Turbulence Modelling for Smoothed Particle Hydrodynamics



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Dual Degree Project (Stage I) - Presentation

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Introduction

Turbulent Flow

- Characterization
 - High Reynolds number flows
 - Random spatial & temporal velocity fluctuations
 - Rotational & 3D velocity field
 - Large mixing capacity of the flow
 - Chaotic nature of solutions

Modelling

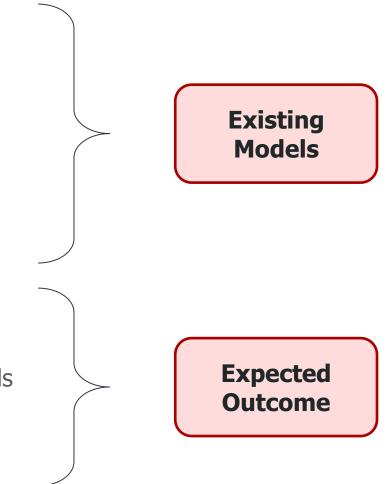
- Lacks analytical solutions except for simple cases
- CFD simulations required for complex flows
- Typical modelling techniques
 - Governing equations → Averaged or filtered
 - Closure problem → Fluctuating components modelled using mean flow properties
 - Stochastic methods
- Models mostly based on Eulerian framework

Lagrangian Modelling – SPH

- No background mesh
- Handles large deformations, complex boundary dynamics
- Simplified model implementation
- Highly & efficiently parallelizable

Project Objectives

- Turbulence Modelling in SPH
 - Lacks robust & accurate models
 - Shortcomings of current models:
 - Cannot be generalized to various types of turbulence-based problems
 - Issues in scaling to 3D turbulent flows
 - Accuracy & computational constraints
 - Boundary conditions & treatment not well established
- Project Objective
 - Review state of the art turbulence models in SPH
 - Provide advantages & disadvantages of the major categories of models
 - Extend promising models to robust & accurate SPH schemes^[1]
 - Analyze & study its performance in bounded turbulent flow
 - Improve overall scheme using recent developments of SPH



Project's Progress

- Surveyed research papers detailing work on turbulence models for SPH (c. 2000 – 2022)
- Classified 5 major categories of turbulence models
- o Identified a systematic, model-evaluation method
 - ☐ Benchmark problems feasible with SPH
 - Post-simulation analysis techniques

Artificial Viscosity Stochastic Implicit P-Poisson LES Turbulence **Explicit P-EOS** Models Lagrangian-LES **RANS** LANS

Turbulence Modelling

Viscosity-based Models

- Eddy Viscosity Model^[1]
 - One of the first classes of SPH turbulence models
 - Velocities are Reynolds-averaged
 - First-order closure model:
 - Reynolds stress tensor & mean velocity gradients
 - Turbulent eddy viscosity considered
 - Simulated Poiseuille flow ($Re = 6.4 \times 10^4$)
 - Comments
 - Reproduced log-law profile near walls
 - Appropriate for shear flows

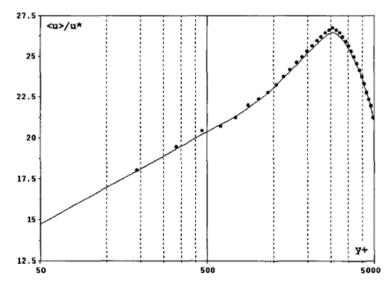


Fig: Computed mean velocity profile of turbulent Poiseuille flow in a pipe (Rep: Violeau et al)

$$\frac{\mathrm{D}\,\mathbf{v}_{i}}{\mathrm{D}\,t} = -\sum_{j} m_{j} \left(\frac{P_{i}}{\rho_{i}^{2}} + \frac{P_{j}}{\rho_{j}^{2}} + \widetilde{\Pi}_{ij} \right) \nabla_{i} W_{h,ij} + \mathbf{F}_{i}$$

$$\widetilde{\Pi}_{ij} = -8 \frac{\nu_{t,i} + \nu_{t,j}}{\rho_{i} + \rho_{j}} \frac{\langle \mathbf{v} \rangle_{ij} \cdot \mathbf{r}_{ij}}{|\mathbf{r}_{ij}|^{2} + \boldsymbol{\xi}^{2}}$$

$$\nu_{t} = L_{m}^{2} ||\underline{\boldsymbol{S}}||_{F} = L_{m}^{2} \sqrt{\langle \underline{\boldsymbol{S}}, \underline{\boldsymbol{S}} \rangle}$$

$$\nabla \langle \mathbf{v} \rangle_i = -\frac{1}{\rho_i} \sum_j m_j \langle \mathbf{v} \rangle_{ij} \otimes \nabla_i W_{h,ij}$$

