Gas Kinetic Scheme for Direct Numerical Simulation of Decaying Compressible Turbulence

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Outline

- Background
- Construction of Gas Kinetic Scheme (GKS)
- GKS for DNS of Decaying Homogenous Isotropic Turbulence (DHIT)
- Conclusions

Objectives, Challenges, Solutions

What we are interested in: To predict transition and turbulence in high-speed flows with Non-Thermochemical-Equilibrium (NTE).

Challenges of NTE turbulence:

- The Kolmogorov paradigm is questionable due to baroclinic-type production of energy at all scales of turbulence
  - Consequences: The premises of large-eddy simulations and other popular closures are not completely valid
  - Solution: Starting from fundamental first principles: Direct Numerical Simulations (DNS)
- High Mach and Reynolds numbers, moderate Knudsen number, high temperature and thermochemical nonequilibrium
  - Consequences: Invalidating Navier-Stokes equations because the assumption of linear constitutive laws and even the basic premises of continuum mechanics begin to break down.
  - Solution: Kinetic methods based on the kinetic theory and Boltzmann equations

Why Kinetic Methods?

- Kinetic methods for CFD are derived from the Boltzmann equation as opposed to the Navier-Stokes (NS) equations.
- Boltzmann equation provides theoretical connection between hydrodynamics and the underlying microscopic physics
- Kinetic methods can include extended hydrodynamics beyond the validity regime of NS equations
- Boltzmann equation is a first-order integro-partial-differential equation with a linear advection term, while NS equation is a second-order partial differential equation with a nonlinear advection term.

GKS: Kinetic Method for Compressible Flows

Kinetic methods for CFD: Lattice Boltzmann Method (LBM) and Gas Kinetic Scheme (GKS)[1]

- LBM: restricted to incompressible flows with low Mach number
- GKS: valid for fully compressible flows
    - Based on the Boltzmann equation and kinetic theory as oppose to Navier-Stokes equations and continuum theory
    - A unified approach for both the continuum and near-continuum flows
    - The fluxes are constructed from the single particle distribution function f in phase space $\mathbf{\Gamma} := (\boldsymbol{x}, \boldsymbol{\xi})$
    - Since f contains both equilibrium and non-equilibrium properties of flows, inviscid and viscous terms are obtained simultaneously

[1] K. Xu, J Comp Phys (2001); Phys Fluids (2002).

Kinetic Theory: Boltzmann Equation

The Boltzmann Equation with BGK approximation:

$$\partial_t f + \boldsymbol{\xi} \cdot \nabla f = \int [f_1' f_2' - f_1 f_2] d\mu \approx -\frac{1}{\lambda}[f - f^{(0)}], \quad f \equiv f(\boldsymbol{x}, \boldsymbol{\xi}, t). \tag{1}$$

The Boltzmann-Maxwellian equilibrium distribution function:

$$f^{(0)} = \rho \, (2\pi RT)^{-D/2} \exp\left[-\frac{(\boldsymbol{\xi} - \boldsymbol{u})^2}{2RT}\right], \tag{2}$$

The macroscopic quantities are the hydrodynamic moments of f or $f^{(0)}$:

$$\rho = \int f d\boldsymbol{\xi} = \int f^{(0)} d\boldsymbol{\xi}, \tag{3a}$$

$$\rho \boldsymbol{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi} = \int \boldsymbol{\xi} f^{(0)} d\boldsymbol{\xi}, \tag{3b}$$

$$\rho \varepsilon = \frac{1}{2} \int (\boldsymbol{\xi} - \boldsymbol{u})^2 f d\boldsymbol{\xi} = \frac{1}{2} \int (\boldsymbol{\xi} - \boldsymbol{u})^2 f^{(0)} d\boldsymbol{\xi}. \tag{3c}$$

