

行政院國家科學委員會補助專題研究計畫期末報告

常壓射頻電容耦合式電漿束之研究(三年)

Development and Characterization of an Atmospheric-pressure Capacitively Coupled Plasma Jet (3 Years)

計畫類別：☒個別型計畫 ☐整合型計畫

計畫編號：NSC-96-2628-E-009-134-MY3

執行期間：96 年 08 月 01 日至 99 年 07 月 31 日

計畫主持人：吳宗信

計畫參與人員：江明鴻 林逸民 洪捷榮 國立交通大學機械
工程學系

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執行單位：國立交通大學機械工程學系

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中文摘要

在過去十年中，大氣電漿逐漸替代低壓電漿作為材料表面處理的應用。其重要性是由於它相對低廉的設備費用，及更容易的操作條件和在更高的靈活性在工業上的應用。其中已經發展的大氣電漿源之中，又以非熱平衡『常壓射頻電容耦合式電漿束』(簡稱常壓電漿束)引起了最多注意。主要乃因為其應用範圍相當廣闊，包括半導體製程光阻去除，清潔，消毒，表面改質，生醫殺菌和薄膜沈積等等，相當廣泛。

本文報告本計畫三年的研究成果。在前兩年主要針對射頻電漿源 (13.56 MHz) 實驗參數特性量測。除傳統氬氣部分亦加入價格較低氬氣做研究分別在電性，光譜，PIV流場量測及2D軸對稱模擬，以便應用部分能更清楚。第三年，在表面處理及表面鍍膜應用以pp film 及SiO₂鍍膜部分探討，在SiO₂鍍膜部分克服氬氣加少許比例氧氣不穩問題，使鍍膜特性調控參數大幅增加。另外針對大面積應用本實驗室另發展以氬氣及空氣為主的平板型介電質常壓電漿束，使用中低頻 (20-60 kHz) 交流電源供應器，解決目前以多支圓管型常壓電漿束使用在大面積不均勻問題，尤其在滅菌及表面清潔使用上，配合所研發的平行模擬程式可以將氬氣電漿電漿特性預測其電流波型，對於透過預測活化基 (radical) 分佈可以更了解應用上電漿應用的機制。

關鍵字：常壓電漿束，氬氣，氬氣，氬氣，空氣，流體數值模擬。

Abstract

In this proposed three-year project, we intend to develop and systematically characterize a non-thermal atmospheric-pressure capacitively coupled plasma jet (APPJ), which is able to generate reactive atoms or radicals of practical interest. Interested radicals may include oxygen- (electronegative) and

nitrogen-based (electropositive) species, which have tremendous practical applications. Research approaches include both experiments and modelings.

In the first two years, in the *experimental part* in the earlier stage we focusdc on examining the post-glow fluid dynamics, plasma physics and chemistry by varying all kinds of test conditions. In later stage, we will shift our focus to study the effects of the discharge by pure helium, pure argon and adding oxygen into the helium. Mechanism of introducing oxygen into the discharge, how to extend the downstream distance of the “alive” reactive oxygen atoms, and increase the oxygen atoms are the three most important tasks. In addition to all the measurements in the first year, distribution of the species concentrations, especially the oxygen atoms, were measured in the post-glow region using the OES system.

Keywords: atmospheric-pressure plasma jet, helium, argon, nitrogen, air, fluid modeling.

一、計畫背景說明

低壓電漿已經在表面改質及半導體製程有廣泛的應用，其優點是在低壓環境產生大量高化學反應活化基及離子相對傳統必須高溫環境才可產生相同反應，對於材料應用有相對優點。最近十年來常壓電漿 (atmospheric-pressure) 吸引許多人的投入[see References in 2000-2005]因為其相對不需如低壓電漿需要昂貴真空設備及為維護成本，針對工業生產線需要連續線生產，常壓電漿有相對優勢[Schutze *et al.*, 1998; Becker *et al.*, 2004; Moravej *et al.*, 2004; 2005a; 2005b; 2006]。但針對電漿反應機制透過模擬及實驗相互驗證的研究團隊，相對少之又少。所以希望透過此計畫能以射頻電源供應器 (13.56 MHz) 常壓電漿束為研究方向，逐步從實驗參數測試及最佳化 (電性，光譜，熱流場)，模擬電漿反應機制，表面改質及鍍膜應用，提供工業界有興趣研發常壓電漿設備作為其參考。另外針對大面積應用本實驗室另發展以氬

氣及空氣為主的平板型介電質常壓電漿束，使用中低頻 (20-60 kHz) 交流電源供應器，解決目前以多支圓管型常壓電漿束使用在大面積不均勻問題，尤其在滅菌及表面清潔使用上，配合所研發的平行模擬程式可以將氮氣電漿電漿特性預測其電流波型，對於透過預測活化基 (radical) 分佈可以更了解應用上電漿應用的機制。

第一年，在實驗部分，我們設計建立和驗證基本常壓電漿束設備。基本先以氦氣及氬氣或是兩者混合氣體做為量測實驗參數定義(電壓-電流、電流-功率參數關係)。我們將在常壓電漿束出口位置使用幾種量測方式定義電漿特性。這幾種量測方式包括使用粒子影像測速儀(PIV)量測速度；使用熱電偶線量測溫度分佈。另外在電漿系統數值模擬部份中我們以流體模擬數值技(fluid modeling)術預測電漿密度及電子溫度分佈。

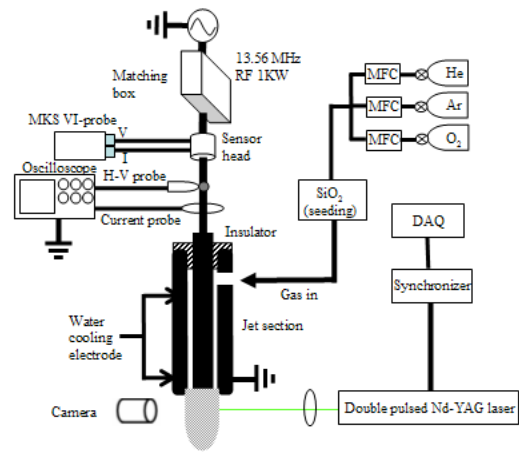
第二年，在實驗部分中，早期焦點放在改變各種測試條件下量測其電漿束出口處電漿相關的流體，化學及物理性質；後期再將焦點放在加入氧氣到原先氬氣與純氦及純氬比較對電漿性質的影響。並分別把氧氣加入常壓電漿束之機制，於出口區域延長自由基氧原子存活距離及增加其成份作為三個重要研究任務。除了重複第一年的量測外，在常氣電漿束出口位置針對不同氣體電漿使用光譜儀(OES)量測自由基原子種類及強度最後針對高分子材料PP film進行表面處理，得到良好親水性結果。

第三年，在實驗部分中，繼續針對現在抗磨損膜二氧化矽薄膜沉積 (deposition) 作研究，因為用氬氣作為電漿工作氣體配合以六甲基二矽氧烷 (HMDSO) 作為前驅物 (precursor)，初步結果發現若加入少許氧氣於氬氣電漿中可以影響SiO₂鍍膜特性。關於氬氣電漿中加入氧氣使電漿不穩定部分，已可以完全克服。

另外過去三年中亦針對工業上大面積應用，本實驗室另發展以氬氣及空氣為主的平板型介電質常壓電漿束解決目前以多支圓管型常壓電漿束使用在大面積不均勻問題，使用20-60 kHz交流(quasi-pulsed) 電源供應器應用在滅菌及表面清潔，所發展模擬程式(fluid modeling)可以了解氮氣電漿電漿內活化基 (radical) 的分佈情形。因為活化基的種類及強度分佈對實際工業應用上佔了主要影響，電子及離子離開電場後在後放電區域的應用相對活化基強度相對低了許多。

二、研究成果

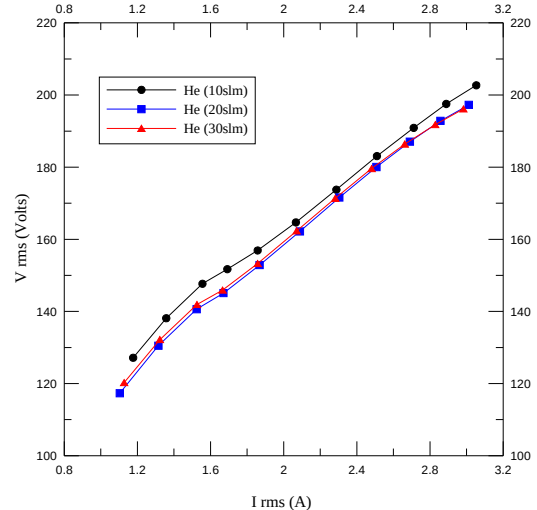
圖一為射頻常壓電漿同軸管使用 PIV 量測流場及相關電性量測設備示意圖。內電極為金屬材料外徑 12 mm，連接 RF power，外電極為金屬材料內徑 14.4 mm，電極間隙為 1.2 mm。另外在第二年使用外電極無冷卻設計內電極外徑 3 mm，外電極內徑 5 mm，電極間隙為 1mm。More details can be found in the midterm report of the 1st year and the 2nd year.



圖一 射頻常壓電漿束設備圖

(一) 同軸管 He、Ar 電漿流量對放電特性影響

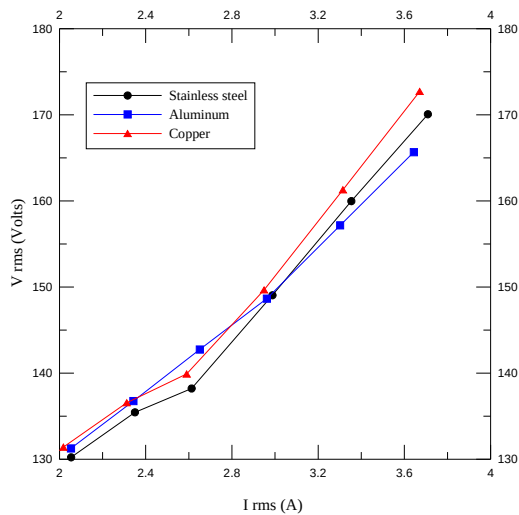
圖二表示氬氣電漿電壓與電流的關係，流量對氬氣電漿電性影響差異不大，而氦氣電漿則有些許差異，但整體而言流量對兩種氣體電性影響還是很小。除此之外，在相同電流下，氬氣的崩潰電壓較氦氣為高與文獻資料相符。



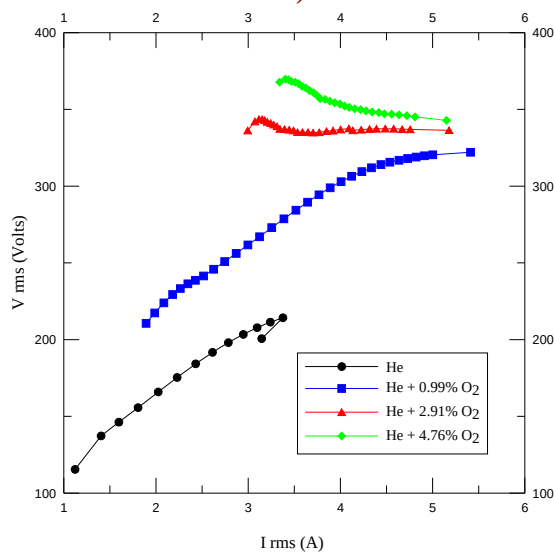
圖二 氣體流量改變其電壓與電流的關係(氬氣)

