A priori testing of subgrid-scale models for a two-phase turbulent flow: Droplets in Homogeneous-Isotropic Turbulence

Suhas S Jain and Sanjiva K Lele

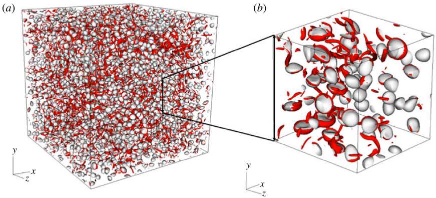
ME461: Advanced Topics in Turbulence,
Stanford University

14th December 2017

Stanford University

Introduction and Motivation

- Turbulent two-phase flows are ubiquitous.
- DNS is expensive.
- Need for a good LES model.
- First Step ⇒ *A priori* testing.



DNS data:

- Droplets in decaying homogeneous-isotropic turbulence
- $Re = 6.42 \times 10^4$, $We = 1.53 \times 10^4$
- 3130 Taylor length scale size droplets
- density ratio = 10, viscosity ratio = 10 and $We_{rms} = 1$
- $1024 \times 1024 \times 1024$ grid
- ≈ 32 grid points per diameter of the drops

Ref: Dodd & Ferrante (2016)

Stanford University

Objectives

- Derivation of governing equations - ”one-fluid formulation”
- Filtering the equations and deriving the unclosed terms.
- Choose filters and filter sizes.
- Order of magnitude analysis of the unclosed terms.
- Choose sub-grid scale model and compute correlation coefficients.

Stanford University

Unfiltered equations

Interface:

$$f^k(\vec{x},t) = 0$$

Sharp phase-indicator function:

$$\chi^k = H(f^k)$$

Two-fluid formulation

$$\frac{\partial \chi^k \rho^k}{\partial t} + \vec{\nabla}\cdot(\chi^k \rho^k \vec{u}^k) = \rho^k(\vec{W} - \vec{u}^k)\cdot \vec{n}^k \delta_i,$$

$$\frac{\partial \chi^k \rho^k \vec{u}^k}{\partial t} + \vec{\nabla}\cdot[\chi^k(\rho^k \vec{u}^k \otimes \vec{u}^k + p^k \mathbb{1} - \underline{\underline{\tau}}^k)] - \chi^k \rho^k g = [\rho^k \vec{u}^k \otimes (\vec{W}^k - \vec{u}^k) + p^k \mathbb{1} - \underline{\underline{\tau}}^k]\cdot \vec{n}^k \delta_i$$

One-fluid variable:

$$\phi = \sum_k \chi^k \phi^k$$

One-fluid formulation

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot(\rho \vec{u}) = 0,$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \vec{\nabla}\cdot(\rho \vec{u}\otimes \vec{u} + p\mathbb{1} - \underline{\underline{\tau}}) - \rho g = [\sigma \vec{n}^k(\nabla_s \cdot \vec{n}^k) - \nabla_s \sigma]\delta_i.$$

Stanford University

Filtered equations

Filtering

$$\overline{u(\vec{x},t)} = \int_{-\infty}^{t}\int_{\Omega} G(\overline{\Delta}, \vec{x}-\vec{x'}, t-t')u(\vec{x'})dx'dt'$$

Filtered equations

$$\frac{\partial\overline{\rho}}{\partial t} + \vec{\nabla}\cdot(\overline{\rho}\widetilde{\vec{u}}) = 0.$$

$$\frac{\partial\overline{\rho}\widetilde{\vec{u}}}{\partial t}+\vec{\nabla}\cdot(\overline{\rho}\widetilde{\vec{u}}\otimes\widetilde{\vec{u}}+\overline{p}\mathbb{1}-\overline{\mu}\overline{S_D}+\underline{\underline{\tau}}_{fl_{\rho uu}}+\underline{\underline{\tau}}_{fl_{\mu S}} = [\overline{\sigma}^s\overline{\vec{n}}^s\overline{(\nabla_s\cdot\vec{n})}^s-\overline{\nabla_s}^s\overline{\sigma}^s]\overline{\delta_i}+\underline{\underline{\tau}}_{r_{\sigma n}}+\underline{\underline{\tau}}_{r_{\sigma t}}$$