Viscosity-based Models

- Generalized Langevin Model^[1]
 - Prescribed the particle velocity as a random process
 - Acceleration → Function of a random vector (noncorrelated with velocity)
 - \circ Simulated Poiseuille flow ($Re = 6.4 \times 10^4$)

- Mean operator appeared to behave like a LES filter
- Large deviations observed in mean velocity profile $(\propto k^{0.5})$
- Can be generalized to various types of turbulent flows, & not only shear flows

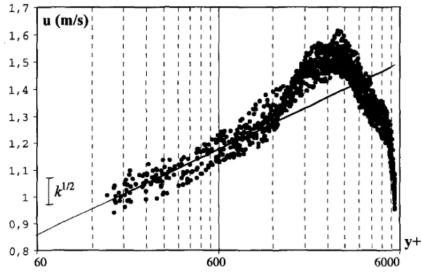


Fig: Computed mean velocity profile of turbulent Poiseuille flow in a pipe (Rep: Violeau et al)

$$\frac{\mathrm{D}\,\mathbf{v}_i}{\mathrm{D}\,t} = -\sum_j m_j \left(\frac{\langle P \rangle_i}{\rho_i^2} + \frac{\langle P \rangle_j}{\rho_j^2}\right) \nabla_i W_{h,ij} - \frac{1}{2} C_1 \frac{\epsilon_i}{k_i} \mathbf{v}_i' + C_2 \nabla \langle \mathbf{v} \rangle_i \cdot \mathbf{v}_i' + \sqrt{\frac{C_0 \epsilon_i}{\Delta t}} \vec{\xi}_i$$

$$\epsilon_i = 2\nu_{t,i} + ||\underline{\boldsymbol{S_i}}||_F^2$$

$$k_i = \frac{\epsilon_i \nu_{t,i}}{C_\mu} \quad , \quad C_\mu = 0.009$$

Viscosity-based Models

- Modified-SPH (mSPH)^[1]
 - Observation: Absence of viscosity → Noisy particle motion
 - Finite viscosity → Over-prediction of dissipation
 - Modified EOS & MOM eqs. → Particle distribution homogenised
 - Simulated:
 - 2D Taylor-Green Vortex (TGV) ($Re = \infty$, $N_i = 64^2$)
 - 3D Taylor-Green Vortex (TGV) (Re = 400, $N_i = 64^3$)

Fig: Velocity vector plot at t=2 (left) and t=30 (right). (Rep: Adami et al)

- Merging of vortices observed
- Energy cascade (Kolmogorv scale) slopes reproduced
 - mSPH (-3); standard SPH (1)
- Transitional flow simulated with reasonable dissipation rate
- mSPH ~ Eddy viscosity model below numerical resolution

- Implicit Pressure Poisson-based Models^[1,2]
 - Assumption: Incompressible flow
 - Navier-Stokes (NS) eqs. → Spatially filtered
 - Stress tensor → Closed using Boussinesq's hypothesis
 - Eddy viscosity → Estimated using modified Smagorinsky model
 - Model modified to include wall effects
 - Predictive-corrective time integrator
 - Requires implicit solution of pressure poisson eq
 - Simulated: $(Re \approx 10^6, N_i \approx 10^4)$
 - 2D wave interaction with partially immersed breakwater^[1]
 - 2D wave breaking on a beach^[2]

- Accurately tracked free surfaces with large deformation
- Surfaces did not exhibit numerical diffusion
- Scheme's accuracy: $O(\Delta t + \Delta x^{1.25})$