(二) 同軸圓管電極材料對電漿電性影響

圖三表示在流量 30 slm 氬氣電漿條件下，改變不同內電極金屬材料其電壓與電流關係。結果顯示內電極材料材料改變對電性影響很小，然而在較高電流操作條件有些許差異。所以下面文章敘述如特別說明外，測試條件均以紅銅作為內外電極材料。



圖三 電極材料改變其電壓與電流的關係 (Ar, 30 slm)



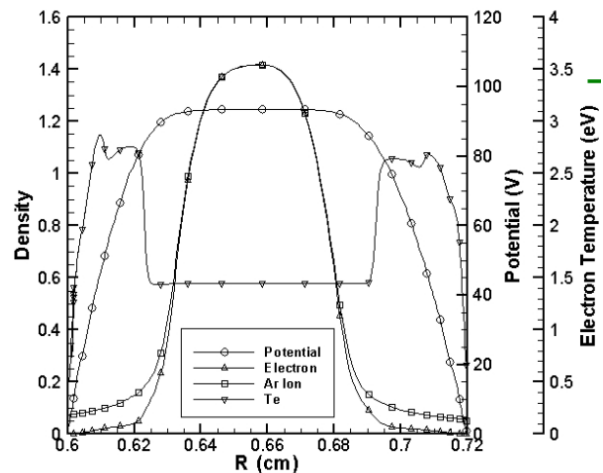
圖四 氬氣電漿加入不同氧氣濃度其電壓與電流的關係 (10 slm)

(三) 同軸圓管 He 與 O₂ 比例對電漿電性影響

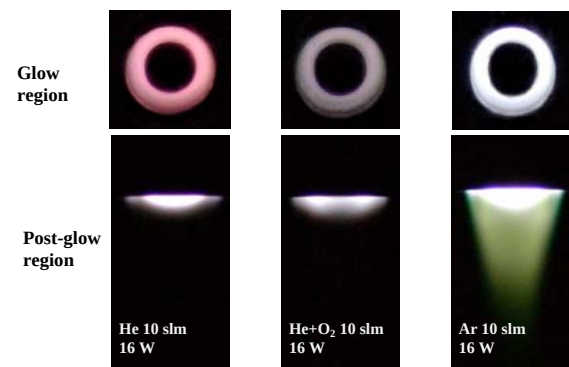
圖四表示流量 10 slm 氬氣電漿加入不同比例的氧氣其電壓與電流的關係。清楚發現加入氧氣會使原本氬氣電漿電性明顯改變，在不同添加氧氣比例 0%，0.99%，2.91% 及 4.76%，其對應的崩潰電壓分別為 120, 210, 340 及 370 伏特，主要是氧氣是負電型電漿會吸引電子吸附其表面。當氧氣加入比例至 0.99% 可以發現如文獻顯示非正常放電現象 (abnormal discharge) 其電壓與電流曲線為正斜率，隨著輸入電流增加電壓也跟著增加。若氧氣比例再增加至 2.91%，電壓與電流曲線正斜率區間變窄，當電流增加反而電壓稍微為降為負斜率，最後觀察到就如文獻正常放電現象 (normal discharge) 斜率為零。氧氣比例若加至 4.76%，電壓與電流曲線正斜率區間變更窄，負斜率區域轉至零斜率區間不明顯最後轉變成電弧 (arc) 放電，關於氧氣加入惰性氣體電性變化現象未來配合更進一步以電漿化學與電漿物理模擬解釋。

(五) 模擬 RF 氬氣電漿其電極間平均週期電漿密度分佈

圖五表示一個平均週期電漿特性分佈，電漿電位約為 94V，不均勻對稱的鞘層在內電極表面厚度約 0.3 mm 而外電極表面 0.4 mm，在準中性區域中間電子溫度約 1.5 eV，但出現兩個極值約 2.5 eV 在與鞘層區域交界處，因此電漿密度的分佈不如期望相當對稱。



圖五 模擬 RF 氬氣電漿其電極間平均週期電漿密度分佈



圖六 放電區 (glow region) 及後放電區 (post-glow) 照片 (a) He, 10 slm; (b) He+0.3% O₂, 10 slm; (c) Ar, 10 slm

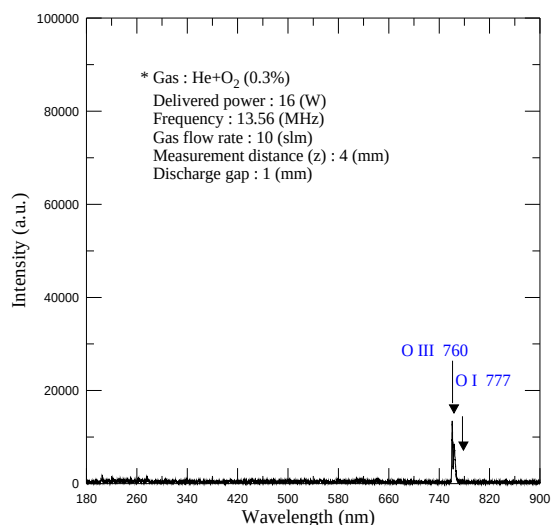
(六) 同軸圓管 He 與 Ar 電漿放電區後放電區照片

圖六表示氬氣、氬氣加 0.3% 氧氣及氬氣電漿典型輝光放電區域 (glow discharge) 及後輝光放電 (post-discharge) 照片，第二年開始使用鋁製內電極 (外徑 3 mm) 以及不鏽鋼製外電極 (內徑 5 mm)，因為電極尺寸縮小外電極不用冷卻水路可達到低溫電漿，相對操作功率降低。氣體流量為 10 slm，操作功率 16 W。從照片來看氬氣電漿亮度較亮相對氬氣及氬氣加 0.3% 氧氣電漿。氬氣加 0.3% 氧氣電漿亮度較純氬氣暗，因為氧氣為負電型電漿，這些現象可以從接下來光譜量測解釋。

(七) 同軸圓管 He 與 Ar 光譜比較

圖七表示流量 10 slm 功率 16 W 氬氣電漿加入 0.3% 氧氣其 200-900 nm 光譜分佈，因為氧氣為負

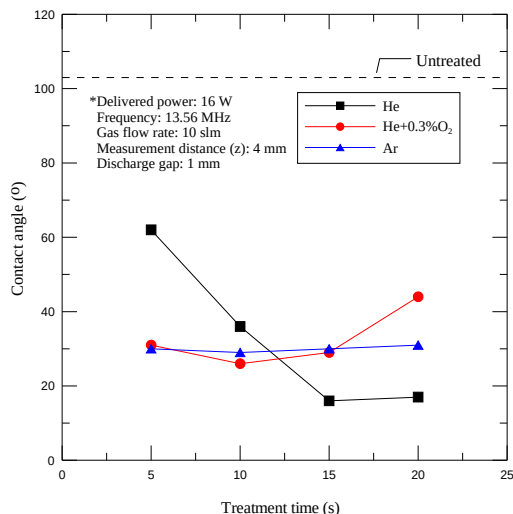
電型電漿，其中所有光譜強度幾乎都降低，所以未何從照片亮度比純氧氣電漿為暗的理由。依舊可以觀察到 760 nm 的 O III 放射光譜及 777 nm 的 O 放射光譜。



圖七 He+0.3% O₂ 電漿 180-900 nm 光譜分佈 (後放電區域 z=4mm)

(八) 同軸圓管 He 與 Ar 對 pp 表面親水性影響

圖八表示經由常壓電漿束在靜止情況下處理 pp film 5 至 20 秒觀察其接觸水滴角變化，可以看到經過氬氣電漿處理 5 秒後接觸角即可從原先 104 度降至 15 至 20 度，其可能的機制為 UV 會打斷原先 pp film 表面碳氧化合物鍵結，另外 UV 區域 250 nm 會被產生臭氧吸收產生 O₃P 的活化基，還有原先其他 O 的活化基 (741、672 及 777 nm) 與表面反應。

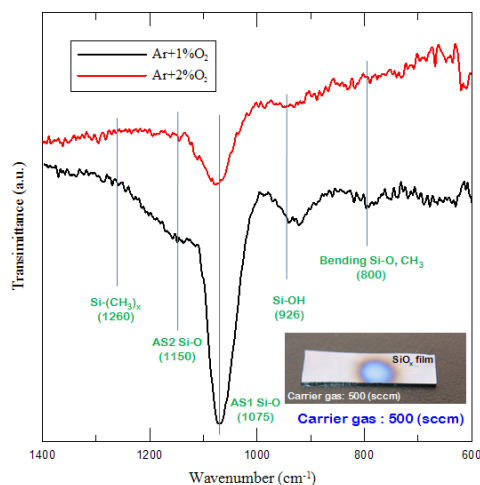


圖八 不同常壓電漿處理 pp film 表面時間與接觸水滴角關係 (10 slm)

(九) 同軸圓管 Ar 與 O₂ 比例電漿與 HMDSO 其 SiO_x 鍍膜 FTIR 分析

在第三年計畫，主要針對二氧化矽薄膜沉積 (deposition) 做研究，電極設備沿用第二年設計，圖九表示氬氣電漿加入不同氧氣比例與前驅物 (HMDSO) 其 FTIR 關係，從相關文獻要在常壓下氬氣電漿內加入氧氣會引起電漿不穩定，主要還

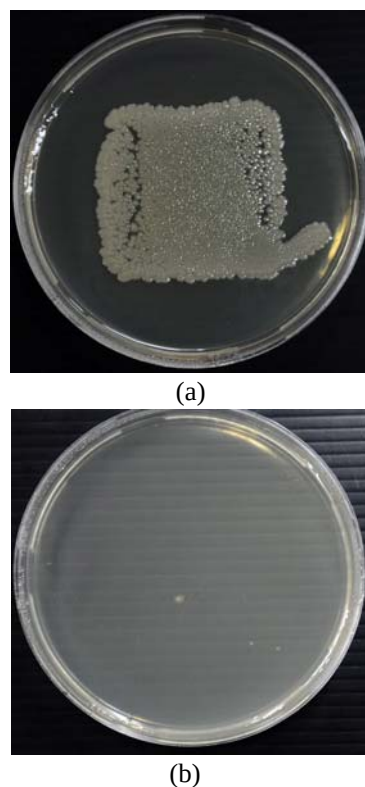
是因為氧氣為負電型電漿，研究中發現若加入介電質材料可以穩定電漿，如此一來使射頻常壓電漿束應用在相關氧化薄膜沉積多一個可控制參數，對於相關製程應用有幫助，從 FTIR 可以觀察在 1% 氧氣 AS1 Si-O (1075 cm⁻¹) 訊號較 2% 為強。



圖九 氬氣電漿加入不同氧氣比例與前驅物 500 sccm (HMDSO) 反應其 FTIR 分佈

(十) 平板型介電質常壓電漿束其滅菌應用

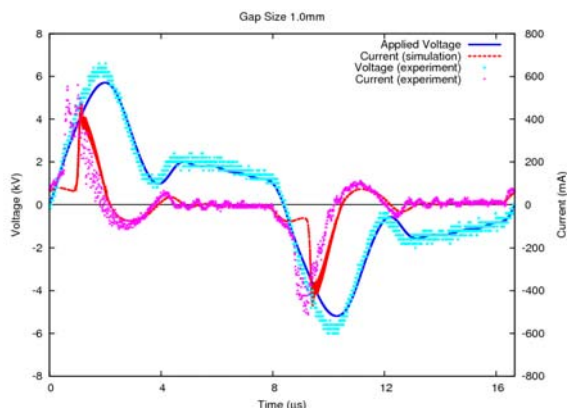
圖十為使用平板型空氣電漿束作大腸桿菌滅菌測試，測試條件 10 slm、電漿溫度 25 度、培養皿移動速度 1cm/s、培養皿與電漿距離 20 mm，菌液濃度 10⁶ CFU/plate，菌液面積 4 cm × 4 cm 可以觀察處理來回 5 次後，即可得到滅菌效果。