Favre average:

$$\widetilde{u} = \overline{\rho u}/\overline{u}$$

Surface filtering:

$$\overline{\phi}^s = \frac{\int_{\Omega}\delta_i\phi d\vec{x}}{\int_{\Omega}\delta d\vec{x}} = \frac{\overline{\delta_i\phi}}{\overline{\delta_i}}$$

Stanford University

Assumptions

- Only two phases.
- Incompressible fluids, hence ρ is constant in each phase.
- No mass transfer.
- Isothermal and no chemical reactions, hence μ is constant in each phase and σ is constant.
- No sliding between the phases, hence filtering and gradient operators commute.
- Immiscible fluids.

Stanford University

Unclosed terms

Convective tensor

$$\underline{\underline{\tau}}_{fl_{\rho uu}} = \overline{\rho \vec{u} \otimes \vec{u}} - \overline{\rho} \widetilde{\vec{u}} \otimes \widetilde{\vec{u}}$$

Viscous tensor

$$\underline{\underline{\tau}}_{fl_{\mu S}} = \overline{\mu S_D} - \overline{\mu} \widetilde{S_D}$$

Surface tension vector

$$\underline{\underline{\tau}}_{r_{\sigma n}} = \overline{\delta_i \vec{n} (\nabla_s \cdot \vec{n})} - \overline{\delta_i}\ \overline{\vec{n}}^s \overline{(\nabla_s \cdot \vec{n})}^s$$

Stanford University

Filters and filter sizes

- Drops are of $\approx 32\Delta x$ in diameter
- Five filter sizes $\overline{\Delta} = 2\Delta x, 4\Delta x, 16\Delta x, 32\Delta x$ and $64\Delta x$
  - $\overline{\Delta} < 32\Delta x \rightarrow$ drops resolved by LES.
  - $\overline{\Delta} = 32\Delta x \rightarrow$ drops are of approximately the same size as of the LES grid.
  - $\overline{\Delta} > 64\Delta x \rightarrow$ drops are fully sub-grid.
- Filtering in frequency space.
  - Physical space $\rightarrow \approx 1$ day for $\overline{\Delta} = 4\Delta x$
  - Frequency space $\rightarrow \approx 10$ min, given the memory is $> \approx 150GB$

Filters

Gaussian:

$$G_{gauss} = \begin{cases} 1 & nk\Delta x < \pi/2 \\ 0 & else. \end{cases}$$

Spectrally sharp:

$$G_{sharp} = exp\Big[- \frac{(nk\Delta x)^2}{4} \Big],$$

$n = 1, 2, 8, 16$ and 32

Order of magnitude analysis: Previous studies

Summary:

- Convective tensor $\underline{\underline{\tau}}_{fl_{\rho uu}}$ increases with the filter size.
- Shear stress tensor $\underline{\underline{\tau}}_{fl_{\mu S}}$ is small for all filter sizes.
- Surface tension tensor $\underline{\underline{\tau}}_{r_{\sigma n}}$ is very small and decreases with the filter size.

[*Ref: Vincent et al. (2008), Toutant et al. (2006), Labourasse et al. (2007) and McCaslin and Desjardins (2014)*]

Classification of the terms in the momentum equation for different filtering sizes