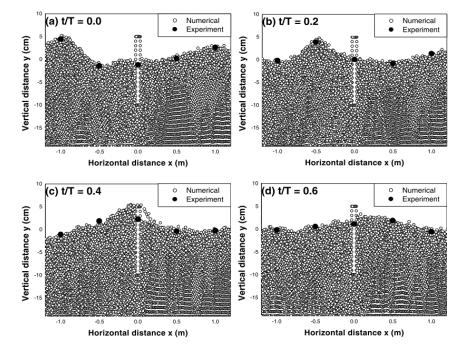


Fig: Time sequences of wave profile. (Rep: Gotoh et al)

$$\frac{\mathbf{D}\,\overline{\mathbf{v}}}{\mathbf{D}\,t} = -\frac{1}{\rho}\nabla\overline{P} + \nu\Delta(\overline{\mathbf{v}}) + \frac{1}{\rho}\nabla\cdot\underline{\boldsymbol{\tau}} + \mathbf{F}$$
$$\frac{1}{\rho}\underline{\boldsymbol{\tau}} = 2\nu_t\underline{\boldsymbol{S}} - \frac{2}{3}k\underline{\boldsymbol{I}}$$

$$\nu_t = \min(C_s \Delta x, \kappa d_{wall})^2 \sqrt{2\langle \underline{S}, \underline{S} \rangle}$$

$$\nabla \cdot \left(\frac{1}{\rho_*} \nabla \overline{P}_{t+1}\right) = \frac{\rho_o - \rho_*}{\rho_o \Delta t^2}$$

- Explicit Pressure EOS-based Models^[1,2]
 - Assumption: Compressible flow
 - NS eqs → Favre averaged
 - Observation: Density variations → Unphysical behaviour on free surfaces
 - Shepard filtering of density performed periodically
 - Simulated: $(Re \approx 10^6, N_i \approx 10^4)$
 - Weakly plunging breaker in 2D & 3D^[1]
 - 2D green-water overtopping, 2D & 3D wave breaking,
 3D dam break^[2]

- Model predicted regions of high vorticity in 2D
- Model captured vertically oriented eddies in 3D
- Accurate for flow separation or splash-based problems
- Requires large N_i & very small Δt
- Uncertain regarding scalability to large-scale problems

$$\frac{\mathrm{D}\,\overline{\rho}}{\mathrm{D}\,t} = -\overline{\rho}\nabla\cdot\widetilde{\mathbf{v}}$$

$$\frac{\mathrm{D}\,\widetilde{\mathbf{v}}}{\mathrm{D}\,t} = -\frac{1}{\overline{\rho}}\nabla\overline{P} + \frac{1}{\overline{\rho}}(\nabla\cdot\overline{\rho\nu}\nabla)\widetilde{\mathbf{v}} + \frac{1}{\overline{\rho}}\nabla\cdot\underline{\boldsymbol{\tau}} + \mathbf{F}$$

$$\underline{\boldsymbol{\tau}} = \overline{\rho} \left(2\nu_t \underline{\boldsymbol{S}} - \frac{2}{3} \operatorname{tr}[\underline{\boldsymbol{S}}] \underline{\boldsymbol{I}} \right) - \frac{2}{3} \overline{\rho} C_I \overline{\Delta}^2 \underline{\boldsymbol{I}}$$

$$\rho_i = \frac{\sum_j \rho_j W_{h,ij} \mathcal{V}_j}{\sum_j W_{h,ij} \mathcal{V}_j}$$

- Explicit Pressure EOS-based Models^[1]
 - Observation: Standard Smagorinsky model cannot enforce
 - Wall conditions
 - Non-vanishing stresses with laminar flows
 - Devised Wall-adapting local eddy viscosity model (WALE)
 - \circ Simulated an array of cylinders in 2D flow ($Re \approx 10^2$, $N_i \approx 10^4$)

- LCS captured reasonably well
- Observed merging of vortices to larger structures
- Interactions of vortices with opposing strengths → Vorticity cancellation
- Claim: Complex vortex interactions → Possible difficulty in interpreting the energy spectrum

