

**INVESTIGATING SMALL SCALE  
TURBULENCE PROCESSES IN  
COMPRESSIBLE FLOWS USING GAS  
KINETIC METHOD AND MACHINE  
LEARNING**

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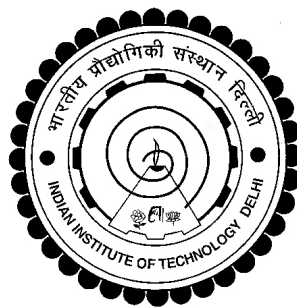
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## CERTIFICATE

This is to certify that the thesis entitled “**Investigating Small Scale Turbulence Processes in Compressible Flows using Gas Kinetic Method and Machine Learning**”, being submitted by **Nishant Parashar** to the Indian Institute of Technology Delhi for the award of the degree of **Doctor of Philosophy**, is a record of the bonafide research carried out by him which has been prepared under our supervisions in conformity with the rules and regulations of the Indian Institute of Technology Delhi. The research reports and results presented in the thesis has not been submitted for any degree or diploma in any other university or institute.

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## ABSTRACT

In a turbulent flow velocity field and its gradients at small scales are closely related to key nonlinear turbulence processes like mixing, intermittency, energy cascade, material element deformation, etc. Thus, the velocity gradient tensor has been a subject of fundamental interest. Various studies have been performed to understand the evolution of velocity gradients in turbulent flows primarily for incompressible flows. These studies have not only contributed to an improved understanding of small-scale motion in turbulent flows, but they have also helped in the development of useful turbulence closure models for incompressible flows. However, very limited studies have been performed for compressible flows.

Compressibility adds more complexity to the dynamics of velocity gradients due to the interaction of shock with turbulence processes. While in incompressible flows, the pressure field depends on the velocity field alone, in compressible turbulence pressure field depends on the temperature and density field as well. Further, in compressible turbulence a significant level of dilatation can exist, which is absent in incompressible flows. Hence, it becomes important to understand the influence of compressibility on the dynamics of velocity gradients.

To perform fundamental study of velocity gradient dynamics at small-scales, we need access to compressible turbulence data at varied Mach numbers and Reynolds numbers. However, very limited experimental data is available for compressible flows; thus there is a need to perform direct numerical simulation (DNS) of canonical compressible turbulent flows. To generate these canonical compressible turbulence datasets, an appropriate numerical scheme must be employed that can robustly handle the presence of extreme discontinuities in the flow-field. Further, these methods need to be ported on parallel computing platforms like graphical processing unit (GPU) clusters to perform high-fidelity DNS simulations.

The Lagrangian approach is known to be more insightful in understanding the dynamics of velocity gradients. However, it is very difficult to generate Lagrangian flow fields. Alternately, the Lagrangian field can also be produced with the help of simulated Eulerian field data and a Lagrangian particle tracker. Following this approach, we generate Lagrangian field data from DNS data of compressible turbulent flows and perform Lagrangian analysis of velocity gradients and its associated processes.

In recent years, machine learning-based techniques have evolved as a viable tool for discovering key relationships from data. Recently, data-driven techniques have become very popular in the turbulence community, motivated by the recent

success, which has led to improved accuracy of turbulence models assisted with machine learning. These machine learning methods can be of paramount importance in learning hidden physical mappings between velocity gradients and the processes governing its dynamics.

In this work, we identify three objectives towards both understanding of velocity gradient dynamics and modelling the governing processes:

1. Study A: GPU-accelerated DNS of compressible turbulence using GKM integrated with a Lagrangian particle tracker.
2. Study B: Lagrangian investigation of velocity gradients in compressible turbulence:
  - Study B1: Vorticity-strain rate dynamics.
  - Study B2: Lifetime of flow-field topologies.
  - Study B3: Evaluations of viscous models for velocity gradient dynamics in non-stationary turbulence.
3. Study C: Data-driven modelling of Pressure Hessian from velocity-gradient information using neural networks.