Kinetic Theory: Chapman-Enskog Analysis

Chapman-Enskog expansion:

$$f = \sum_{n=0}^{\infty} \varepsilon^n f^{(n)}, \qquad \partial_t = \sum_{n=0}^{\infty} \varepsilon^n \partial_{t_n} \qquad \varepsilon := \mathrm{Kn} \tag{4}$$

with the following constraints

$$\int d\boldsymbol{\xi} f^{(0)} \left(1,\, \boldsymbol{\xi},\, \frac{1}{2}(\boldsymbol{\xi} - \boldsymbol{u})^2\right) = (\rho,\, \rho\boldsymbol{u},\, \rho\varepsilon)\,, \tag{5a}$$

$$\int d\boldsymbol{\xi} f^{(n)} \left(1,\, \boldsymbol{\xi},\, \frac{1}{2}(\boldsymbol{\xi} - \boldsymbol{u})^2)\right) = (0,\, \mathbf{0},\, 0)\,, \qquad n \geq 1\,. \tag{5b}$$

Non-equilibrium Flow: a Multi-scale Problem

Through Chapman-Enskog expansion, hydrodynamic equations can be derived from Boltzmann equation at different orders,

$$
\begin{aligned}
&\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) = 0 \\
&\partial_t (\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla \cdot \sum_{n=0}^{\infty} \varepsilon^n \mathsf{P}^{(n)} \\
&\partial_t (\rho E) + \nabla \cdot (\rho \boldsymbol{u} E) = -\nabla \cdot (\boldsymbol{u} \cdot \sum_{n=0}^{\infty} \varepsilon^n \mathsf{P}^{(n)}) - \nabla \cdot \sum_{n=0}^{\infty} \varepsilon^n \boldsymbol{Q}^{(n)}
\end{aligned}
\tag{6}
$$

Here, pressure tensor P and heat flux $\boldsymbol{Q}$ are expanded to n-th order,

$$\mathsf{P} = \sum_{n=0}^{\infty} \varepsilon^n \mathsf{P}^{(n)} \qquad \text{and} \qquad \boldsymbol{Q} = \sum_{n=0}^{\infty} \varepsilon^n \boldsymbol{Q}^{(n)}$$

$\mathsf{P}^{(n)}$ and $\boldsymbol{Q}^{(n)}$ present multi-scale nature of the non-equilibrium flows

For $n = 0$ and 1 $\longrightarrow$ Euler and Navier-Stokes equations

For $n = 2$ and 3 $\longrightarrow$ Burnett and super-Burnett equations

Integral Solution of Continuous Boltzmann Equation

Rewrite the Boltzmann BGK Equation in the form of ODE:

$$D_t f + \frac{1}{\tau} f = \frac{1}{\tau} f^{(0)}\,, \qquad\qquad D_t \equiv \partial_t + \boldsymbol{\xi}\cdot\nabla\,. \tag{7}$$

Integrate Eq. (7) over a time step (from 0 to t) along characteristics:

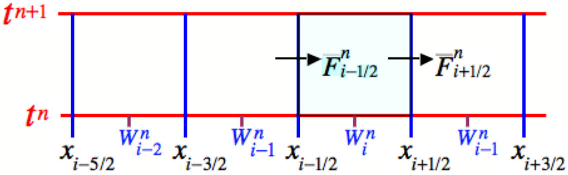
$$\begin{aligned} f(\boldsymbol{x}+\boldsymbol{\xi}t,\, \boldsymbol{\xi},\, t) = e^{t/\tau}\, f(\boldsymbol{x},\, \boldsymbol{\xi},\, t) \\ + \frac{1}{\tau} e^{-t/\tau} \int_0^t e^{t'/\tau}\, f^{(0)}(\boldsymbol{x}+\boldsymbol{\xi}t',\, \boldsymbol{\xi},\, t+t')\, dt'\,. \end{aligned} \tag{8}$$

LBM: Finite difference.
GKS: Finite volume.