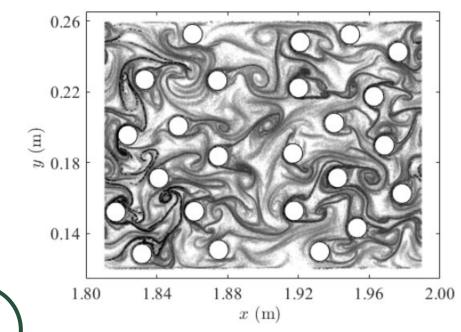


Fig: Backward-in-time FTLE field. (Rep: Canelas et al)

$$\nu_t = \rho (C_w \Delta x)^2 \frac{\langle \underline{S}^d, \underline{S}^d \rangle^{3/2}}{\langle \underline{S}, \underline{S} \rangle^{5/2} + \langle \underline{S}^d, \underline{S}^d \rangle^{5/4}}$$

$$\underline{\boldsymbol{S}^d} = \frac{1}{2} \left((\nabla \mathbf{v})^2 + \left((\nabla \mathbf{v})^T \right)^2 \right) - \frac{1}{3} \operatorname{tr}[(\nabla \mathbf{v})^2] \underline{\boldsymbol{I}}$$

- Explicit Pressure EOS-based Models^[1]
 - Reinterpret SPH → Lagrangian quadrature technique for explicit LES
 - ➤ Kernel scale limits SPH's physical resolution → Unsuitable DNS alternative
 - Navier-Stokes (NS) eqs. → Spatially filtered
 - Compared multiple Smagorinsky models
 - (standard, σ , MCG-form)
 - Simulated 3D TGV ($Re \approx 10^4$, $N_i = 200^3 500^3$)

- Smagorisnky models reduced averaged kinetic energy
- Dissipation rates not predicted accurately
- SPH can capture turbulence up to kernel scale (high cost)
- Explicit SGS models remove kinetic energy → Increases energy deficit of standard SPH
- "SGS models in SPH framework only degrade the quality of the subsonic turbulent flow approximation"[2]

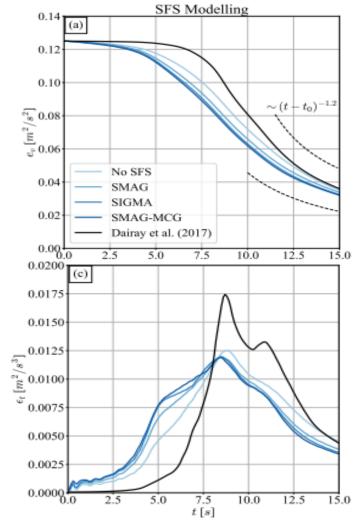


Fig: Density-weighted averaged kinetic energy (top), averaged dissipation rate (bottom). (Rep: Okraschevski et al)

Lagrangian LES-based Models

- Lagrangian form of LES^[1,2]
 - Assumption: Weakly compressible flow
 - Lagrangian filter φ (compact support, even) introduced
 - φ decomposed into independent spatial & temporal components
 - Governing eqs. written using spatially filtered terms
 - Temporal terms of higher order neglected
 - Continuity eq. closed using Fick-like diffusion term
 - MOM eq. closed using Yoshizawa-model for the stress tensor
 - Considered δ -SPH formulation
 - Simulated:
 - 2D TGV ($Re \approx 10^3 10^6$, $N_i \approx 10^3 10^6$)
 - 3D homogenous turbulence ($Re \approx 10^3$, $N_i = 64^3 256^3$)

- The model overcomes issues of spurious high-frequency noise & onset of tensile instability (High *Re* flows)
- The energy spectra agrees well with theoretical decay rate
- Wall functions need to be incorporated to deal with boundaries
- Higher-order approach can significantly improve the performance

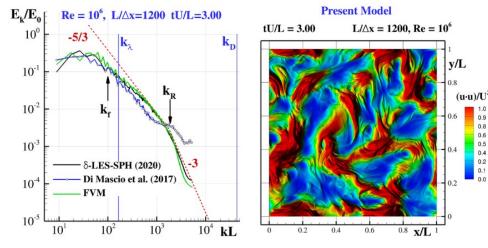


Fig: Energy spectrum (left), k field (right). (Rep: Colagrossi2021)

$$\frac{\overline{D}\,\widetilde{\rho}}{\overline{D}\,t} = -\widetilde{\rho}\langle\nabla\cdot\widetilde{\mathbf{v}}\rangle + C_1 + C_2$$

$$\frac{\overline{D}\,\widetilde{\mathbf{r}}}{\overline{D}\,t} = \widetilde{\mathbf{v}}$$