圖十 空氣電漿處理大腸桿菌滅菌 (a) 對照組; (b) 電漿處理後 (z=20 mm, loop 5, 1cm/s)

(十) 平板型介電質 N_2 電漿束電性模擬與電漿特性分析

圖十一為模擬氮氣平板型介電質常壓電漿束電極間電漿分佈情形，測試條件頻率 60 kHz，圖十一中紅色實線為預測出來電漿內電流與實驗粉紅色虛線幾乎一致。此證明所研發的電漿模擬軟體相當準確。



圖十一 平板型氮氣電壓與電流隨時間分佈情形模擬與實驗比較

三、學術成果

關於RF及DBD常壓電漿束的研究以自己實驗室發展軟體配合自己實驗室實驗能對整個電漿物理及化學機制更加清楚，對於後續相關常壓電漿設備研發將可提供清楚電漿反應機制。在本計畫資助之下，本人已成功在交通大學建立一個具國際水準的低溫電漿研究團隊，同時研究成果亦相當豐碩。總計在過去三年中(2007-2010)發表12篇的SCI期刊論文 [8-19]，5篇準備中的SCI期刊論文 [20-24]及19篇國際會議論文及[25-43; Two are invited speeches.]。主要包括fluid modeling, 電漿實驗及在表面處理, 鍍膜, 殺菌等應用。在此不詳述, 可詳見上述論文[8-43]。

四、技術推廣及運用的價值

後放電區(post-discharge)常壓電漿應用不受限物件大小，可以安置於連續式生產線，不論是單點式或是平面均可使用，可用表面親水處理 (pp film 及 ITO glass)、滅菌 (*E. coli*、*B. subtilis*、*spore*)、 SiO_2 鍍膜 (HMDSO)，解決舊有方式需要真空設備耗能問題及化學方式處理環境污染問題，常壓電漿束是個很好環保生產設備。

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行政院國家科學委員會補助國內專家學者出席國際學術會議報告

99年 1 月 20日

附件三

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時間會議地點	10-14 January 2010 Hong Kong, China	本會核定補助文號	NSC-96-2628-E-009-136-MY3
會議名稱	(中文)(英文) The 8th Asian Computational Fluid Dynamics Conference		
發表論文題目	(中文)(英文) Overview of the Kinetic-based Quiet Direct Simulation (QDS) Method for Gas Flow Computation (Attached at the end of this report, pp. 9-27)		

報告內容應包括下列各項：

一、參加會議經過

This conference has been organized for more than a decade. This is the 8th Asia CFD Conference held in Hongkong organized by Prof. C.-C. Hsu of HKUST in the period of January 10-14, 2010. There are more than 130 papers presented in the conference, in which there were 15 papers from Taiwan. More than 50 papers were presented from China, which is the largest group from Asia. There were also some papers from areas other than Asia countries such as France and USA.

二、與會心得

1. I was invited to join the International Advisory Committee meeting of Asia CFD Conference by Prof. C.C. Hsu along with Prof. J.-Y. Yang (NTU) and Prof. C.-A. Lin (NTHU) during the conference. I was elected as one of International Advisory Committee Member starting in January 2010. Decision was also made that all committee member must attend the conference at least once four years. Otherwise, he/she will be removed from the list.
2. I have presented a paper entitled “Overview of the Kinetic-based Quiet Direct Simulation (QDS) Method for Gas Flow Computation” with quite a good turnout.
3. I also served as one of the session chair for New Algorithm on the 2nd day of the conference.

三、考察參觀活動(無是項活動者省略)

N/A

四、建議

1. N/A

五、攜回資料名稱及內容

Printed version of Asia CFD-8 Proceedings..

六、其他

N/A

Overview of the Kinetic-based Quiet Direct Simulation (QDS) Method for Gas Flow Computation

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Abstract

An overview of the current status of the kinetic-based QDS method is presented. The recent progress of QDS as a Eulerian flow solver is presented, which includes: (1) a novel second order extension to the QDS scheme, 2) the QDS extension to axisymmetric flow - the world's first true-direction, two-dimensional axisymmetric solver, 3) extension to Nth order QDS scheme, 4) a parallel QDS scheme using the distributed-memory MPI library, and 5) the large reduction of computational time possible using graphic processor units (GPUs) which enable speedup approaching ~100-300 times. At the end, several ideas for future extensions of the QDS method are briefly outlined.

Keyword: *Quiet Direct Simulation, Maxwell-Boltzmann Distribution Function, Parallel Computation, Graphic Processing Unit.*

1. Introduction

There are a number of approaches for the simulation of gas flows and a large variety of solution methods depending on the nature and level of rarefaction of the flow. Computational fluid dynamics (CFD) codes typically use a finite volume method to solve a set of discretized governing equations, usually the Euler or Navier-Stokes equations. Contemporary finite volume CFD codes divide the computational domain into a grid of finite volumes and fluxes of mass, momentum and energy are calculated through the interfaces between these volumes. The technique suffers from the major disadvantage that poor alignment of the grid with the flow field results in large errors since fluxes can only occur between elements which share an interface. Thus, CFD requires careful grid design to ensure accurate results, convergence and stability.

Alternative approaches take into account kinetic theory and the particle-based nature of gases in simulating the flow field. Recently, the Quiet Direct Simulation (QDS) method was invented by Albright *et al.* [1] as a method for modeling plasma physics. They subsequently applied QDS to the simulation of Eulerian fluids for Sod's one dimensional shock tube problem and a simple two dimensional blast wave problem. Since then little further work has been done, the only example being by Peter [2] for simulating a typical diffusion equation using random time step for particle movement. In the QDS method, the effect of sampling using random numbers is replaced by using the weights and abscissas of a Gauss-Hermite quadrature. Thus, QDS is a particle- and kinetic-based Euler solver which exhibits negligible statistical scatter, has a large dynamic range, is easily extended to multi-dimensions and multi-species, is computationally inexpensive, is easily implemented on parallel computers and, since it is a particle-based method, does not require direction decoupling like conventional finite volume method. The major disadvantage is the scheme is inherently very diffusive. Albright *et al.* named the technique the Quiet DSMC (QDSMC) method; however the present authors feel this is a misnomer as there is no random number (or Monte Carlo) component to the algorithm and, unlike DSMC, it is valid only when thermal equilibrium can be assumed.

The QDS method employs trial particles to carry fluxes of mass, momentum and energy in physically realistic directions regardless of the underlying computational grid. Particle velocities are determined through an analytical discretization of the Maxwell-Boltzmann distribution without the use of

stochastic (random) processes like the DSMC method [3], thus removing all statistical scatter traditionally associated with such schemes. The analytical foundation of the particle property calculation and zero statistical scatter allows the number of particles to be small: 3 or 4 particles are usually sufficient. Following the convention of other kinetic-theory founded schemes, particles are permitted to move unobstructed during the free flight or flux phase of the simulation resulting in a solver with very high locality, making the method ideal for large-scale distributed-memory and/or vector computing. This nature also makes the QDS method a true direction coupling numerical scheme, which is very difficult for the conventional finite volume methods in CFD to achieve.

There are several advantages to particle-based Euler solvers. Firstly, hybridization between the solver and a pure DSMC solver which is capable of simulating the non-continuum regions of flow is relatively simple. Several authors have developed such particle-based hybrid methods including Macrossan [4], Chen [5], Smith [6] and Wu [7]. The second major advantage is that particle-based methods can exchange fluxes between any two cells on the grid for any given time step. Direction decoupled computational fluid dynamics (CFD) methods only allow fluxes to be exchanged between cells sharing a common interface. This obviously unphysical treatment often results in non-physical results in CFD simulations [8].

Recently, Wu's group [9] has applied the second order reconstruction using slope limiters to reduce the numerical diffusion of the QDS method, which was validated using several 1D and 2D cases. Later, the 2D QDS method was further extended to simulate axisymmetric 2D flow by the same group [xx], which, to the best knowledge of the authors, is the world's first true-direction, two-dimensional axisymmetric solver. Several interesting and important studies are also currently under investigation in Wu's group, which include: extension to multi-species, a parallel QDS scheme using the distributed-memory MPI library, and the even larger reduction of computational time by combing graphic processor units (GPUs) and distributed-memory machines. In addition, several ideas for future extensions of the QDS method are briefly presented, which include: 1) extension to N-th order spatial reconstructions to further reduce the numerical diffusion, 2) extension to viscous flow simulation using Chapman-Enskog distribution, 3) hybridization with the DSMC method for rarefied-continuum flow simulation. It is thus the objective of this paper to provide an overview the QDS method and its outlook as a gas flow solver.

The remainder of this paper is organized as follows. The QDS method is first introduced briefly and then followed by its extension using the 2nd order spatial reconstruction. Several 1D and 2D gas flows are presented, which include 1D Sod's problem, 2D explosion and implosion problems and 2D blast wave simulation. Next, its extension to simulate the axisymmetric gas flow problems are presented and validated by computing several 1D-radial and 2D-axisymmetric flows. Later, two strategies in reducing the computational time are introduced, which include parallel computing using distributed-memory machines and by combining GPUs and distributed-memory machines. Finally, several possible research directions are outlined at end of the paper.

2. The QDS Method and Its Extensions

2.1 First Order Particle Based Scheme

The normal random variable $N(0,1)$ is defined by the probability density:

$$p(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}} \quad (1)$$

By using a Gaussian quadrature approximation, the integral of equation (1) over its limits can be approximated by:

$$\int_{-\infty}^{\infty} \frac{e^{-x^2/2}}{\sqrt{2\pi}} f(x) dx \approx \sum_{j=1}^J \frac{w_j}{\sqrt{\pi}} f(\sqrt{2}q_j) \quad (2)$$

where w_j and q_j are the weights and abscissas of the Gaussian quadrature (also known as the Gauss-Hermite parameters). The abscissas are the roots of the Hermite polynomials which can be found tabulated in reference [13] or can be defined by the recurrence equation:

$$H_{n+1}(q) = 2qH_n - 2nH_{n-1} \quad (3)$$

where $H_{-1}=0$ and $H_0=1$. The weights can be determined from:

$$w_j = \frac{2^{n-1} n! \sqrt{\pi}}{n^2 [H_{n-1}(q_i)]^2} \quad (4)$$

Equation (2) becomes exact when the function $f(x)$ is a linear combination of the $2J-1$ polynomials $x^0, x^1, \dots, x^{2J-1}$.