In Study A, we develop a direct numerical simulation (DNS) solver for isotropic compressible turbulent flow integrated with a Lagrangian particle tracker (LPT). The Lagrangian field data produced using this solver will be utilized for performing Lagrangian analysis of the velocity gradient tensor (Study B). Towards this goal, we first employ a variant of the gas kinetic method (GKM) called the Analytical gas kinetic method (AGKM) which has been recently developed by Xuan and Xu (2013). We extensively compare and evaluate DNS results against high-order accurate Navier–Stokes based DNS results of Honein and Moin (2004) and Samtaney *et al.* (2001) over a range of turbulent Mach numbers (0.3-0.5) and Reynolds number (30-175). Further, we evaluate the speed-up and scalability of AGKM on GPU platform using compute unified device architecture (CUDA) application programming interface (API) developed by NVIDIA.

We found that the AGKM scheme cannot simulate very high Mach number turbulent flows. To enhance the capability of the numerical solver to simulate high Mach number flows, we switch to GKM-WENO scheme developed by Kumar *et al.* (2013). Considering the computational requirements of the GKM-WENO scheme, we added distributed computing capability in our solver using message passing interface (MPI) along with CUDA for performing multi-node and multi-GPU computations on the IIT Delhi HPC cluster. At last, we integrate a cubic-spline based Lagrangian particle tracker (LPT) with the DNS code to save immense Lagrangian post-processing time (required for Study B).

In Study B1, we investigate the influence of compressibility on vorticity-strain rate dynamics. Well-resolved direct numerical simulations of compressible homogeneous isotropic turbulence performed over a cubical domain of  $1024^3$  are employed for this study. To identify the influence of compressibility on the time-dependent dynamics (rather than on the one-time flow field), we employ a well-validated Lagrangian particle tracker. The tracker is used to obtain time correlations between the instantaneous vorticity vector and the strain-rate eigenvector system of an appropriately chosen reference time. In this work, compressibility is parameterized in terms of both global (turbulent Mach number) and local parameters (normalized dilatation-rate and flow field topology).

Our investigations reveal that local dilatation rate significantly influence these statistics. In turn, these observed influences of dilatation rate are predominantly associated with rotation dominated topologies (unstable-focus-compressing, stable-focus-stretching). We find that an enhanced dilatation rate (in both contracting and expanding fluid elements) significantly enhances the tendency of the vorticity vector to align with the largest eigenvector of strain-rate. Further, in fluid elements where the vorticity vector is maximally misaligned (perpendicular) at the reference time, vorticity does show a substantial tendency to align with the intermediate eigenvector as well. Authors attempt to provide physical explanations of these observations (in terms of the moment of inertia and angular momentum) by performing detailed calculations following tetrads (approach of Chertkov *et al.* (1999) and Xu *et al.* (2011)) in a compressible flow field.

In Study B2, we perform Lagrangian investigations of the dynamics of velocity gradients in compressible decaying turbulence. Specifically, we examine the evolution of the invariants of the velocity gradient tensor. We employ well-resolved direct numerical simulations over a range of Mach number along with a Lagrangian particle tracker to examine trajectories of fluid particles in the space of the invariants of the velocity gradient tensor. This allows us to accurately measure the lifetimes of major topologies of compressible turbulence and provide an explanation of why some selective topologies tend to exist longer than the others. Further, the influence of dilatation on the lifetime of various topologies is examined. Finally, we explain why the so-called conditional mean trajectories (CMT) used previously by several researchers fail to predict the lifetime of topologies accurately.

In Study B3, we focus specifically on two models meant for the incumbent viscous process: the linear Lagrangian diffusion model (LLDM) and the recent fluid deformation closure model (RFDM). Performance of both the models have indeed been examined earlier, but most evaluations have been restricted to statistical stationary flow fields. In this work, we subject these models to further scrutiny in non-stationary turbulence. Our evaluation procedure (i) uses direct numeri-

cal simulation data of decaying isotropic (non-stationary) turbulence, (ii) follows identified fluid particles (the so-called Lagrangian evolution), (iii) uses both compressible and nearly incompressible flow fields. In nearly incompressible regime, the RFD model is found to be satisfactory, while the LLDM model overestimates viscous effects at late times. In the compressible regime, both the models show inadequacies. For compressible flows, we propose an alternative modelling strategy which shows improvement over both LLD and RFD models.