$$\widetilde{P} = F(\widetilde{\rho})$$

$$C_2 \approx \nabla\cdot(\nu_\delta\nabla\widetilde{\rho})$$

$$\frac{\operatorname{D}\widetilde{\mathbf{v}}}{\operatorname{D}t} = -\frac{\langle \nabla P \rangle}{\widetilde{\rho}} + \nu \langle \Delta(\widetilde{\mathbf{v}}) \rangle + (\lambda' + \nu) \langle \nabla(\nabla \cdot \widetilde{\mathbf{v}}) \rangle + M_1 + M_2$$
$$M_2 = \nabla \cdot \underline{\mathbf{T}}_l = \nabla \cdot \left(-\frac{k^2}{3} \underline{\mathbf{I}} - \frac{2}{3} \nu_t \operatorname{Tr}[\underline{\widetilde{\mathbf{S}}}] \underline{\mathbf{I}} + 2\nu_t \underline{\widetilde{\mathbf{S}}} \right)$$

^[1] A. Di Mascio, M. Antuono, A. Colagrossi, and S. Marrone, "Smoothed particle hydrodynamics method from a large eddy simulation perspective," Phys. Fluids, vol. 29, no. 3, 2017, doi: 10.1063/1.4978274.

^[2] A. Colagrossi, "Smoothed particle hydrodynamics method from a large eddy simulation perspective. Generalization to a quasi-Lagrangian model Smoothed particle hydrodynamics method from a large eddy simulation perspective. Generalization to a quasi-Lagrangian model," vol. 015102, no. December 2020, 2021, doi: 10.1063/5.0034568.

RANS-based $k - \epsilon$ **Models**

- $k \epsilon$ Models^[1,2]
 - Considered incompressible, unsteady RANS equations
 - Predictive-corrective time integrator
 - Requires implicit solution of pressure poisson eq
 - Simulated:
 - 2D wave breaking and overtopping of sloping wall^[1] ($Re \approx 10^6$, $N_i = 6000$)
 - 2D solitary wave propagating over a bottom-mounted barrier^[2] ($Re \approx 10^6$, $N_i \approx 1.3 \times 10^5$)

- Accurately tracks free-surfaces
- $k \epsilon$ coefficients (empirically derived from quasi-steady state) perform sub-optimally in transient flow
- Model requires a sensitivity analysis for the turbulence model
 & spatial resolution for improved performance
- Underpredicts max k & is sensitive to initial seeding of k
- Effects of viscous dissipation & numerical dissipation need to be balanced

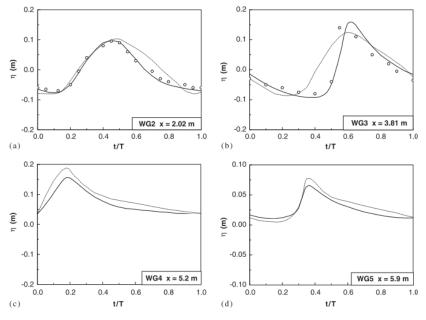


Fig: Water surface elevations. (Rep: Shao et al)c

$$\nu_t = c_d \frac{k^2}{\epsilon}$$

$$\frac{\mathrm{D}\,k}{\mathrm{D}\,t} = \nabla \cdot \left(\frac{\nu_t}{\sigma_k} \nabla k\right) + P_k - \epsilon$$

$$\frac{\mathrm{D}\,\epsilon}{\mathrm{D}\,t} = \nabla \cdot \left(\frac{\nu_t}{\sigma_\epsilon} \nabla \epsilon\right) + c_{1\epsilon} \frac{\epsilon}{k} P_k - c_{2\epsilon} \frac{\epsilon^2}{k}$$

$$P_k = 2\nu_t \langle \underline{S}, \underline{S} \rangle$$

LANS-based Models

- Lagrangian-averaged NS eqs. (LANS- α) Models^[1,2,3,4]
 - Lagrangian-averaging^[1]: Performed at the level of variational principle from which NS eqs. are derived
 - lacktriangleright α denotes scale of rapid fluctuations in the flow map
 - ∘ SPH- α model^[2] → Initial models based on LANS- α eqs.
 - Particle transport → Smoothed velocity
 - MOM eq. solved iteratively
 - ∘ SPH- ϵ model^[3,4] → Improvement of SPH- α model
 - Explicit MOM eq. with viscous term
 - Simulated 2D flow past a cylinder moving along a Lissajous curve^[4] $(Re \approx 10^3, N_i \approx 10^4)$