Derivation of GKS: 1-D Example

- GKS is a Finite Volume Method (FVM) for compressible flows
- In a FVM, W_i^n is allowed to change only due to fluxes at the boundary of the control volumes

$$W_i^{n+1} = W_i^n - \frac{1}{\Delta x}(\bar{F}_{i+1/2}^n - \bar{F}_{i-1/2}^n) \tag{9}$$



- Different from usual FVMs, GKS computes $\bar{F}_{i\pm 1/2}$ at cell interface from distribution function f — solution of Boltzmann equation

$$F_\alpha^{i+1/2} = \int \xi_\alpha \Psi f(x_{i+1/2}, t) d\boldsymbol{\xi} \qquad \bar{F}_\alpha^{i\pm 1/2} = \int_0^{\Delta t} F_\alpha^{i\pm 1/2} dt \tag{10}$$

Construction of Gas Kinetic Scheme

- Integral solution of continuous Boltzmann equation in 1-D

$$f(x,t) = \underbrace{e^{-t/\tau} f_0(x - \xi t)}_{\text{initial part}} + \underbrace{\frac{1}{\tau}\int_0^t f^{(0)}(x', t') e^{-(t-t')/\tau} dt'}_{\text{inhomogeneous part}} \tag{11}$$

  where $x' := x - \xi(t - t')$

- Procedures of constructing f at cell interface $(x_{i+1/2} = 0)$:
  - Initial data: hydrodynamic variables $(\rho, \rho \boldsymbol{u}, \rho E)$ and their 1st order gradients at $(x_{i+1/2} = 0)$
  - 1) Compute $f_0(x)$ up to Navier-Stokes order by Chapman-Enskog expansions: $f_0(x) = f_0^{(0)} + \tau f_0^{(1)} = (1 - \tau D_t) f_0^{(0)}(x)$
    2) Taylor-expand $f_0^{(0)}(x)$ from $(x, 0)$ to cell interface $(x_{i+1/2} = 0, 0)$
  - Taylor-expand $f^{(0)}(x,t)$ from (x,t) to $(x_{i+1/2} = 0, 0)$
  - $f^{(0)}(x_{i+1/2} = 0, 0)$ can be determined by initial data
  - $f(x_{i+1/2} = 0, t)$ is determined with $f_0(x)$ and $f^{(0)}(x,t)$ determined

Boundary and Initial Conditons of DHIT

Domain of size $L^3 = (2\pi)^3$ with periodic boundary conditions, mesh size N^3, a divergence-free random initial velocity field $\boldsymbol{u}_0(\boldsymbol{x})$ is specified with its rms:

$$u' := \frac{1}{\sqrt{3}} \sqrt{\langle \boldsymbol{u} \cdot \boldsymbol{u} \rangle} \tag{12}$$

The initial energy spectrum $\tilde{E}_0(k)$ in the Fourier space $\boldsymbol{k}$:

$$\tilde{E}_0(k) = A k^4 \exp(-2k^2/k_0^2) \tag{13}$$

where $A = 1.3 \times 10^{-4}$ and $k_0 = 8$. At $t = 0$:

$$\mathrm{Re}_\lambda := \frac{\langle \rho \rangle u' \lambda}{\langle \mu \rangle}, \quad \mathrm{Ma_t} := \frac{\sqrt{3} u'}{\langle c_s \rangle} = \frac{\sqrt{3} u'}{\sqrt{\gamma R T_0}}$$

With u', Re_λ and $\mathrm{Ma_t}$ given at $t = 0$, the initial values of ρ_0, T_0, and μ_0 can be determined.

Statistical Quantities of Turbulence

Energy spectrium $\tilde{E}$, kinetic energy K, dissipation ε, transverse Taylor-microscale length λ, Kolmogorov scale η: [2,3]

$$\tilde{E}(\boldsymbol{k}, t) := \frac{1}{2}\tilde{\boldsymbol{u}}(\boldsymbol{k}, t) \cdot \tilde{\boldsymbol{u}}^{\dagger}(\boldsymbol{k}, t), \tag{14a}$$

$$K(t) := \frac{1}{2}\langle \rho \boldsymbol{u} \cdot \boldsymbol{u} \rangle \tag{14b}$$

$$\varepsilon(t) := 2\left\langle \frac{\mu}{\rho}\boldsymbol{u} \cdot \nabla^2 \boldsymbol{u} \right\rangle \tag{14c}$$

