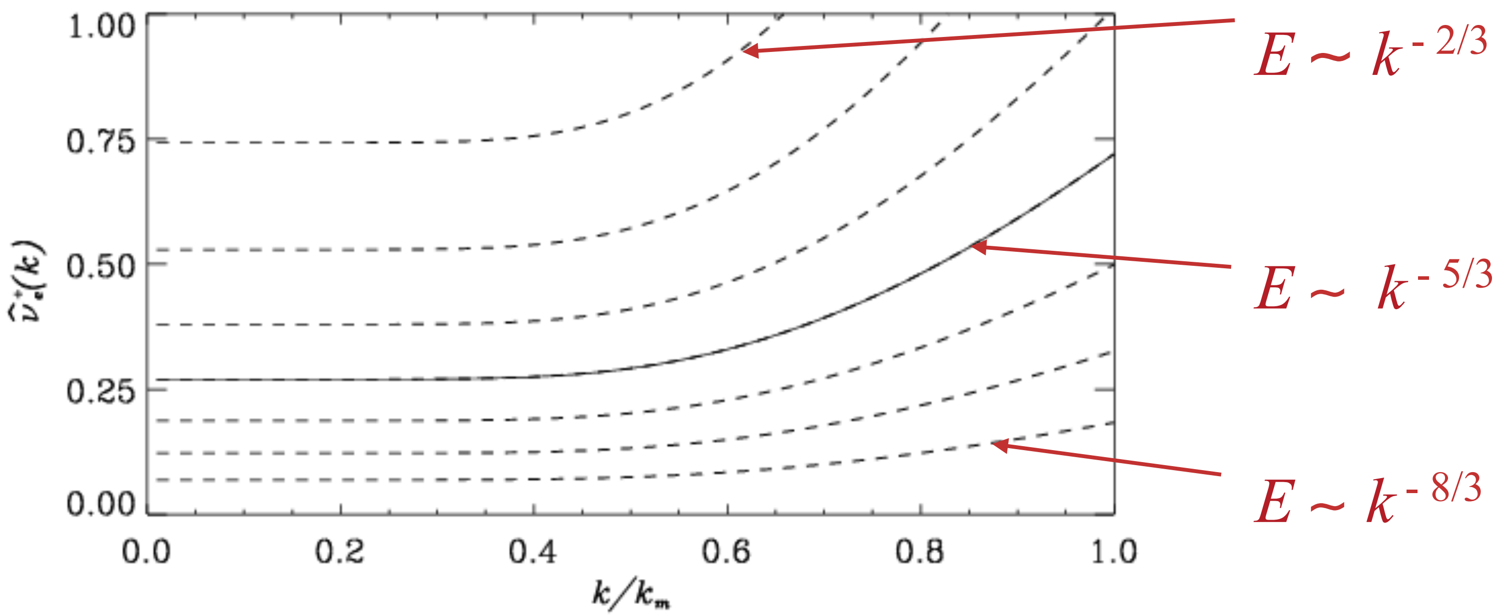
- With C_K=1.41 this gives $C_S \cong$ 0.18.

Queen's University

Smagorinsky model

- Predicts overall dissipation fairly accurately
  - *Except near solid walls, during transition or re-laminarization or in other cases in which the small scales are not in equilibrium.*
- Does not account for local interactions.
- The Smagorinsky constant needs to be adjusted in the presence of shear, in transitional flows, near solid walls etc.

Two-point closures



- Eddy viscosity in wave space
  - *Plateau: distant interactions.*
  - *Peak: local interactions.*
- Chollet-Lesieur (1981) EDQNM eddy-viscosity:

$$\widehat{\nu}(k) = C_K^{-3/2}\left[0.441 + 15.2\exp\left(-3.03k_m/k\right)\right]\left[E(k_m)/k_m\right]^{1/2}$$

Structure-function model

- The EDQNM eddy viscosity must be implemented in spectral space.
- Métais & Lesieur (1992) derived the structure function model, that can be implemented in real space.