- Bounded (*no-slip*) flow implies v is neither periodic/isotropic → Author prefers correlation functions over energy spectrum
- Satisfactory results for velocity correlation functions, energy spectrum & mixing with half the particle resolution of DNS
- Flows with larger Reynolds numbers & other boundary conditions, such as free surfaces need to be studied

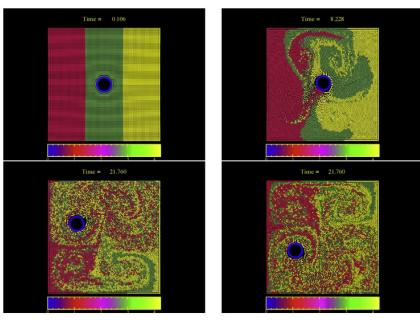


Fig: Stirring of coloured particles. (Rep: Monaghan2017)

$$\widehat{\mathbf{v}}_i = \mathbf{v}_i - \varepsilon \sum_j \frac{m_j}{M_o} \mathbf{v}_{ij} K_{h',ij}$$

^[1] J. E. Marsden and S. Shkoller, "Global well-posedness for the Lagrangian averaged Navier-Stokes (LANS-a) equations on bounded domains," Philos. Trans. R. Soc. A Math. Phys. Eng. Sci., vol. 359, no. 1784, pp. 1449–1468, 2001, doi: 10.1098/rsta.2001.0852

^[2] J. J. Monaghan, "SPH compressible turbulence," vol. 852, pp. 843–852, Apr. 2002, doi: 10.1046/j.1365-8711.2002.05678.x.

^[3] J. J. Monaghan, "A turbulence model for smoothed particle hydrodynamics," Eur. J. Mech. B/Fluids, vol. 30, no. 4, pp. 360–370, 2011, doi: 10.1016/j.euromechflu.2011.04.002. [4] J. J. Monaghan, "SPH-ε simulation of 2D turbulence driven by a moving cylinder," Eur. J. Mech. B/Fluids, vol. 65, pp. 486–493, 2017, doi: 10.1016/j.euromechflu.2017.03.011.

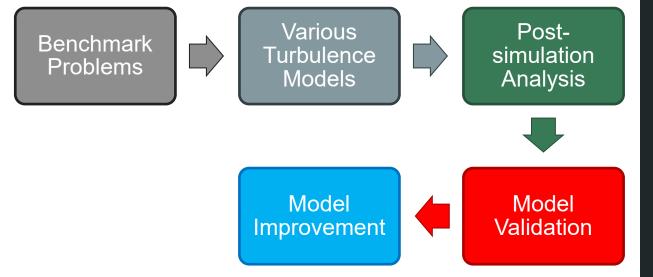
Miscellaneous Models

- Viscosity-based vorticity correction model^[1]
 - Aimed primarily towards benefiting the CGI community
 - Faster computational time & simplified system of equations
 - Research focuses more on visual artifacts of the flow, not quantified metrics
 - Builds on the fact that rotational kinetic energy ≤ translational kinetic energy

- Hybrid-SPH (hrSPH)^[2]
 - Particle data interpolated onto Eulerian mesh grids
 - Rate of change of flow properties computed on mesh grid
 - Updated mesh values interpolated onto particles
 - Advection of particles using the updated properties
 - Remeshing is performed when particles cluster to ensure uniform particle distribution
 - Information from the model cannot help improve traditional SPH schemes

^[2] A. Obeidat and S. P. A. Bordas, "Three-dimensional remeshed smoothed particle hydrodynamics for the simulation of isotropic turbulence," Int. J. Numer. Methods Fluids, vol. 86, no. 1, pp. 1–19, 2018, doi: 10.1002/fld.4405.