Thus the basic first-order one-dimensional QDS algorithm consists of three basic steps (the method can be readily extended to higher dimensions) [6]:

(1) Particles undergo a “quiet start”. Here $j = 1, \dots, J$ particles are generated on the grid point x_i from the known grid quantities of density (ρ_i), velocity (u_i), velocity variance (σ_{vi}^2) and energy (E_i). The particles masses, velocities and internal energies are, respectively:

$$m_{ij} = \frac{\rho_i \Delta x w_j}{\sqrt{\pi}} \quad (5)$$

$$v_{ij} = u_i + \sqrt{2\sigma_{vi}^2} q_j \quad (6)$$

$$\varepsilon_{ij} = \frac{(\xi - \Omega)\sigma_{vi}^2}{2} \quad (7)$$

where Δx is the uniform grid size, ξ is the total number of degrees of freedom ($\xi = 2(\gamma-1)^{-1}$) and Ω is the number of simulated translation degrees of freedom (i.e. for one-dimensional simulation, $\Omega = 1$). Any unused translational and other non-translational degrees of freedom are thus treated as internal structural degrees of freedom.

(2) Particles are advanced to their new position over a time step Δt such that:

$$x_{ij}(t + \Delta t) = x_i + v_{ij}\Delta t \quad (8)$$

(3) The grid properties are updated by linearly distributing the properties carried by the particles on to the grid. The grid properties of mass, momentum and energy can be calculated from the individual particle mass (m_p), velocity (v_p) and internal energy (ε_p) with:

$$m_i = \sum_P m_p W_{Pi} \quad (9)$$

$$p_i = \sum_P m_p v_p W_{Pi} \quad (10)$$

$$E_i = \sum_P m_p W_{Pi} \left(\frac{1}{2} v_p^2 + \varepsilon_p \right) \quad (11)$$

The macroscopic equilibrium temperature, T_i , is calculated in each cell in the manner used by conventional finite volume solvers:

$$T_i = \frac{1}{C_v} \left(\frac{E_i}{m_i} - \frac{1}{2} \left(\frac{p_i}{m_i} \right)^2 \right) \quad (12)$$

where C_v is the specific heat under constant volume ($C_v = R(\gamma-1)^{-1}$). Other macroscopic fluid quantities can be calculated from these values. The linear weights W_{Pi} for each particle are calculated assuming uniform conditions across each cell by:

$$W_{Pi} = \begin{cases} (x_p - x_{i-1})/(x_i - x_{i-1}) & \text{if } x_{i-1} < x_p \leq x_i \\ (x_{i+1} - x_p)/(x_{i+1} - x_i) & \text{if } x_i < x_p \leq x_{i+1} \\ 0 & \text{otherwise} \end{cases} \quad (13)$$

This linear interpolation scheme is the mathematical representation of the assumption that each particle represents a very large number of particles with identical velocities uniformly distributed across the source cell. Such a scheme is inherently first order accurate in space. The interpolation routine implemented by Albright et al. [1] in the original QDS does no more than effectively replace the free flight phases of molecular motion which is an assumption present in many modern kinetic

theory based flow solvers. The introduction of a higher order interpolation scheme on data which is linearly varying (in space, in this instance) will, at best, perform no better than a linearly interpolating scheme. In addition, no information regarding gradients of conserved or primitive variables appears in either linear or higher order interpolation routines.

2.2 Extension to a Second Order Scheme

In order to extend the scheme to high order accuracy in a more conventional fashion, the estimates of flux values are improved by adjusting the particle mass, velocity and internal energy in equations (5) to (7) by considering the gradient values calculated at the previous time step using a second order flux reconstruction scheme. Thus, as an example, the particle mass becomes:

$$m_{ij} = \frac{\left(\rho_i + \frac{d\rho}{dx} \Delta x_L \right) \Delta x w_j}{\sqrt{\pi}} \quad (14)$$

where Δx_L represents the location in the cell from where the flow properties are taken.

This is demonstrated in Figure 1 showing the addition of a linear variation of density within a cell. Since QDS is essentially a direction coupled volume-to-volume solver, conditions within a region of space are required. Particles moving to a region right of the source cell are likely to have their properties defined by a region in the right half of the cell. In the present implementation, fluxes moving to the right are assumed to take their quantities from the reconstructed state $\Delta x_L = 0.5(\Delta x - v_{ij}dt)$ to the right of the cell center. This corresponds to the centre of mass of the flux which moves into the destination cell. Left moving fluxes have properties constructed in a similar fashion. Particles are then moved in free flight, justifying the use of a linear interpolation routine.

To prevent unphysical and unstable oscillations in the solution, the gradients are calculated using slope limiters. In this scheme, gradients are first determined using the MINMOD (Minimum Modulus) and the MC (Monotonized Central Difference) scheme [10]. Using density as an example, the gradient using the MC slope limiter is:

$$\frac{d\rho}{dx} = \text{MINMOD} \left[\frac{\rho_{i+1} - \rho_{i-1}}{2\Delta x}, \text{MINMOD} \left(2 \frac{\rho_{i+1} - \rho_i}{\Delta x}, 2 \frac{\rho_i - \rho_{i-1}}{\Delta x} \right) \right] \quad (15)$$

where the MINMOD scheme is:

$$\text{MINMOD}[a, b] = \begin{cases} 0 & \text{IF SIGN}(ab) < 0 \\ a & \text{IF (SIGN}(ab) > 0) \text{ AND } (|a| < |b|) \\ b & \text{IF (SIGN}(ab) > 0) \text{ AND } (|b| < |a|) \end{cases}$$

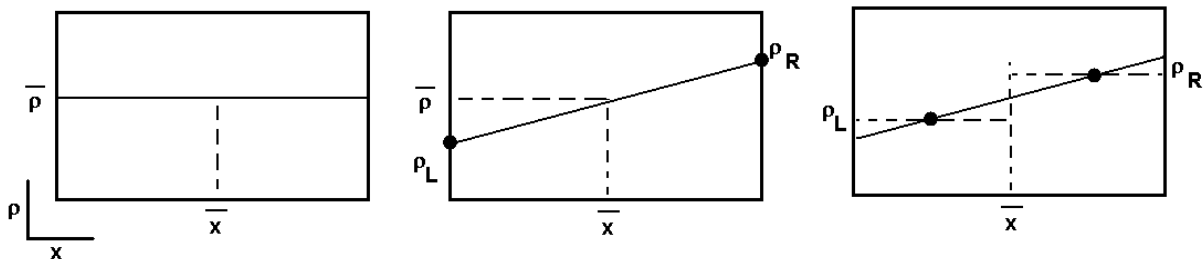


Fig. 1: Examples of addition of in-cell gradients. a) No gradient, conventional first order scheme, b) conventional finite volume implementation where fluxes are calculated at cell interfaces and c) implementation when calculated fluxes are volume to volume (direction decoupled) as opposed to calculated at flux interfaces.

The extension of the scheme to two-dimensions is relatively straight-forward; however, at this stage it becomes convenient to move away from the concept of a particle whose properties are interpolated onto a grid towards a conventional finite volume approach. In this approach, conserved quantities such as mass, momentum and energy are exactly conserved by tracking fluxes from source volumes to destination volumes. Discrete simulation particles are now considered as a very large number of smaller particles uniformly (or linearly) distributed over the source cell. If the particle position distributions (i.e gradients of density in the flow) are known, the flux from the source region to any arbitrary destination volume can be calculated. This concept is illustrated in [Figure 2](#) for a 2D case. The amount of mass, momentum and energy moving from the source to the destination cell is proportional to the ratio of the area (or volume for 3D) of the overlap to the area of the original cell. This scheme requires minimal computation, works between arbitrarily sized source and destination cells (which makes it suitable for adaptive mesh refinement). Using this concept, the particle mass and velocities in equations (5) and (6) become:

$$m_{ijk} = \frac{\rho_i \Delta x \Delta y w_j w_k}{\pi} \quad (16)$$

$$v_{ij} = u_x + \sqrt{2\sigma_{vi}^2} q_j \quad (17)$$

$$v_{ik} = u_y + \sqrt{2\sigma_{vi}^2} q_k \quad (18)$$

where there are $k = 1, \dots, K$ particles in the y -coordinate direction.

The internal energy remains identical to the one dimensional case, allowing for a corresponding increase in Ω to account for the extra simulated dimension.

As shown in [Figure 2](#), the fraction of mass from the source cell which fluxes to the destination cell can be determined by the overlap area $A = v_{xj(new)} v_{yj(new)} dt^2$ divided by the source cell area $dx dy$ for the 2D case. Thus the amount of mass m_{flux} , energy E_{flux} and momentum in each coordinate direction $p_{x,flux}$ and $p_{y,flux}$ which must be added to the destination cell and subtracted from the source cell are given by:

$$m_{flux} = \frac{A}{A_S} m_{ijk} \quad (19)$$

$$E_{flux} = \frac{A}{A_S} m_{ijk} \left[\frac{1}{2} (v_{ij}^2 + v_{ik}^2) + \varepsilon_{ijk} \right] \quad (20)$$

$$p_{flux,x} = \frac{A}{A_S} m_{ijk} v_{ij} \quad (21)$$

$$p_{flux,y} = \frac{A}{A_S} m_{ijk} v_{ik} \quad (22)$$

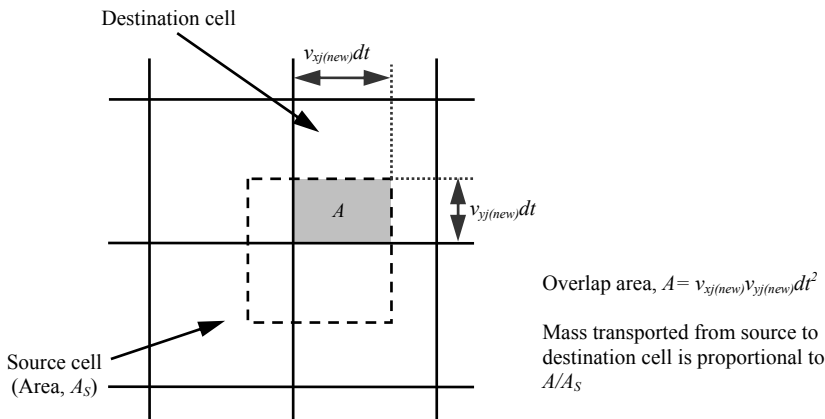


Fig. 2: Schematic showing the way fluxes of conserved quantities between source and destination cells are calculated using the “overlap” function in QDS.

2.3 Extension to a Second Order Axisymmetric Scheme

The simple method for calculating the overlap function becomes more complicated for axisymmetric flows. Two corrections must be applied, since cells at different radii have different volumes, even if their cross-sectional area is the same. The first correction is applied to the momentum of each cell to account for the variation in the force due to static pressure across the top and bottom interfaces of the cell, as shown in Figure 3. At each time step, an amount of momentum is added to each cell which is given by:

$$\Delta M = P\alpha\Delta r\Delta x\Delta t \quad (23)$$

where $P (= \rho RT)$ is the pressure in the cell, Δr is the radial size of the cell, Δt is the simulation time step and the arbitrary angle α is set to π in the current implementation of the QDS code. If this difference is not accounted for, an artificial flow will be set up towards the axis of symmetry, even for flows with zero bulk radial velocity.