Structure-function model

- Express the spectrum $E(k_m)$ in terms of the second-order structure function

$$\overline{F_2}(\mathbf{x};\overline{\Delta}) = \langle [\overline{u}_i(\mathbf{x}+\mathbf{r}) - \overline{u}_i(\mathbf{x})]\, \langle [\overline{u}_i(\mathbf{x}+\mathbf{r}) - \overline{u}_i(\mathbf{x})] \rangle,$$

  where <•> is an ensemble-average taken over all points such that $|\mathbf{r}| = \overline{\Delta}$.

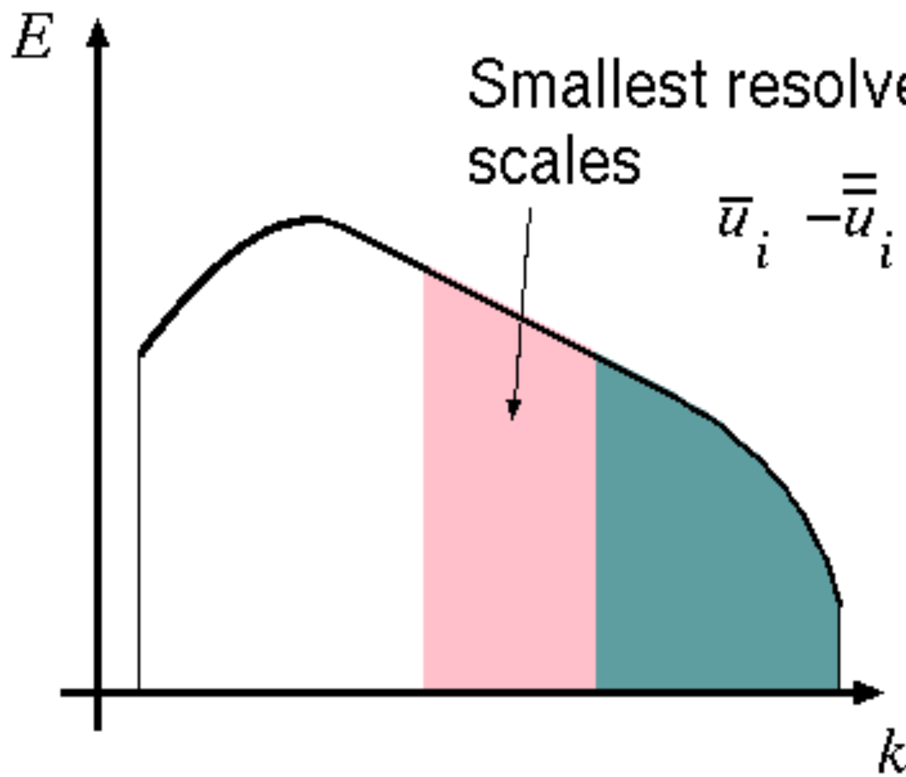
- This gives $\nu_T(\mathbf{x}) = 0.063\overline{\Delta}^2 \left(|\overline{S}|^2 + |\omega|^2\right)^{1/2}$.

Structure-function model

- Smagorinsky-like model. Strain-rate replaced by velocity gradient.
- For isotropic flows, the model is less dissipative than the Smagorinsky model.
- For sheared flows the structure function may be excessively dissipative.
- Improved results were obtained by applying a Laplacian filter to remove the contribution of the largest eddies to the velocity gradient before computing the structure function (Ducros et al. 1996).

