Extension of Unified Gas Kinetic Scheme for handling complex geometries and turbulent flows

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Certificate

This is to certify that the thesis entitled **"Extension of Unified Gas Kinetic Scheme for handling complex geometries and turbulent flows"**, being submitted by **Lokesh Kumar Ragta** 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

Many engineering applications involving complicated geometries often encounter flows in more than one regime viz: continuum, slip, transition and rarefied such as re-entry vehicles, flows in micro-channels, thruster-plumes etc. These flow situations demand the development of accurate and robust numerical techniques which can seamlessly simulate flows in different regimes. The Unified Gas Kinetic Scheme (UGKS) is a potential technique with an ability of seamlessly solving flows from the hydrodynamic regime to free molecular flow regime.

Although UGKS has the ability to simulate flows corresponding to various Knudsen numbers, its recent applications have been limited to simulate canonical flow problems only. This is due to the reason that UGKS is computationally expensive both in terms of time and substantial memory requirements. Moreover, UGKS has primarily been developed for structured meshes and has not been systematically developed for simulating flows past complicated geometries. A final lacuna that remains in extending UGKS to practical flows is the lack of any validation for its applicability to turbulent flows.

The overarching aim of the current thesis is to remove the above mentioned limitations of UGKS, enable it to handle flow past complicated geometries at various Knudsen numbers and extend its application to simulate turbulent flows. Both these require, in turn, the development of a parallelization strategy for UGKS. Accordingly, the thesis first focuses on developing an efficient parallelisation technique for UGKS using an application programming interface called message passing interface (MPI). The MPI based parallelisation procedure developed in this work utilises a three dimensional domain de-

composition technique called the cubic decomposition. The parallel 3D UGKS solver is first validated by simulating both the 2D and 3D laminar flows. Thereafter, it is used to perform the direct numerical simulation of turbulent flows. The numerical results demonstrate that with efficient parallelisation, UGKS can be used to simulate even the turbulent flows.

The thesis then focuses on simulating the flow past complicated geometries in different regimes. This is achieved by combining the UGKS solver with a suitably derived Cartesian Grid Method (CGM) and developing a novel UGKS-CGM solver. The CGM presented here satisfies the boundary conditions at wall by using a constrained least square interpolation procedure. Moreover, it differs from the usual, continuum Cartesian Grid Methods in two ways. Firstly, in order to capture the non-continuum effects at the boundaries, the CGM used herein interpolates the microscopic velocity distribution function in addition to the macroscopic variables. Secondly, even for the macroscopic variables, a gas-kinetic method based density interpolation procedure is used at the boundaries which allows the CGM to interface well with the UGKS method. The method is then tested for its robustness and efficacy by using it to simulate flows past arbitrary shaped immersed boundaries at various Knudsen numbers ranging from continuum to transition regimes. The numerical results demonstrates that the newly developed UGKS-CGM solver is capable of simulating viscous, compressible flows (with intermediate Mach numbers) upto transition regime quite well. In summary, the development of a parallelization strategy, a Cartesian grid methodology for complex geometries, and demonstration of applicability to turbulent flows, in conjunction, are expected to aid in the application of UGKS to practical flow scenarios.

सार

जटिल ज्यामितियों से जुड़े कई अभियांत्रिकी अनुप्रयोग अक्सर ऐसे होते हैं जिनमे द्रव एक से अधिक रिजीम में प्रवाह करता है अर्थात: सातत्य. स्लिप, संक्रमण और कम घना जैसे कि पुनः प्रवेश वाहन, सूक्ष्म-चैनलों में प्रवाह, थ्रस्टर प्लूम आदि। ये प्रवाह स्थितियां ऐसे संख्यात्मक तकनीकों के विकास की मांग करती हैं जो विभिन्न द्रवों के प्रवाह को सटीकता से सीमांकित कर सकें। यूनिफाइड गैस काइनेटिक स्कीम (यूजीकेएस) एक ऐसी संभावित तकनीक है जो द्रव प्रवाह को हाइड्रोडायनामिक रिजीम से स्वतंत्र आणविक रिजीम तक एकीकृत तरीके से सुलझाने की क्षमता रखती है।

यद्यपि यूजीकेएस विभिन्न नुड्सन संख्याओं के अनुरूप प्रवाह को अनुकरण करने की क्षमता रखती है, इसके हाल के अनुप्रयोग केवल वैमानिक प्रवाह समस्याओं को अनुकरण करने तक ही सीमित हैं। इसका कारण यह है कि यूजीकेएस समय और पर्याप्त मेमोरी आवश्यकताओं के मामले में कम्प्यूटेशनल रूप से महंगा है। इसके अलावा, यूजीकेएस मुख्य रूप से संरचित जाल के लिए विकसित किया गया है और जटिल ज्यामितियों के ऊपर बहने वाले द्रव प्रवाह के अनुकरण के लिए व्यवस्थित रूप से विकसित नहीं हुआ है। व्यावहारिक प्रवाह के लिए यूजीकेस को विस्तारित करने के लिए एक अंतिम कमी है इसकी प्रयोज्यता को अशांत प्रवाह के अनुकरण के लिए सिद्ध करना।