Category	FiSm	FiAv	FiLa	FiHu
Large	$\nabla \cdot \overline{\rho u \otimes u + p}$	$\nabla \cdot \overline{\rho u \otimes u + p}$ $\nabla \cdot \tau_{l\rho uu}$	$\nabla \cdot \overline{\rho u \otimes u + p}$ $\nabla \cdot \tau_{l\rho uu}$	$\nabla \cdot \overline{\rho u \otimes u + p}$ $\nabla \cdot \tau_{l\rho uu}$
Medium	$\nabla \cdot \tau_{l\rho uu}$ $\nabla \cdot \overline{\tau}$	$\boxed{\frac{\partial \tau_{l\rho u}}{\partial t}}$	$\boxed{\frac{\partial \tau_{l\rho u}}{\partial t}}$	
Small	$\boxed{\frac{\partial \tau_{l\rho u}}{\partial t}}$ $\nabla \cdot \tau_{l\mu S}$	$\nabla \cdot \overline{\tau}$ $\nabla \cdot \tau_{l\mu S}$	$\nabla \cdot \overline{\tau}$ $\nabla \cdot \tau_{l\mu S}$ τ_{rnn}	$\nabla \cdot \overline{\tau}$ $\nabla \cdot \tau_{l\mu S}$
Negligible	τ_{rnn}	τ_{rnn}		τ_{rnn} $\boxed{\frac{\partial \tau_{l\rho u}}{\partial t}}$

Figure 1: Table 4 from Labourasse et al. (2007) showing the order of magnitude of convective, shear and surface tension unclosed terms for filter sizes $FiSm = 2\Delta x$, $FiAv = 10\Delta x$, $FiLa = 20\Delta x$ and $FiSm = 100\Delta x$, using the DNS data of phase inversion in a closed box on 512×512 grid.

Stanford University

Order of magnitude analysis: Present study

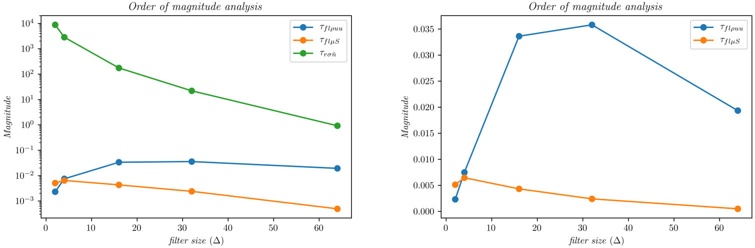


Figure 2: Order of magnitudes of convective $< |\vec{\nabla} \cdot \underline{\underline{\tau}}_{fl_{\rho uu}}| >$, viscous $< |\vec{\nabla} \cdot \underline{\underline{\tau}}_{fl_{\mu S}}| >$ and surface tension unclosed terms $< |\underline{\underline{\tau}}_{r_{\sigma n}}| >$ using a Gaussian kernel, where $<>$ denotes a spatial mean.

Stanford University

Order of magnitude analysis: Present study

- Surface tension term dominates.
  - Previous studies use volume filtering.
  - McCaslin and Desjardins (2014) $\rightarrow$ volume filtering underpredicts the surface tension terms.
  - Explanation: Filtering moves the interface location.
- Convective tensor is the second dominant term.
  - Increases for $\overline{\Delta} < 32\Delta x$
  - Decrease for $\overline{\Delta} > 32\Delta x$
  - Strong dependence on the interfacial scales in the flow
- Viscous term is small and consistent with previous studies.

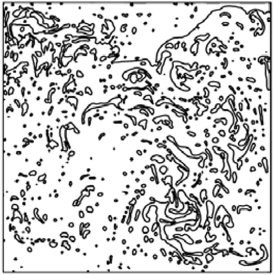


Figure 3: Wide range of interfacial scales seen in the case of phase inversion in a closed box from Figure 8 of Labourasse et al. (2007).

Stanford University

Order of magnitude analysis: Present study

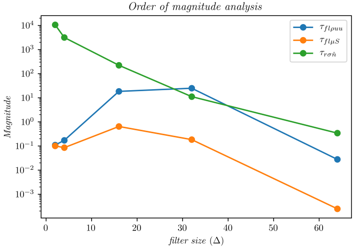


Figure 4: Order of magnitudes of convective $< |\vec{\nabla} \cdot \underline{\underline{\tau}}_{fl_{\rho uu}}| >$, viscous $< |\vec{\nabla} \cdot \underline{\underline{\tau}}_{fl_{\mu S}}| >$ and surface tension unclosed terms $< |\underline{\underline{\tau}}_{r_{\sigma n}}| >$ using a spectrally sharp kernel, where $<>$ denotes a spatial mean.