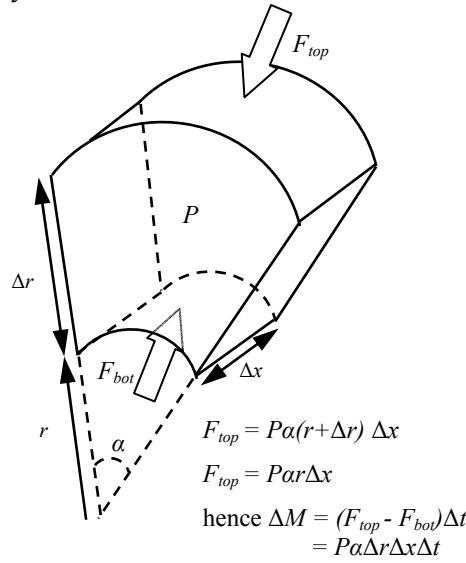


Fig. 3: Schematic of the forces due to static pressure P on an axisymmetric cell leading to the requirement for a momentum correction ΔM at every QDS time step Δt .

The second correction accounts for fact that the simple overlap method described above must now be corrected for radial components of fluxes which will result in the mass, momentum and energy moving to differing cell volumes (i.e. fluxes which move away from the axis must expand into a larger cell volume and vice-versa). It can be shown from Figure 4 that for a flux having radial velocity v_r over a time step Δt , the ratio between the displaced volume V_d , having a centroid at radius r and a radial width Δr , to the volume where this mass originated V_0 is:

$$\frac{V_d}{V_0} = \frac{v_r\Delta t(2r + \Delta r - v_r\Delta t)}{2r\Delta r} \quad \text{for } v_r > 0 \quad (24)$$

$$\frac{V_d}{V_0} = \frac{v_r\Delta t(-2r + \Delta r + v_r\Delta t)}{2r\Delta r} \quad \text{for } v_r < 0 \quad (25)$$

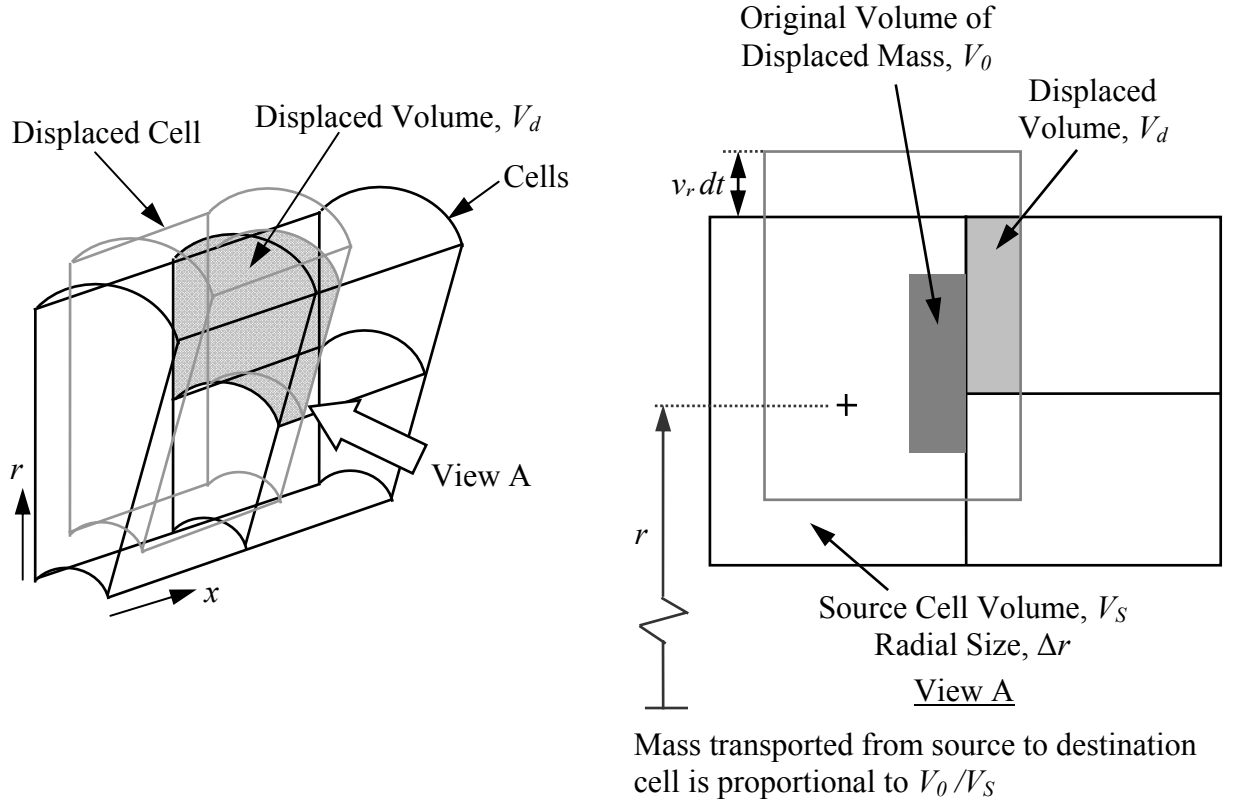


Fig. 4: Schematic showing the relationship between displaced and original volumes used to calculate the fluxes in axisymmetric cells using QDS

These ratios can be multiplied directly to the radial components of mass, momentum and energy fluxes to correct for the difference in radial volumes of source and destination regions.

Equations (24) and (25) are suitable for first order simulations; however in second order the effect of property gradients must be taken into account. **Figure 5** shows the radial flux from a source cell at radius r_{cell} (with upper and lower boundaries r_L and r_R respectively) to a cell of greater radius. Note here that the source cell has a centre of mass at r_{cm} and, given there is a density gradient across the cell of a constant $B = d\rho/dr$, the centre of mass is given by:

$$r_{cm} = \frac{1}{m_{cell}} \int_{r_L}^{r_R} [\rho_{cell} + B(r - r_{cell})] \Delta x r \alpha dr = \frac{\alpha \Delta x}{m_{cell}} \left[\frac{B(r_R^4 - r_L^4)}{4} + \frac{(\rho_{cell} - Br_{cell})(r_R^3 - r_L^3)}{3} \right] \quad (26)$$

where m_{cell} is the total mass of the cell. In **Figure 5**, the mass contained in the element between r and $r + \Delta r$ is given by the expression:

$$mass(r \rightarrow r + \Delta r) = [\rho_{cm} + B(r - r_{cm})] \Delta x r \alpha \Delta r = \alpha \Delta x [Br^2 + Cr] \Delta r \quad (27)$$

where the constant $C = \rho_{cm} - Br_{cm}$. Integrating this expression between r_1 and r_R gives the net mass available to flux between the two cells:

$$Net \text{ mass} = \alpha \Delta x \int_{r_1}^{r_R} (Br^2 + Cr) dr = \alpha \Delta x \left[\frac{B}{3} (r_R^3 - r_1^3) + \frac{C}{2} (r_R^2 - r_1^2) \right] \quad (28)$$

The mass associated with this bucket is hence:

$$m_{rj} = \frac{\alpha \Delta x \left[\frac{B}{3} (r_R^3 - r_1^3) + \frac{C}{2} (r_R^2 - r_1^2) \right] w_{yj}}{\sqrt{\pi}} \quad \text{for } v_r > 0 \quad (29a)$$

The expression for fluxes moving toward the axis can be determined in a similar manner:

$$m_{rj} = \frac{\alpha \Delta x \left[\frac{B}{3} (r_1^3 - r_L^3) + \frac{C}{2} (r_1^2 - r_L^2) \right] w_{yj}}{\sqrt{\pi}} \quad \text{for } v_r < 0 \quad (29b)$$

Thus, for an axisymmetric simulation, radial fluxes are calculating using equations (29a) and (29b) while axial fluxes use equation (9). These are combined in a $2N$ flux formulation to obtain the fluxes to the eight surrounding neighbor cells.

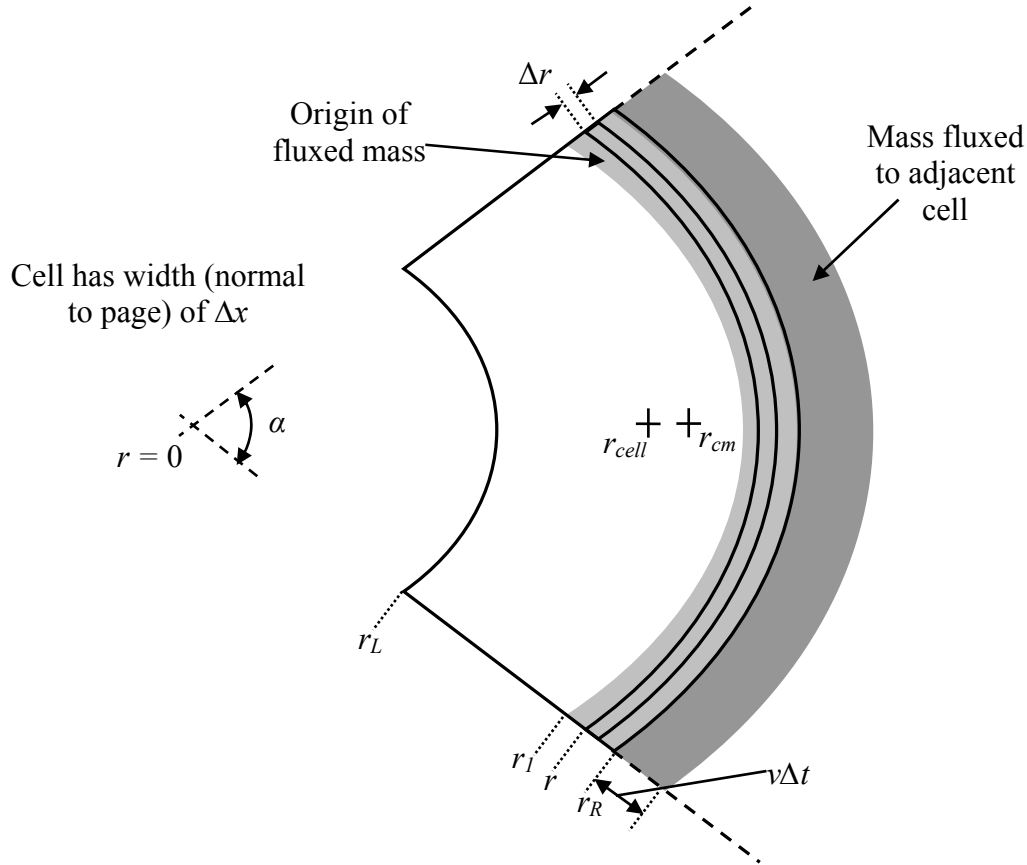


Fig. 5: Schematic for the derivation of second order expressions for axisymmetric QDS simulations.

2.4 Parallel Implementation Using Distributed-memory Machines

For large scale computation using QDS, proper parallelization is necessary to reduce the runtime for a meaningful simulation. By applying the spatial domain decomposition method, the QDS method itself is perfect for parallel implementation using distributed-memory machines through MPI libraries because of: 1) explicit in time marching scheme and 2) highly local flux scheme inherited in the scheme. In the present paper, we have simply divided the computational domain by enforcing approximately equal number of cells in each processor.

2.5 Parallel Implementation by Combining Distributed-memory Machines and GPUs

GPUs have been playing very important role in gaming software design because of the high speed calculation due to hardware computing, and low cost due to mass production in the IT industry. Recently, several disciplines of scientific computing have taken advantage of this fast development, which include astronomy, molecular dynamics, lattice Boltzmann method, and CFD, to name a few. Unlike the conventional finite-volume method in CFD, the QDS method may have much larger potential in applying this new technique because of similar reasons as mentioned in previous sections: explicit in time and highly local scheme. In addition, by combining the distributed-memory machines and GPUs, very large reduction of computational time can be expected. However, some paradigm shift

of the QDS scheme is required to suit the hardware structure of the GPUs. All the GPU codes were programmed through the use of CUDA, which is developed by Nvidia Inc. The modifications are described briefly in the following.