Scale-similar and mixed models

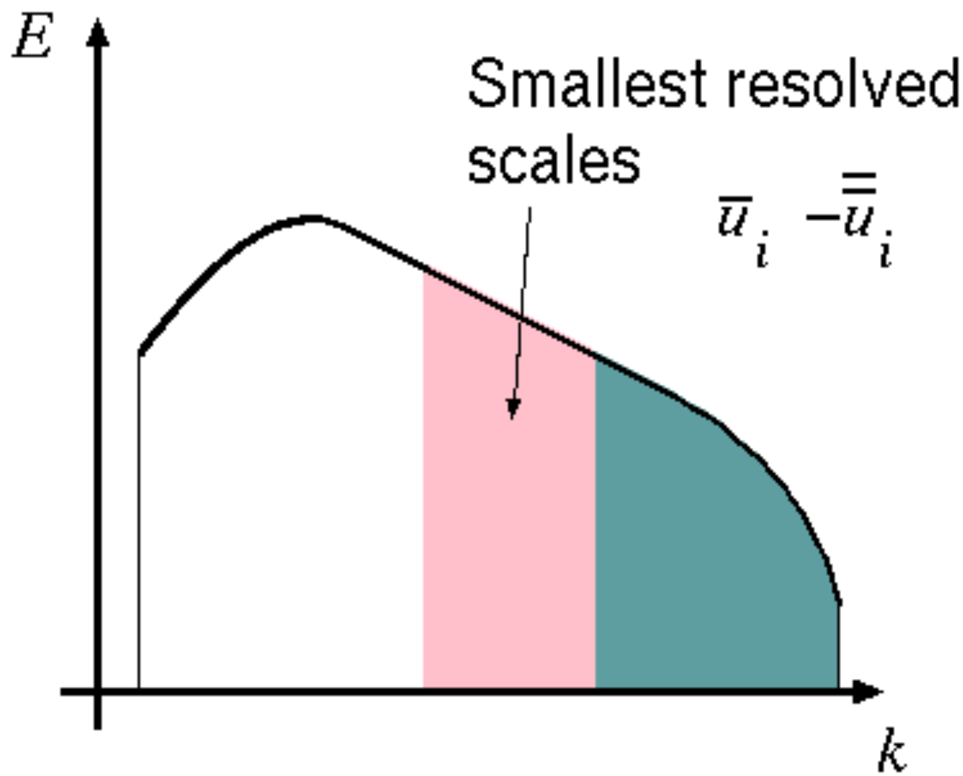
- Scale-similar models are based on the following assumptions (Bardina et al. 1980):
  - *The most active subfilter scales are those closer to the cutoff.*
  - *The scales with which they interact most are those right above the cutoff.*



Scale-similar and mixed models

- The largest subfilter scales can be obtained by filtering the SFS velocity $u_i' = u_i - \overline{u}_i$ to obtain

$$\overline{u_i'} = \overline{u}_i - \overline{\overline{u}}_i$$



- A Smagorinsky model is added to represent the dissipative effect of the small scales, to give

$$\tau_{ij} - \frac{\delta_{ij}}{3}\tau_{kk} = C_B\left[\overline{\overline{u}_i\overline{u}_j} - \overline{\overline{u}}_i\,\overline{\overline{u}}_j - \frac{\delta_{ij}}{3}\left(\overline{\overline{u}_k\overline{u}_k} - \overline{\overline{u}}_k\,\overline{\overline{u}}_k\right)\right] - 2\nu_T\overline{S}_{ij}.$$