Stanford University

Sub-grid model evaluation

- No sub-grid models for surface tension unclosed terms.
- Convective dominates viscous terms.
- Vincent et al. (2008), Toutant et al. (2006), Labourasse et al. (2007) computed effective eddy viscosity → dispersive.

$$\mu_{ef} = \frac{\underline{\underline{\tau}}_{fl_{\rho uu}} : \vec{\nabla}\vec{u}}{S : \vec{\nabla}\vec{u}}$$

- Choose → Mixed Bardina-Smagorinsky type model.
- Model L → scale-similarity hypothesis and $C + R$ → eddy-viscosity hypothesis.

Germano decomposition (Germano (1986))

$$\overline{\phi\psi} - \overline{\phi}\;\overline{\psi} = L + C + R,$$

where,

$$L = \overline{\overline{\phi}\;\overline{\psi}} - \overline{\overline{\phi}}\;\overline{\overline{\psi}}$$

$$C = \overline{\overline{\phi}\;\psi'} - \overline{\overline{\phi}}\;\overline{\psi'} + \overline{\phi'\;\overline{\psi}} - \overline{\psi'}\;\overline{\overline{\psi}}$$

$$R = \overline{\phi'\;\psi'} - \overline{\phi'}\;\overline{\psi'}$$

Stanford University

Model and correlation coefficients

Scale similarity model

$$\underline{\underline{\tau}}_{fl_{\rho uu}} = \overline{\overline{\rho}\tilde{\tilde{\vec{u}}} \otimes \tilde{\tilde{\vec{u}}}} - \overline{\overline{\rho}}\tilde{\tilde{\tilde{\vec{u}}}} \otimes \tilde{\tilde{\tilde{\vec{u}}}},$$

where,

$$\tilde{\tilde{\tilde{\vec{u}}}} = \frac{\overline{\overline{\rho}\tilde{\tilde{\vec{u}}}}}{\overline{\overline{\overline{\vec{u}}}}}.$$

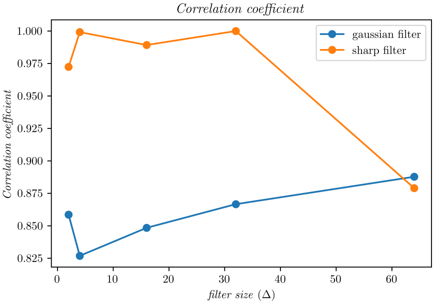


Figure 5: Correlation coefficients for scale-similarity model based on Gaussian kernel and spectrally sharp kernel.

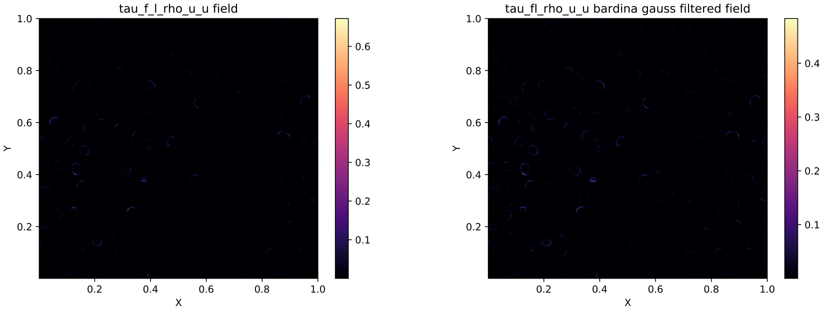


Figure 6: Unclosed term computed from DNS data and predicted by model for filter size $\overline{\Delta} = 2\Delta x$.