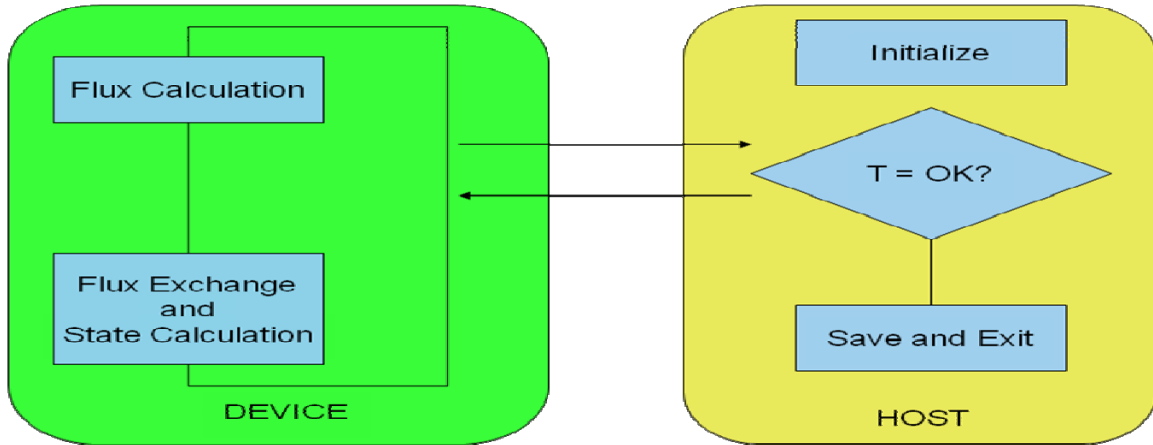
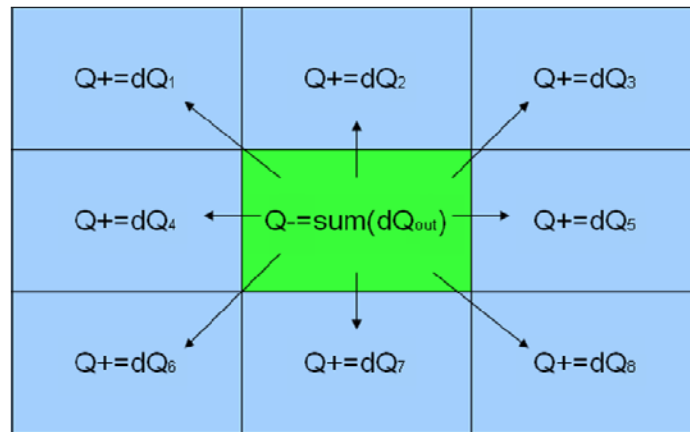


Fig. 6: Basic algorithm of QDS computation using GPUs.

The major idea of a successful GPU computation of the QDS scheme strongly relies on the possibility of conducting all the computations (flux calculations, flux exchange and state calculations) on the device after the initiation from the host, which is shown in Figure 6. This is mainly caused by the fact that the data exchange between device and host is very inefficient. Most important of all, since each cell is an independent **thread** on GPUs, all communications between the cells becomes inefficient because of the slow communication between **threads**. Thus, to conduct an efficient GPU computation, some modification of the serial QDS scheme is necessary to avoid any possible data exchange between host and device. One feasible and easy way is to collect and add all incoming fluxes from neighbor cells (Figure 7b), rather than to store outgoing fluxes to the destination cells (Figure 7a). Since the Cartesian grids are used in the present QDS scheme, all incoming fluxes from all neighbor cells can be calculated easily and stored once the macroscopic properties of the neighbor cells are known. In addition to the computation of QDS on GPUs, we have also demonstrated that it is possible to do the computation by combining conventional distributed-memory machines (through MPI libraries) and GPUs (through CUDA).



(a)

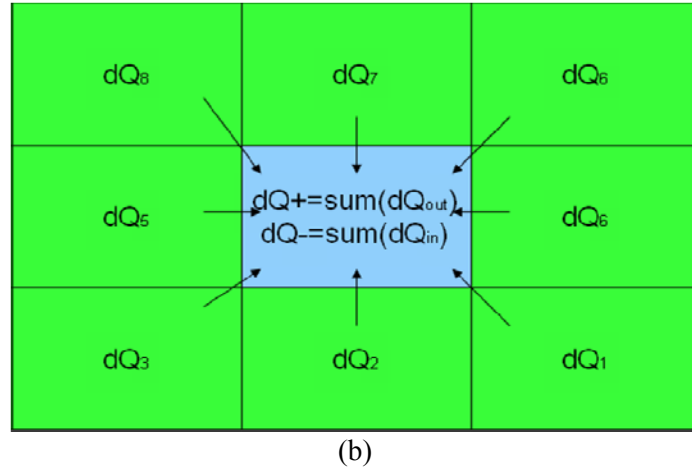


Fig. 7: Schematic diagram of flux exchange. (a) Serial computation (b) parallel GPU computation.

3. Results and Discussion

3.1 The Second Order Extension

Figure 8 illustrates the typical results of density profiles of Sod's problem using different numerical schemes as compared to the analytical Riemann solution. Results clearly demonstrate that the 2nd order QDS using slope limiters improves the solution greatly with only minimal amount of extra computational cost. Figure 9 shows that simulated density profiles using different CFL numbers (0.1, 0.5 and 1.0). Results show that the present 2nd order QDS scheme is relatively insensitive to the variation of CFL number less than 1.0, although a slight bump occurs at the edge of the right-moving shock.

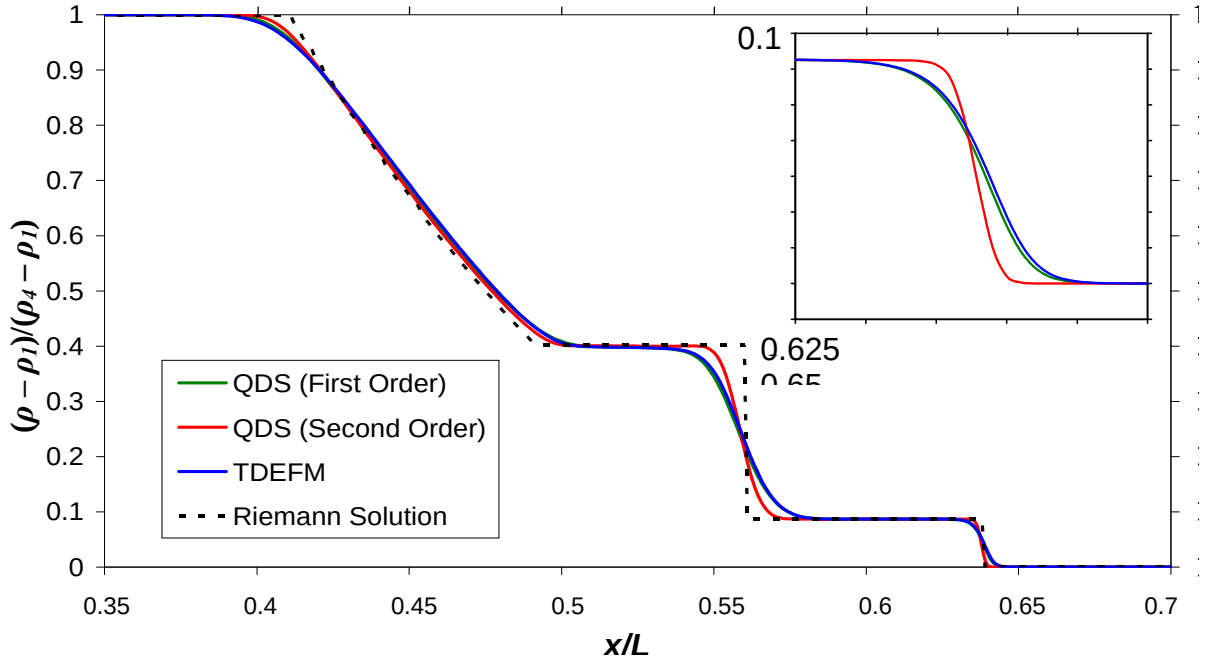


Fig. 8: Shock tube density profile as generated by QDS (first and second order) and TDEFM compared to the Riemann solution. The inset shows the profile in the region of the shock.

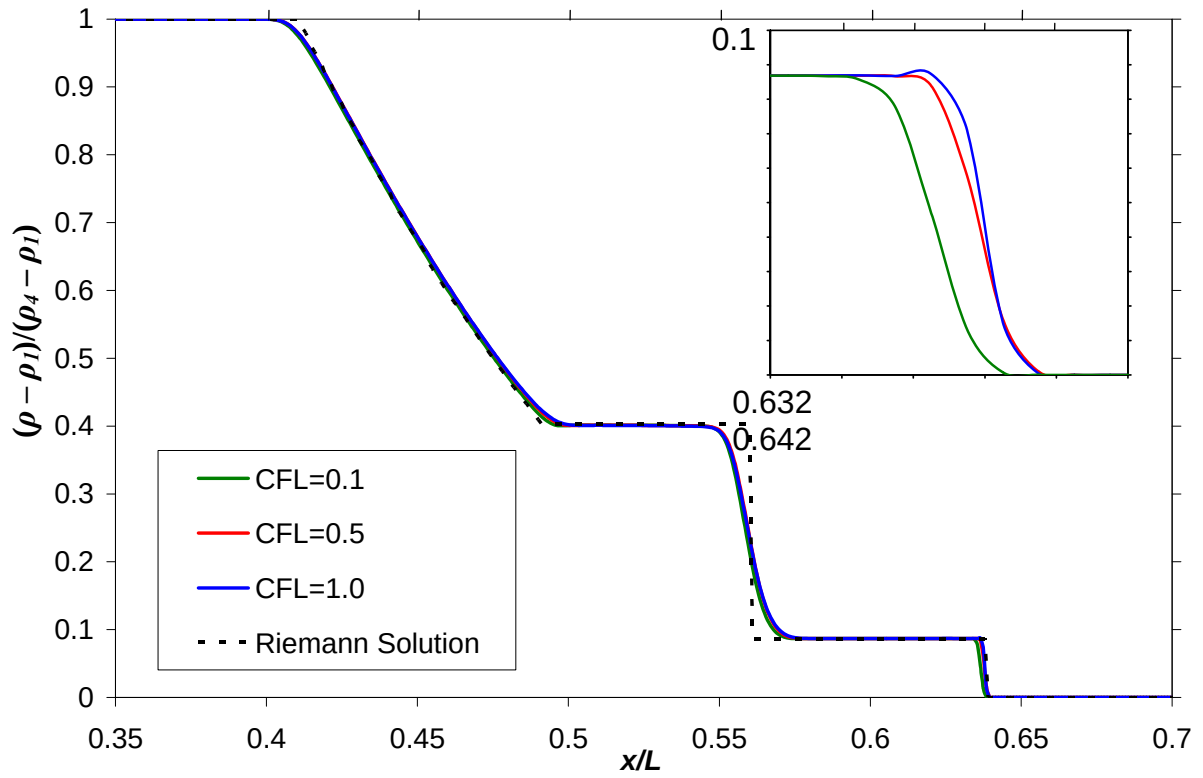


Fig. 9: Shock tube density profile as generated by second order QDS showing the effect of varying CFL number (via time step variation) on the solution. The inset shows the profile in the region of the shock.