In Study C, we first demonstrate the limitations of the RFDM in estimating the pressure-Hessian. Further, we employ a tensor basis neural network (TBNN) developed by Ling *et al.* (2016) to model the pressure-Hessian from the velocity gradient tensor itself. The neural network is trained on high-resolution data obtained from direct numerical simulation (DNS) of isotropic turbulence at Reynolds number of 433 (JHU turbulence database, JHTD). The predictions made by the TBNN are tested against three different isotropic turbulence datasets at Reynolds number of 433 (JHTD) and 315 (UP Madrid turbulence database, UPMTD) and 70. The evaluation of the neural network output is made in terms of the alignment statistics of the predicted pressure-Hessian eigenvectors with the strain-rate eigenvectors for turbulent isotropic flow. Our analysis of the predicted solution leads to the discovery of ten unique coefficients of the normalized tensor basis of strain-rate and rotation-rate tensors, the linear combination over which accurately captures key alignment statistics of the pressure-Hessian tensor.

## सारांश

एक टर्बुलेंट फ्लो में वेग क्षेत्र और छोटे पैमानों पर इसके ग्रेडिएंट्स का निकटतम संबंध मुख्य नॉन लीनियर टर्बुलेंस प्रक्रियाओं जैसे मिक्सिंग, इंटरमिटेंसी, एनर्जी कैस्केड, मटेरियल एलिमेंट डीफॉर्मेशन आदि से होता है। इस तरह से, वेग ग्रेडिएंट टेंसर मौलिक रुचि का विषय है। मुख्य रूप से टर्बुलेंट फ्लो में वेग ग्रेडिएंट के विकास को समझने के लिए विभिन्न अध्ययन प्रस्तुत किये गये हैं। इन अध्ययनों ने न केवल एक बेहतर योगदान दिया है टर्बुलेंट प्रवाह में छोटे पैमाने पर गति को समझने के लिए, उन्होंने इनकंप्रेसिबल प्रवाह के लिए उपयोगी टर्बुलेंस मॉडल के विकास में भी सहायता की है। हालांकि, कम्प्रेसिबल प्रवाह के लिए बहुत सीमित अध्ययन किए गए हैं।

कंप्रेशन और टर्बुलेंस के साथ आपसी संबंध की वजह से वेग ग्रेडिएंट्स की गतिशीलता में अधिक जटिलता शामिल है। जहां इनकंप्रेसिबल प्रवाह में, दबाव क्षेत्र अकेले वेग क्षेत्र पर निर्भर करता है, कम्प्रेसिबल टर्बुलेंस दबाव क्षेत्र में तापमान और घनत्व क्षेत्र पर भी निर्भर करता है। इसके अलावा, संकुचित करने योग्य कम्प्रेसिबल में एक महत्वपूर्ण स्तर का फैलाव मौजूद हो सकता है, जो कम्प्रेसिबल प्रवाह में अनुपस्थित है। इसलिए, वेग ग्रेडिएंट्स की गतिशीलता पर कम्प्रेसिबिलिटी के प्रभाव को समझना महत्वपूर्ण हो जाता है।

छोटे पैमाने पर वेग ढाल की गतिशीलता का मौलिक अध्ययन करने के लिए, हमें विभिन्न मॉक संख्याओं और रेनॉल्ड्स नंबरों पर कंप्रेसिबल टर्बुलेंस डेटा तक पहुंच की आवश्यकता होती है। हालांकि, कम्प्रेसिबल प्रवाह के लिए बहुत सीमित प्रयोगात्मक डेटा उपलब्ध है; इस प्रकार, कम्प्रेसिबल टर्बुलेंट प्रवाह का डायरेक्ट न्यूमेरिकल सिमुलेशन करने की आवश्यकता है। इन कैनोनिकल कम्प्रेसिबल टर्बुलेंस डेटासेट को उत्पन्न करने के लिए, एक उपयुक्त संख्यात्मक योजना को नियोजित किया जाना चाहिए जो फ्लो-फील्ड में अत्यधिक असंतोष की उपस्थिति को मजबूती से संभाल सके। इसके अलावा, इन विधियों को उच्च-निष्ठा सिमुलेशन सिमुलेशन प्रदर्शन करने के लिए ग्राफिकल प्रोसेसिंग यूनिट क्लस्टर जैसे समानांतर कंप्यूटिंग प्लेटफार्मों पर पोर्ट किए जाने की आवश्यकता है।