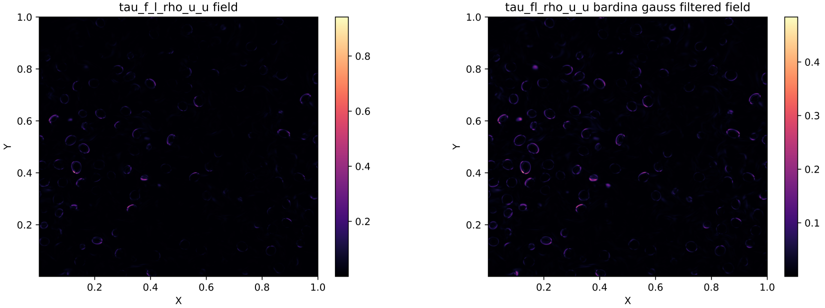
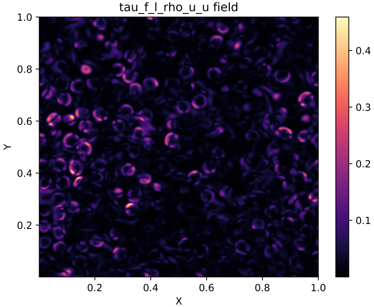


Figure 7: Unclosed term computed from DNS data and predicted by model for filter size $\overline{\Delta} = 4\Delta x$.



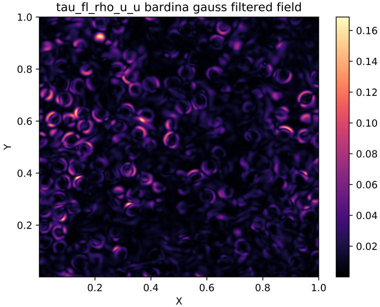


Figure 8: Unclosed term computed from DNS data and predicted by model for filter size $\overline{\Delta} = 16\Delta x$.

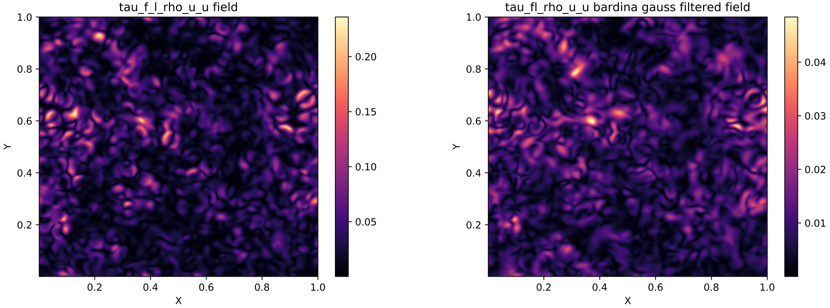


Figure 9: Unclosed term computed from DNS data and predicted by model for filter size $\overline{\Delta} = 32\Delta x$.

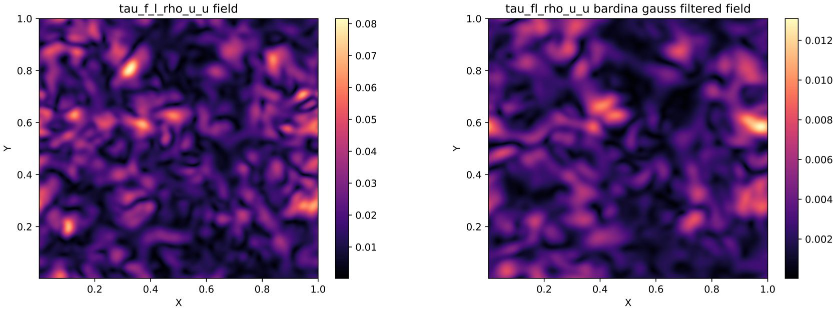


Figure 10: Unclosed term computed from DNS data and predicted by model for filter size $\overline{\Delta} = 64\Delta x$.

Stanford University

Summary and Conclusion

A priori testing to evaluate SGS model for turbulent two-phase flows.

- Droplets in a homogeneous-isotropic turbulence in a triply-periodic box
- Derived the filtered governing equations for two-phase turbulent flows based on "one-fluid formulation"
- Recognized the convective, viscous and surface tension unclosed terms
- Performed the order of magnitude analysis of these terms for different filters and filter size
  - Magnitude of the convective term depends on the interfacial scales in the flow.
- Scale-similarity model and computed the correlation coefficients $\rightarrow$ Good
- Overall $\Rightarrow$ Insights on choosing a filter, filter size, and the SGS model

Stanford University

THANK YOU

Acknowledgements:

Dr. Micheal Dodd

Aditya Ghate