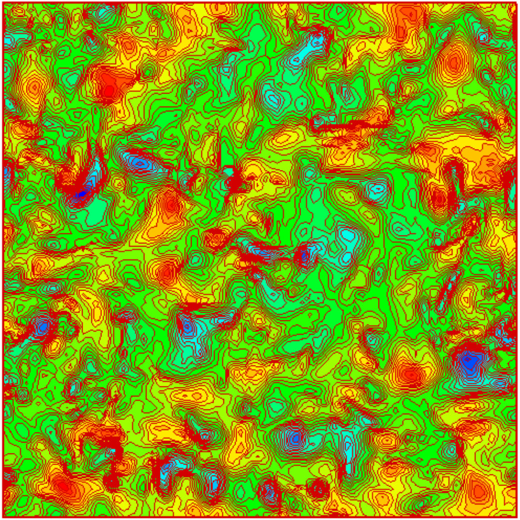
$$\lambda := \sqrt{\frac{10\nu K(t)}{\varepsilon(t)}} \tag{14d}$$

$$\eta := (\langle \mu/\rho \rangle^3/\varepsilon)^{1/4} \tag{14e}$$

[2] R. Sarkar *et al.* J. Fluid Mech. **227**:473-493 (1991).

[3] R. Santaney, D. I. Pullin, and B. Kosović. Phys. Fluids **13**(5):1415-1430 (2001).

Shocklets in Compressible DHIT



Density contours at $Re_\lambda = 72$, $Ma_t = 0.5$

Two-Point and "Shocklet" Statistics

The two-point longitudinal velocity difference:[4]

$$\delta u(\boldsymbol{r}|\delta\boldsymbol{r}) := \delta\hat{\boldsymbol{r}} \cdot [\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{r}+\delta\boldsymbol{r})], \quad \delta\hat{\boldsymbol{r}} := \frac{\delta\boldsymbol{r}}{\|\delta\boldsymbol{r}\|} \tag{15}$$

The normal upstream shock Mach number $\mathrm{Ma}_\perp$ is defined by

$$\frac{\delta u}{c_s} = -\frac{2}{1+\gamma}\left(\mathrm{Ma}_\perp - \frac{1}{\mathrm{Ma}_\perp}\right) \tag{16}$$

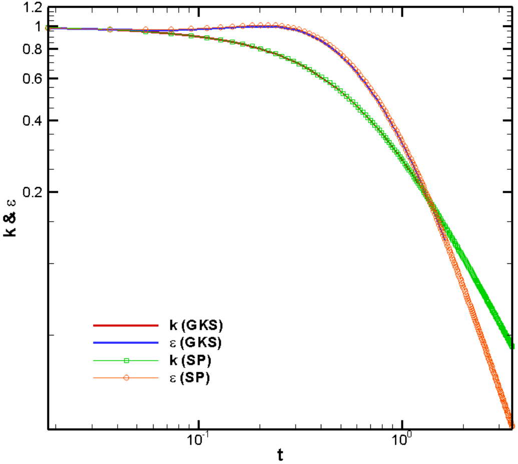
The shock strength χ is defined as

$$\chi := (\mathrm{Ma}_\perp - 1) \tag{17}$$

To compute Probability Distribution Functions (PDF) of δu and χ from DNS results.

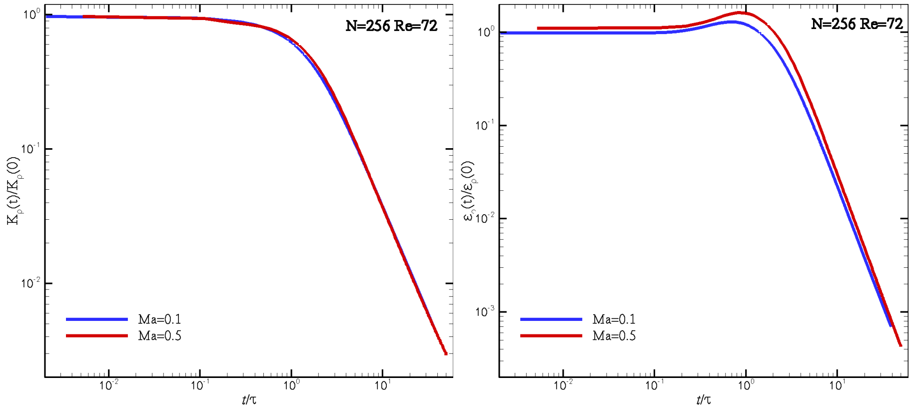
[4] R. Santaney, D. I. Pullin, and B. Kosović. Phys. Fluids **13**(5):1415-1430 (2001).