वर्तमान थीसिस का व्यापक उद्देश्य यूजीकेस की उपर्युक्त सीमाओं को दूर करना है, इसे विभिन्न नुड्सन संख्याओं पर जटिल भौमितिकी पर बहने वाले द्रव प्रवाह को संभालने के लिए सक्षम बनाना है और इसकी प्रयोज्यता को अशांत प्रवाह के अनुकरण के लिए विस्तार करना है। इन दोनों उद्देश्यों की आवश्यकता है यूजीकेएस के लिए एक समानांतर रणनीति का विकास। तदनुसार, थीसिस पहले एक संदेश प्रोग्रामिंग अंतरफलक (एमपीआई) नामक एक प्रोग्रामिंग इंटरफ़ेस का उपयोग करते हुए यूजीकेएस के लिए एक कुशल समानांतर तकनीक विकसित करने पर केंद्रित है। इस काम में विकसित की गई एमपीआई आधारित समानांतर प्रक्रिया तीन अपघटन तकनीक का इस्तेमाल करती है जिसे घनीय अपघटन कहा जाता है। समानांतर तीन आयामी यूजीकेएस सॉल्वर को पहले दो आयामी और तीन आयामी पटलीय प्रवाहों का अनुकरण करके मान्य किया गया है। इसके बाद इसे अशांत

प्रवाहों का प्रत्यक्ष संख्यात्मक अनुकरण करने के लिए प्रयोग किया गया है। संख्यात्मक परिणाम दर्शाते हैं कि कुशल समांतरता के साथ यूजीकेएस का इस्तेमाल भी अशांत प्रवाह को अनुकरण करने के लिए किया जा सकता है।

इसके बाद थीसिस अलग-अलग जटिल ज्यामितियों पर द्रव प्रवाह का अनुकरण करने पर केंद्रित है। यह उद्देश्य यूजीकेएस सॉल्वर को एक उपयुक्त रूप से व्युत्पन्न कार्टेशियन ग्रिड विधि (सीजीएम) के साथ जोड़कर और एक यूजीकेएस-सीजीएम सॉल्वर विकसित करके प्राप्त किया गया है। यहां प्रस्तुत सीजीएम दीवार पर सीमा की शर्तों को एक सीमित कम से कम वर्ग प्रक्षेप प्रक्रिया का उपयोग करके संतुष्ट करता है। इसके अलावा, यह सामान्य, सातत्य कार्टेशियन ग्रिड तरीके से दो तरह से अलग है। प्रथम, सीमाओं पर गैर-सातत्य प्रभावों को अधिकृत करने के लिए यहां प्रयोग किए जाने वाला सीजीएम मैक्रोस्कोपिक वेरिएबल्स के साथ-साथ माइक्रोस्कोपिक वेग डिस्ट्रिब्यूशन फ़ंक्शन को भी इंटरपोलेट करता है। दूसरा, इस तकनीक में सीमाओं पर भी मैक्रोस्कोपिक वैरिएबलस के लिए एक गैस-गतिज विधि आधारित घनत्व प्रक्षेप प्रक्रिया का उपयोग किया जाता है जो कि सीजीएम को यूजीकेएस विधि के साथ अच्छी तरह अंतराफलक करने की अनुमति देता है। इसके बाद यूजीकेएस-सीजीएम विधि की प्रभावकारिता को अलग-अलग नुड्सन संख्याओं पर विभिन्न आकार के विसर्जित सीमाओं पर द्रव प्रवाह को सातत्य से लेकर संक्रमण रिजीम तक अनुकरित करके प्रस्तुत किया गया है। संख्यात्मक परिणाम दर्शाते हैं कि नव विकसित यूजीकेएस-सीजीएम सॉल्वर चिपचिपा, संपीड़ित प्रवाह (मध्यवर्ती माक संख्याओं के साथ) संक्रमण प्रणाली तक अनुकरण करने में सक्षम है। संक्षेप में, यूजीकेएस के लिए एक समानांतर रणनीति का विकास, जटिल ज्यामितियों के लिए एक कार्टेशियन ग्रिड पद्धति, और अशांत प्रवाहों के लिए यूजीकेएस की प्रयोज्यता का प्रदर्शन संयोजक रूप से यूजीकेएस को व्यावहारिक प्रवाह परिदृश्यों के उपयोग में सहायक सिद्ध होंगे।

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List of Acronyms

API	=	Application Programming Interface
BC	=	Boundary Condition
BGK	=	Bhatnagar-Gross-Krook
CFD	=	Computational Fluid Dynamics
CGM	=	Cartesian Grid Method
CPU	=	Central Processing Unit
DNS	=	Direct Numerical Simulation
DOM	=	Discrete Ordinate Method
DSMC	=	Direct Simulation Monte Carlo
DVM	=	Discrete Velocity Method
ES-BGK	=	Ellipsoidal Statistical Bhatnagar-Gross-Krook
FDM	=	Finite Difference Method
FEM	=	Finite Element Method
FVM	=	Finite Volume Method
GKM	=	Gas Kinetic Method
GPU	=	Graphics Processing Unit
HS	=	Hard Sphere
IBM	=	Immersed Boundary Method
IP	=	Information Preserving
KFVS	=	Kinetic Flux Vector Splitting
LES	=	Large Eddy Simulation

MD	=	Molecular Dynamics
MPI	=	Message Passing Interface
NS	=	Navier-Stokes
OpenMP	=	Open Multiprocessing
PDE	=	Partial Differential Equation
RAM	=	Random Access Memory
RANS	=	Reynolds-Averaged Navier-Stokes
UGKS	=	Unified Gas Kinetic Scheme
VHS	=	Variable Hard Sphere