लैंग्रेजियन दृष्टिकोण को वेग ग्रेडिएंट्स की गतिशीलता को समझने के लिए अधिक व्यावहारिक माना जाता है। हालांकि, लैंग्रेजियन प्रवाह फ़ील्ड को जनरेट करना बहुत मुश्किल है। वैकल्पिक रूप से, लैंग्रेजियन फ़ील्ड को सिम्युलेटेड यूलरियन फ़ील्ड डेटा और लैंग्रेजियन पार्टिकल ट्रैकर की सहायता से भी उत्पादित किया जा सकता है। इस दृष्टिकोण के बाद, हम संपीड़ित अशांत प्रवाह के डायरेक्ट न्यूमेरिकल सिमुलेशन (डीएनएस) डेटा से लैंग्रेजियन क्षेत्र डेटा उत्पन्न करते हैं और वेग ढाल और इसके संबंधित प्रक्रियाओं का लैंग्रेजियन विश्लेषण करते हैं।

हाल के वर्षों में, मशीन लर्निंग-आधारित तकनीक डेटा से महत्वपूर्ण संबंधों की खोज के लिए एक व्यवहार्य उपकरण के रूप में विकसित हुई है। हाल ही में, मशीन लर्निंग-आधारित तकनीक की सफलता से प्रेरित, टर्बुलेंट समुदाय में डेटा चालित तकनीक बहुत लोकप्रिय हो गई है, जिससे मशीन लर्निंग से सहायता लेने वाले टर्बुलेंट मॉडल की सटीकता में सुधार हुआ है। ये मशीन लर्निंग के तरीके से वेग ग्रेडिएंट्स और इसकी गतिशीलता को नियंत्रित करने वाली प्रक्रियाओं के बीच छिपे हुए भौतिक मानचित्रण सीखने में सबसे महत्वपूर्ण हो सकते हैं।

इस कार्य में, हम तीन अध्ययनों (स्टडी ए, बी और सी) की पहचान करते हैं, जो कि वेग ग्रेडिएंट डायनेमिक्स की समझ और शासी प्रक्रियाओं को मॉडलिंग करते हैं। अध्ययन ए में, हम आइसोट्रोपिक कंप्रेसिबल टर्बुलेंट प्रवाह के लिए एक लैंग्रेजियन कण ट्रैकर (एलपीटी) के साथ डीएनएस को एकीकृत विकसित करते हैं। इस सॉल्वर के उपयोग से उत्पादित लैंग्रेजियन फ़ील्ड डेटा का उपयोग वेग ग्रेडिएंट टेंसर (स्टडी बी) के लैंग्रेजियन विश्लेषण के लिए किया जाएगा। हम उच्च-क्रम सटीक नवियर-स्टोक्स आधारित परिणामों के विरुद्ध डीएनएस परिणामों की बड़े पैमाने पर तुलना और मूल्यांकन करते हैं। इसके अलावा, हम कम्प्यूटरीकृत डिवाइस आर्किटेक्चर एप्लिकेशन प्रोग्रामिंग इंटरफेस का उपयोग करके ग्राफिकल प्रोसेसिंग यूनिट प्लेटफॉर्म पर हमारे सॉल्वर की गति और मापनीयता का मूल्यांकन करते हैं। अंत में, हम डीएनएस कोड के साथ एक

क्यूब-स्प्लिन आधारित लैंग्रेजियन पार्टिकल ट्रैकर को एकीकृत करते हैं जो अपार लेंग्रेजियन पोस्ट-प्रोसेसिंग समय बचाता है।