Figure 10 illustrates the density contours of a two-dimensional blast wave resulting from different numerical schemes. It clearly shows that the 2nd order QDS scheme predicts the flow field symmetrically without the defect caused by the direction decoupling of the conventional finite volume method, such as the Riemann solver.

Figure 11 shows the comparison of the snapshot of density contour at $t=4.0$ s for Mach 3 flow past a square block using the 2nd order QDS scheme with that obtained earlier by Keats and Lien [11], who have applied adaptive mesh refinement.

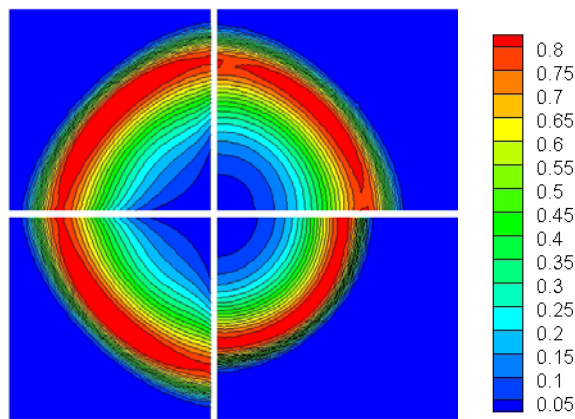


Fig. 10: Contours of density obtained using [left] a 1st order accurate Riemann solver, [upper right] first order QDS and [lower right] second order QDS for a two-dimensional blast wave on a 50x50 grid.

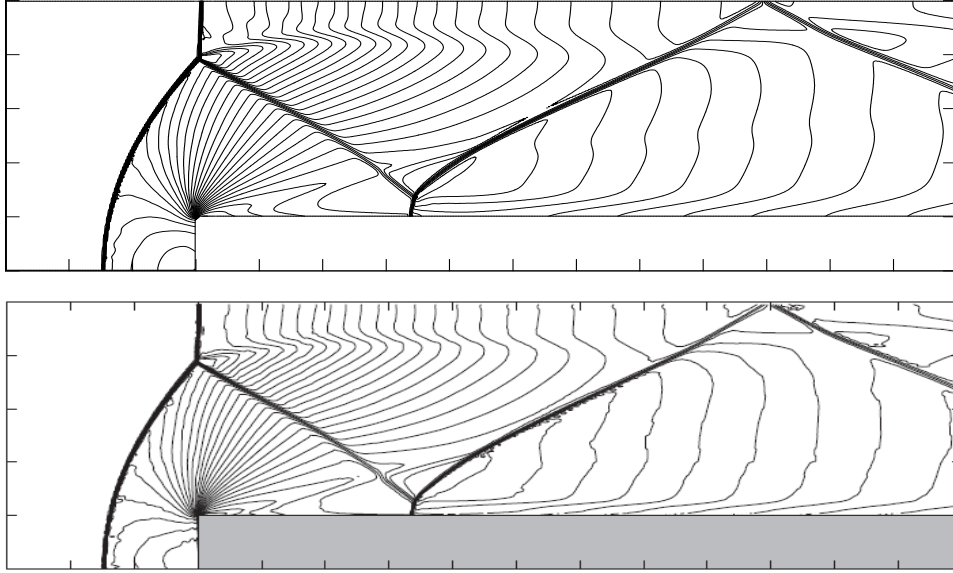


Fig. 11: Contour of density at 4.0s for Mach 3 flow over a forward facing step in a wind tunnel obtained using second order QDS with 4 simulation particles (top) and from the results of Keats and Lien [11].

3.2 The Second Order Axisymmetric QDS

Figure 12 illustrates the comparison of results of a spherical explosion using the 2nd order axisymmetric QDS with other numerical schemes including the 1st order QDS and HLL. Results clearly show that only the 2nd order axisymmetric QDS predicts the flow reasonably because of the inherited true direction coupling. Even with 2nd order HLL scheme, unphysical results also appear at least in the early stage of the evolution. As for the 1st order QDS, it is obviously too diffusive as expected.

Figure 13 presents a series of snapshots of density contour for the simulation of shock propagation through a pipe with a sudden expansion using the second order axisymmetric QDS scheme. All the shock and expansion waves are clearly captured along with the other complicated interaction among these waves. This has also been validated by the good agreement with a direct simulation assuming infinite collision rate, which is shown in Figure 14.

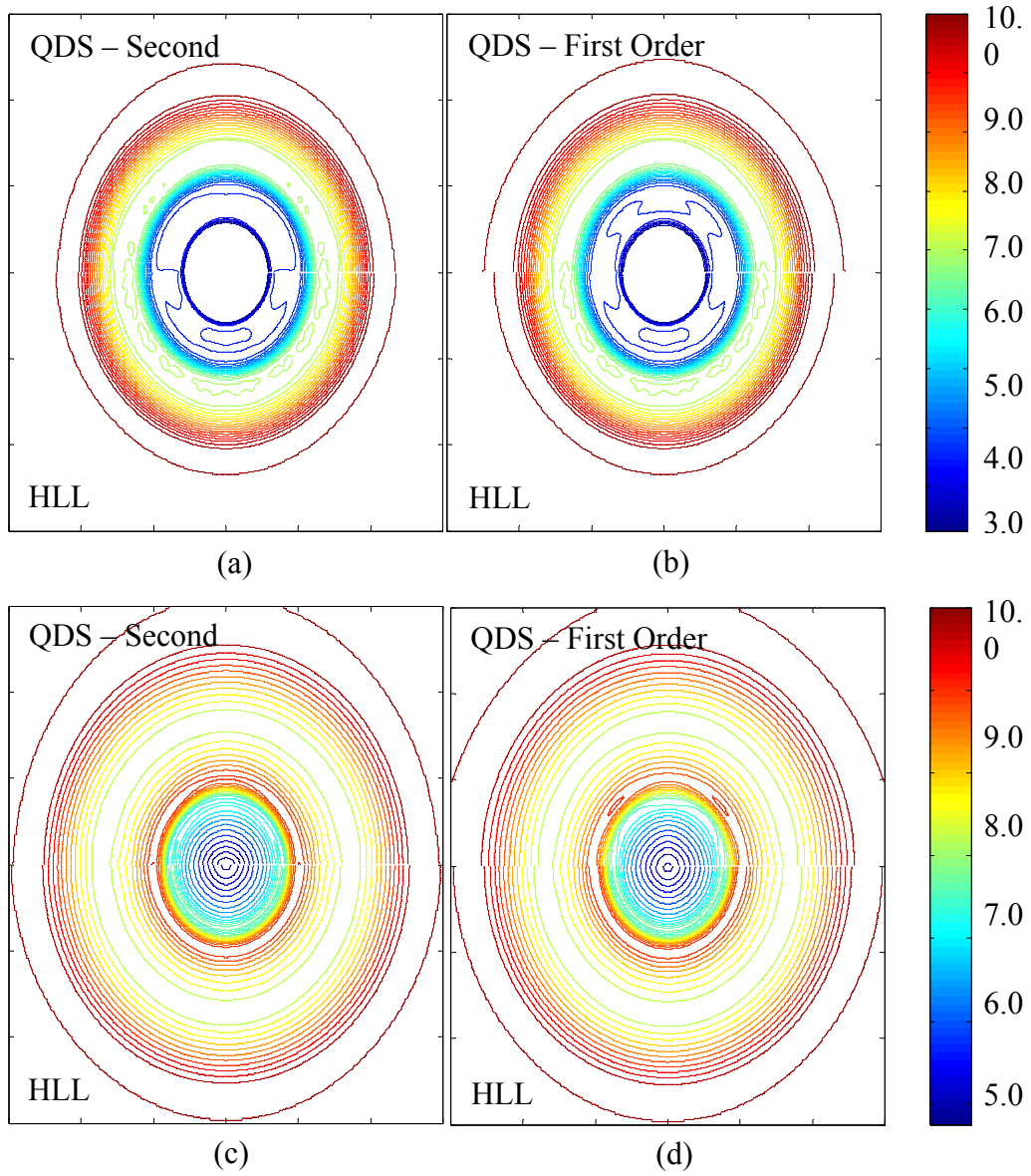


Fig. 12: Comparison of contours of density $[\text{kg/m}^3]$ for a spherical implosion: a) second order QDS and second order HLL at 0.2s, b) first order QDS and second order HLL at 0.2s, c) second order QDS and second order HLL at 0.4s and d) first order QDS and second order HLL at 0.4s.

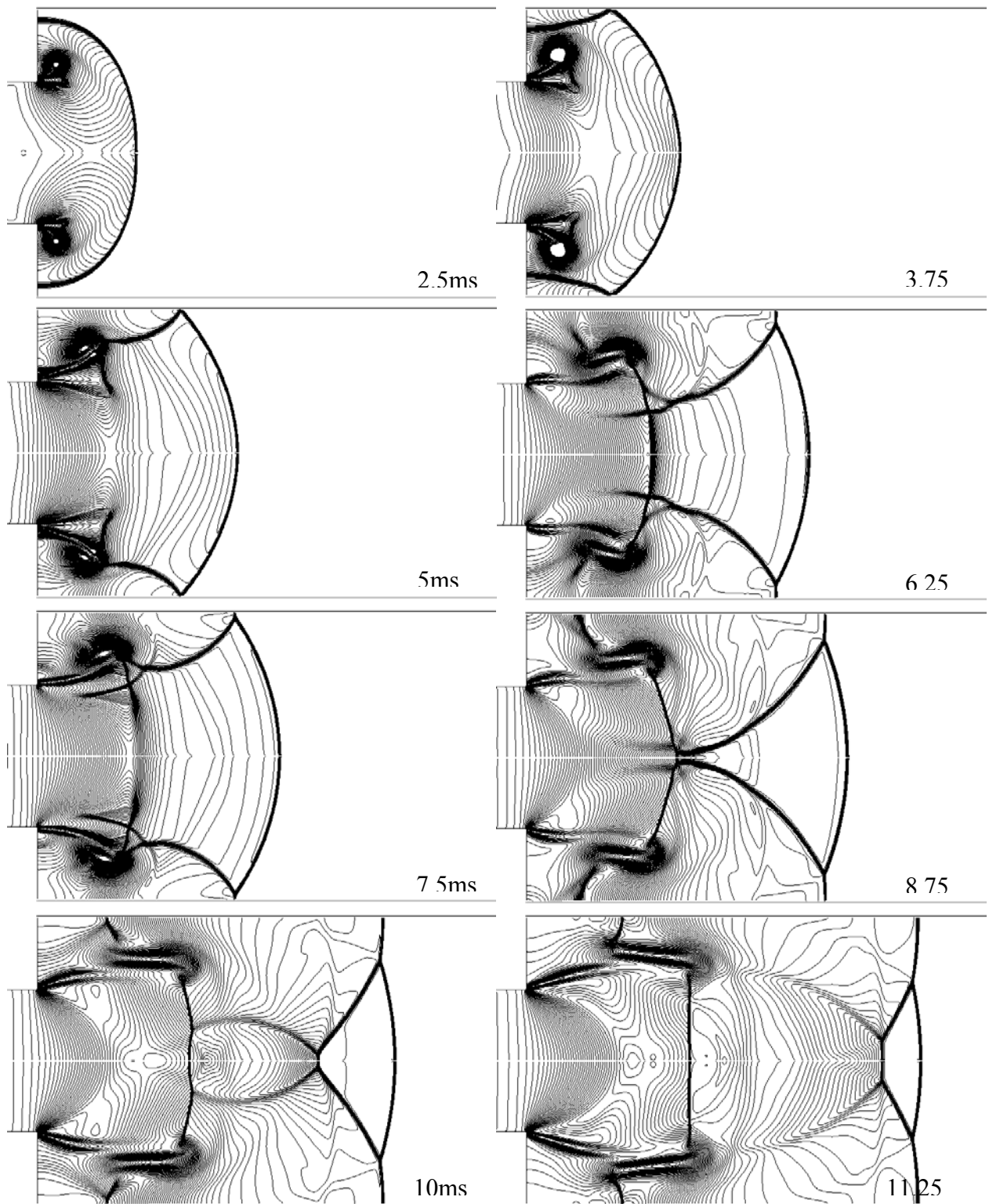


Fig. 13: Contours of log (density) for the propagation of a Mach 2 shock through a pipe with a sudden expansion using 2nd order axisymmetric QDS method.