- Most of Lagrangian turbulent models → Tested for primarily complex, free-surface flows
- A systematic analysis of isotropic turbulence problems provides better insight on the energy spectrum & its cascade across varying length scales
- Appropriate bounded/periodic test cases must be used when analyzing turbulence
- Analyse results with appropriate metrics, and validate the results with experimental or numerical data from literature



Evaluation of Turbulence Models

Benchmark Problems

- Taylor-Green Vortex Problem → Periodic, incompressible flow
 - 2D Case: Analytical solutions known
 - 3D Case: Initial flow conditions can be specified
- Thin Double-Shear Layer
 - Flow under-resolved → Spurious structures are produced
 - Generation of the spurious structure depends on the scheme
- 3D Isotropic Turbulence^[1]
 - DNS dataset from the JHU Turbulence database Cluster
 - Dataset: Incompressible flow with isotropic and forced turbulence.
 - 1024³ spatial points & 1024 time samples spanning one large-scale turnover time
- 2D Confined & Driven Turbulence^[2]
 - 2D fluid confined to a square box enclosing a cylinder
 - Cylinder moves in a predetermined trajectory

Post-Simulation Analysis

- Energy spectral density
 - Velocity field over a grid generated using suitable interpolation of the particle velocity data^[1]
 - Fourier transform of the velocity field → Velocity spectrum as a function of the wave-number
 - Energy spectrum computed from the velocity spectrum
- Velocity gradient-based metrics
 - Iso-vorticity surfaces, Q-criterion, Δ-criterion, etc.
 - Most of the definitions for a vortex \rightarrow Not objective & suitable for studying the flow (esp. 3D flow)^[2]
- Lagrangian coherent structures (LCS)
 - Local velocity fluctuations do not induce noise in LCS
 - ∘ FTLE is formulated in the Lagrangian framework → Better identification of LCSs
 - Provides flexibility in its formulation^[3]
 - Backward-in-time FTLE can be computed using limited resources during run-time concurrently
 - Forward-in-time FTLE can only be computed during post-processing
 - Easily parallelizable

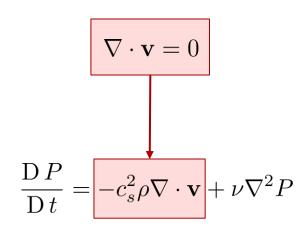
^[1] Y. Shi, X. X. Zhu, M. Ellero, and N. A. Adams, "Analysis of interpolation schemes for the accurate estimation of energy spectrum in Lagrangian methods," Comput. Fluids, vol. 82, pp. 122–131, 2013, doi: 10.1016/j.compfluid.2013.05.003.

^[2] G. Haller, "An objective definition of a vortex," J. Fluid Mech., vol. 525, pp. 1–26, 2005.

^[3] P. N. Sun, A. Colagrossi, S. Marrone, and A. M. Zhang, "Detection of Lagrangian Coherent Structures in the SPH framework," Comput. Methods Appl. Mech. Eng., vol. 305, pp. 849–868, 2016, doi: 10.1016/j.cma.2016.03.027.

Conclusion & Future Work

- Stage I outcome:
 - A reasonable compilation of past SPH turbulence models
 - The corresponding advantages, limitations & potential areas for refinement are understood
- Entropically Damped Artificial Compressibility (EDAC) scheme^[1] →
 Explicit incompressible SPH method
 - Uses a pressure evolution eq. instead of the continuity equation^[2]
 - Produces a smoother & accurate pressure distribution for flows, confined or free
 - Does not require artificial viscosity
- Turbulence Models for EDAC
 - Incompatible with RANS due to incompressibility condition
 - Will consider compressible EDAC scheme to devise a turbulence model
 - Lagrangian LES filtering of the pressure eq → Mixed filtered term obtained; cannot be decoupled further
 - Will investigate potential closure models to decouple/model the mixed term



$$\frac{\mathrm{D}\,\widetilde{P}}{\mathrm{D}\,t} = -c_s^2 \rho \nabla \cdot \widetilde{\mathbf{v}} + \nu \nabla^2 \widetilde{P} + \widetilde{\mathbf{v}} \cdot \nabla \widetilde{P} - \underbrace{\widetilde{\mathbf{v}} \cdot \nabla P}_{f(\widetilde{\mathbf{v}}, \widetilde{P})} \neq \widetilde{f(\mathbf{v}, P)}$$



Thank you!

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