अध्ययन बी १ में, हम वोर्टिसिटी-स्ट्रेन-रेट की गतिशीलता पर संपीड़ितता के प्रभाव की जांच करते हैं। हम तात्कालिक वोर्टिसिटी वेक्टर और एक उचित रूप से चुने गए संदर्भ समय के स्ट्रेन-रेट एंगेक्टर प्रणाली के बीच समय सहसंबंध प्राप्त करते हैं। हम टर्बुलेंट मॉक संख्या और सामान्यीकृत डाइलेटेशन-रेट और प्रवाह क्षेत्र टोपोलॉजी के संदर्भ में कम्प्रेसिबिलिटी को समझते हैं। हमारी जांच से पता चलता है कि स्थानीय डाइलेटेशन-रेट की दर चयनित टोपोलॉजी के लिए इन आंकड़ों को काफी प्रभावित करती है। हम एक संक्षिप्त प्रवाह क्षेत्र में टेट्राद दृष्टिकोण के बाद विस्तृत गणना करके इन टिप्पणियों (जड़ता और कोणीय गति के क्षण के संदर्भ में) के भौतिक स्पष्टीकरण प्रदान करने का प्रयास करते हैं।

स्टडी बी २ में, हम कम्प्रेसेबल डिफ्यूजिंग टर्बुलेंस में वेग ग्रेडिएंट्स की गतिशीलता की लैंग्रेजियन जांच करते हैं। विशेष रूप से, हम वेग ग्रेडिएंट टेंसर के इनवेरिएंट्स के विकास की जांच करते हैं। हम वेग ग्रेडिएंट टेंसर के इनवेरिएंट्स के अंतरिक्ष में द्रव कणों के प्रक्षेपवक्र की जांच करते हैं। यह हमें संपीड़ित अशांति के प्रमुख टोपोलॉजी के जीवनकाल को सटीक रूप से मापने की अनुमति देता है और कुछ चयनात्मक टोपोलॉजी दूसरों की तुलना में लंबे समय तक मौजूद रहने की व्याख्या प्रदान करता है। इसके अलावा, विभिन्न टोपोलॉजी के जीवनकाल पर पड़ने वाले प्रभाव की जांच की जाती है। अंत में, हम बताते हैं कि क्यों कई शोधकर्ताओं द्वारा पहले इस्तेमाल किए गए तथाकथित कंडिशनड मीन ट्राजेक्टोरिस (सीएमटी) टोपोलॉजी के जीवनकाल की सटीक अनुमान लगाने में विफल रहते हैं।

स्टडी बी ३ में, हम विशेष रूप से असाध्य विस्कस प्रक्रिया के लिए दो मॉडल पर ध्यान केंद्रित करते हैं: लीनियर लैंग्रेजियन डिफ्यूजेंट मॉडल (एलएलडीएम) और हाल ही में रीसेंट फ्लूइड डेफॉर्मेशन क्लोज़र मॉडल (आरएफडीएम)। हम इन मॉडलों को गैर-स्थिर टर्बुलेंस में जांच के अधीन करते हैं। हम पाते हैं कि कम्प्रेसिबिलिटी के प्रभाव में, दोनों मॉडल अपर्याप्तता दिखाते हैं। कम्प्रेसिबिलिटी के प्रभाव को समझने के लिए, हम एक वैकल्पिक मॉडलिंग रणनीति का प्रस्ताव करते हैं जो एलएलडी और आरएफडी दोनों मॉडल में सुधार दिखाता है।

अध्ययन सी में, हम पहली बार प्रेशर-हैसियन का आकलन करने में आरएफडीएम की सीमाओं को प्रदर्शित करते हैं। इसके अलावा, हम एक टेंसरल बेसिस न्यूरल नेटवर्क को नियोजित करते हैं, जो कि वेग ग्रेडिएंट टेंसर से ही प्रेशर-हैसियन को मॉडल करता है। तंत्रिका नेटवर्क को ४३३ के रेनॉल्ड्स संख्या में आइसोट्रोपिक टर्बुलेंस के प्रत्यक्ष डीएनएस से प्राप्त उच्च-रिज़ॉल्यूशन डेटा पर प्रशिक्षित किया जाता है। टेंसरल बेसिस न्यूरल नेटवर्क आउटपुट का मूल्यांकन पूर्वानुमानित प्रेशर-हैसियन एंगेक्टर के संरेखण आंकड़ों के संदर्भ में किया जाता है। हमारे विश्लेषण से स्ट्रेन-रेट और रोटेशन-रेट टेन्सर्स के सामान्यीकृत दस अद्वितीय गुणांक की खोज होती है, रैखिक संयोजन जिस पर प्रेशर-हैसियन टेंसर के प्रमुख संरेखण आंकड़ों को सटीक रूप से प्रस्तुत करता है।

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