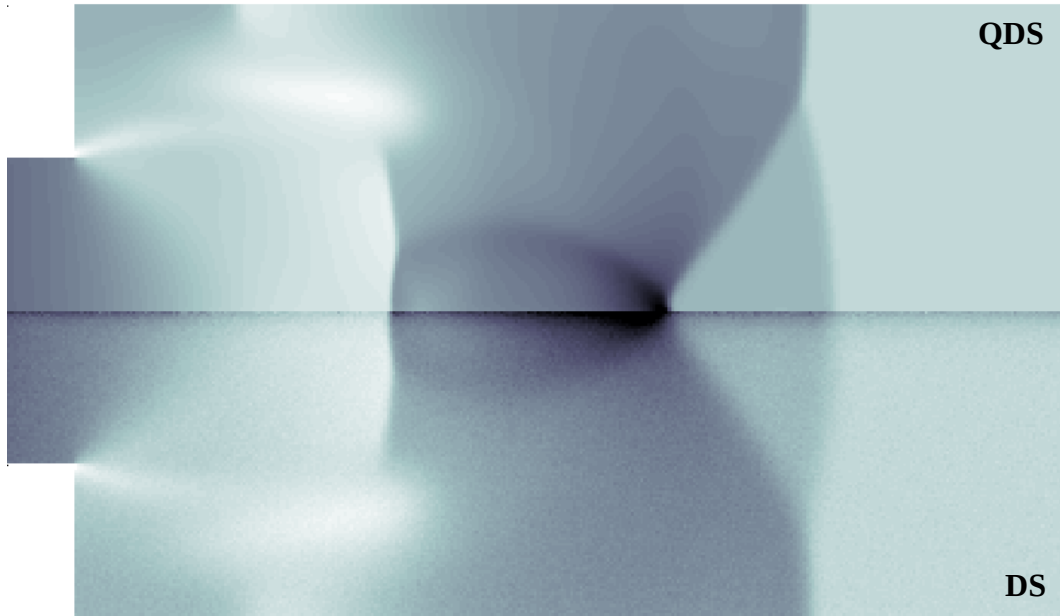


Fig. 14: Density contours $[\text{kg/m}^3]$ for QDS (top) compared with a direct simulation (DS) for the propagation of a Mach 2 shock through a pipe with a sudden expansion.

3.3 Parallel Implementation of the QDS Using Distributed-Memory Machines

Figure 15 shows the parallel performance of Mach 3 flow past a square block using different number of cells. Results show that for the large problem (1,064,700 cells) parallel efficiency can still reach 92% using 128 processors of IBM-1350 (dual processors, dual cores) at National Center for High-Performance Computing, Taiwan. For the small problem (10,647 cells), the parallel efficiency decreases rapidly with increasing number of processors, e.g., 50% using only 36 processors. With this implementation, very large problems can be readily simulated using the 2nd order QDS scheme, which is otherwise very time-consuming.

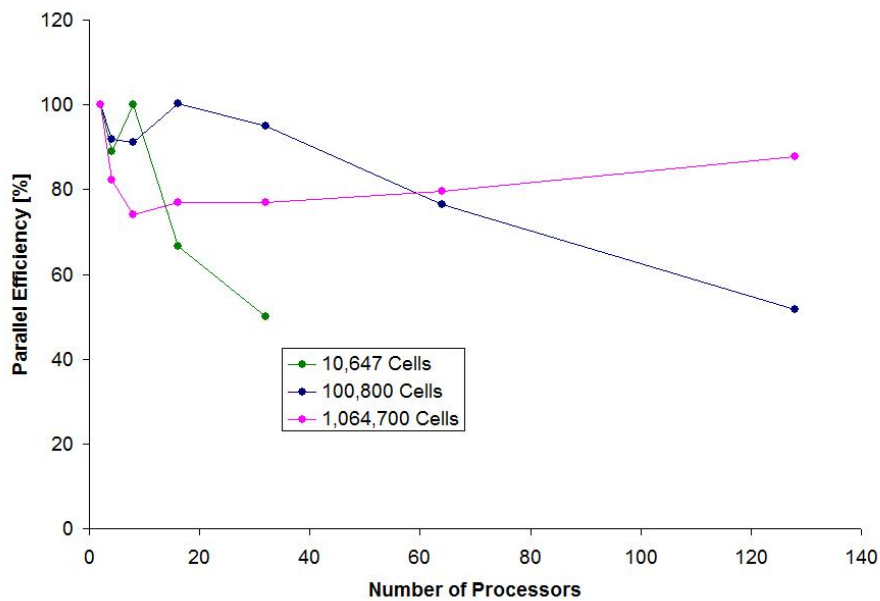


Fig. 15 Parallel performance of the two-dimensional 2nd order QDS scheme for Mach 3 flow past a square block using different number of cells.

2D-QDS Hybrid Speedup rate via CPU vs. GPUs

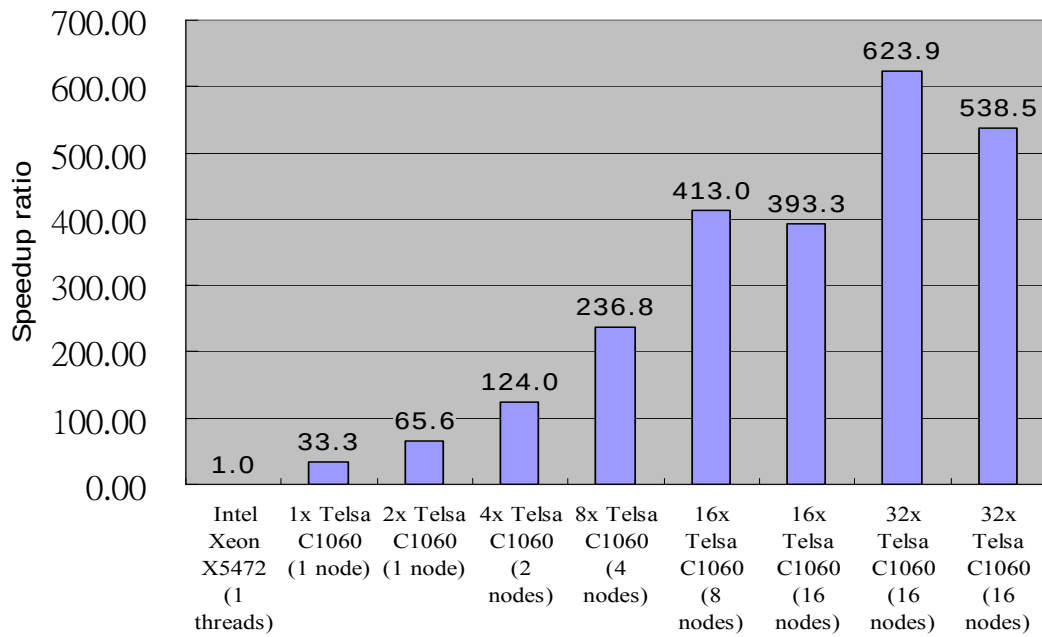


Fig. 16 Speedup of the 2nd order QDS scheme for a blast wave simulation using hybrid computing (Number of cells: 4M).

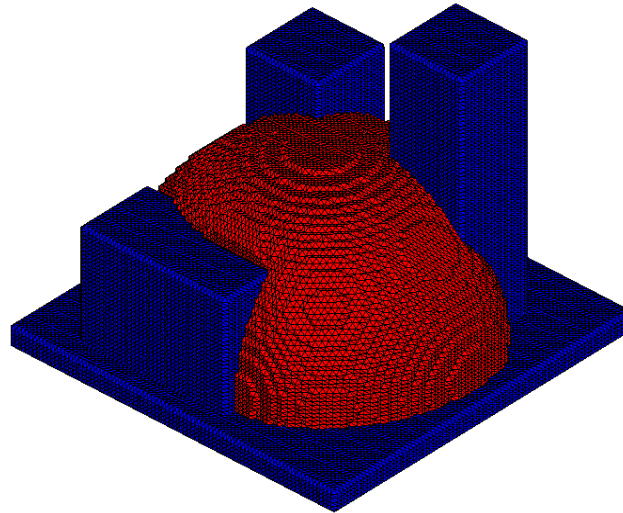


Fig. 17 Snapshot of density distribution of a blast wave propagation under 3D urban environment.

3.4 Hybrid Parallel Computing of the QDS Using MPI and CUDA

Figure 16 shows the speedups of different number of nodes, having one or two GPUs within each node, as compared to a CPU (Intel Xeon X572). Note the protocol for the GPU and network communication is CUDA (developed by NVIDIA Inc.) and MPI library, respectively. Result shows that speedup can reach as high as 623.9 using the combination of 16 nodes with 2 GPUs within each node. Also the speedup is slightly higher as the number of GPUs per node is larger for the same total number of GPUs. This tremendous reduction of computational time by using the hybrid computing approach is very important in some practical applications such as the simulations of a realistic 3D blast wave propagation under the urban environment. One typical example is shown in Figure 17. More details shall be provided in the meeting.

4. Conclusion

In this paper, an overview of the current status and future direction of the QDS method is presented. The recent progress of QDS as a Eulerian flow solver is presented, which includes: (1) a novel second order extension to the QDS scheme, 2) the QDS extension to axisymmetric flow - the world's first true-direction, two-dimensional axisymmetric solver, 3) extension to multi-species, 4) a parallel QDS scheme using the distributed-memory MPI library, and 5) the large reduction of computational time possible using graphic processor units (GPUs) which enable speedup approaching ~ 100 -300 times. Several flows, which include 1D shock tube simulations, 2D explosion and implosion simulations, 2D supersonic flow problems, 2D-axisymmetric pulsed pressure chemical vapor deposition (PP-CVD) simulations, and 2D/3D blast wave propagation in an urban environment, are presented to demonstrate the capability of the QDS method for inviscid fluid simulation.

Several ideas for future extension of the QDS method are briefly outlined as follows, which include: 1) extension to arbitrary N^{th} order spatial reconstructions to further reduce the numerical diffusion, 2) extension to viscous flow simulation using Chapman-Enskog distribution, 3) use of cut cells for simulation of complex geometry whilst maintaining a Cartesian grid, and 4) hybridization with the DSMC method for rarefied-continuum flow simulation.

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