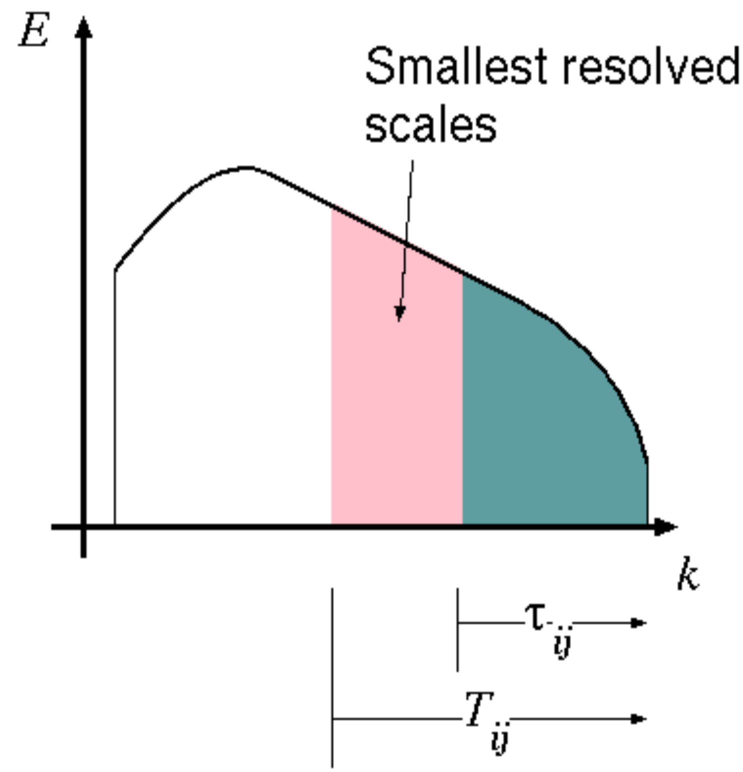
  - C_B=1 to assure Galilean invariance

Scale-similar and mixed models

- Give improved results when graded filters are used.
- Provide an estimate of the SFS energy τ_{kk}.
- Account for the correlation between the resolved Reynolds stress producing events and the SFS energy transfer (local energy transfer).
- Can be coupled to dynamic eddy-viscosity contributions (Zang et al. 1993).

Dynamic models

- Consider the identity
  $$L_{ij} \equiv \widehat{\overline{u}_i \overline{u}_j} - \widehat{\overline{u}}_i \widehat{\overline{u}}_j = T_{ij} - \widehat{\tau}_{ij},$$
- The resolved turbulent stresses L_{ij} are the contribution from the region between test-filter and grid-filter scale.



- The subtest stresses
  $$T_{ij} \equiv \widehat{\overline{u_i u_j}} - \widehat{\overline{u}}_i \widehat{\overline{u}}_j$$
  are obtained by applying the test filter $\widehat{G}$ to the filtered Navier-Stokes equations.

- Substituting for the subfilter and the subtest stresses into the identity yields a system of equations for the model coefficient C.

$$\tau_{ij} = -2C\alpha_{ij}; \quad T_{ij} = -2C\beta_{ij}$$

- The identity can be satisfied only approximately, since the real stresses are replaced by modelling assumptions.
- Lilly (1992) proposed an error minimization that gives

$$C = -\frac{1}{2}\frac{\langle L_{ij}M_{ij}\rangle}{\langle M_{mn}M_{mn}\rangle}; \quad M_{ij} = \beta_{ij} - \widehat{\alpha}_{ij}$$

where the brackets indicate an appropriate average.

- This procedure can be applied to mixed models, or models with more than one coefficient.
- The model gives vanishing eddy viscosity in laminar flows, and has the correct near-wall behaviour.
- The ensemble average $\langle \cdot \rangle$ has the purpose of removing sharp fluctuations of the coefficient.
  - *Germano et al. (1991) used volume or plane averages.*
  - *Ghosal et al. (1995) used an integral formulation.*
  - *Meneveau et al. (1996) proposed a Lagrangian ensemble-average calculating following the fluid particle.*

Deconvolution models

- If a filter G could be inverted, one could obtain the unfiltered velocity from the filtered one:

$$u_i = G^{-1}\overline{u}_i$$

- The SFS stresses could then be computed directly:

$$\tau_{ij} = \overline{u_i u_j} - \overline{u}_i \overline{u}_j$$

- Filters with compact support are not invertible.
- Deconvolution models try to obtain an approximation u_i^* to u_i by an approximate deconvolution process.
- The SFS stresses are then computed as:

$$\tau_{ij} = \overline{u_i^* u_j^*} - \overline{u}_i \overline{u}_j$$

Deconvolution models

- Scale-similar models: $u_i^* = \overline{u}_i$
- Shah and Ferziger (1995): obtained u_i^* as a truncated Taylor series of $\overline{u}_i$
- Domaradzki and co-workers (1997-2000) Subgrid-Scale Estimation model:
  - *Deconvolve the filtered velocity onto a finer grid by interpolation (inversion of the tophat filter).*
  - *Generate new scales by an approximate integration of a linearized non-linear term.*

Deconvolution models

- Stolz and co-workers (1999, 2001) Approximate Deconvolution Model:
  - *Approximate the filter as a truncated series:*

$$Q_N = \sum_{n=1}^{N} (I - G)^n \simeq G^{-1}$$

$$\boxed{u_i^* = Q_N \overline{u}_i}$$

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Implicit LES

- The numerical method provides the dissipation
- Relate the truncation error to the resolved field
- Derive an Effective SFS model
- Truncation errors, Commutation errors and SFS stresses are taken into account together
- Every numerical method is associated with some SFS modelling ansatz
    - *Simple upwind methods: not so good*
    - *Non-Oscillatory Finite Volume schemes are better.*