Verification of GKS for DNS of DHIT



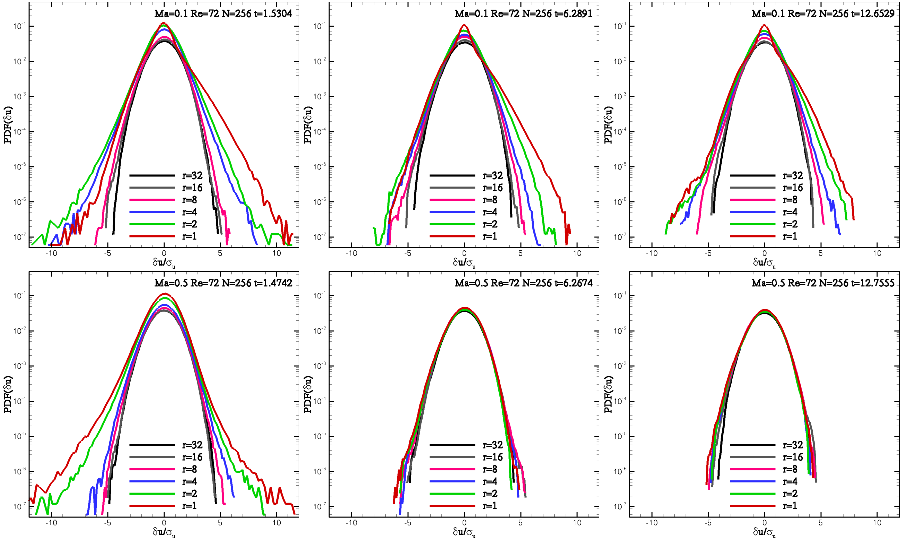
Comparison of GKS and Pseudo Spectrum (SP) Methods for DHIT in the near incompressible region ($Re_\lambda = 24$, $Ma_t = 0.1$).

DHIT: Mach number $\mathrm{Ma_t}$ effect on $K(t)$ and $\varepsilon(t)$

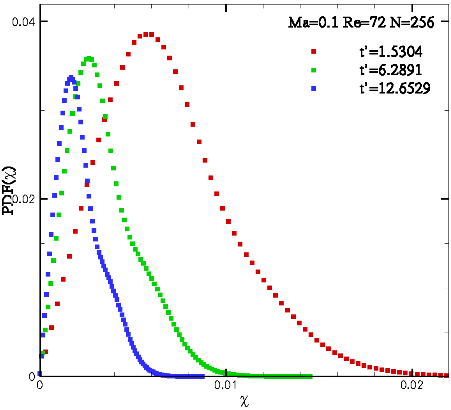


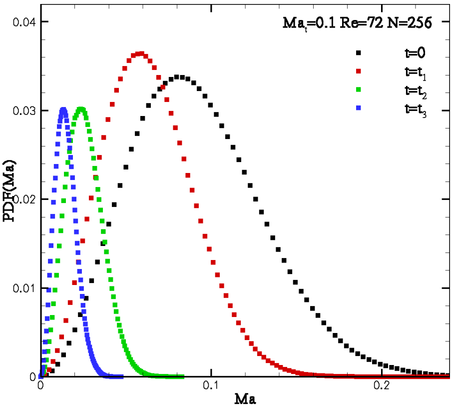
	n_K	n_ε
$\mathrm{Ma_t}(0) = 0.1$	1.4942	1.3950
$\mathrm{Ma_t}(0) = 0.5$	1.4973	1.5169

DHIT: PDF of longitudinal δu, $\mathrm{Ma_t} = 0.1$ and 0.5

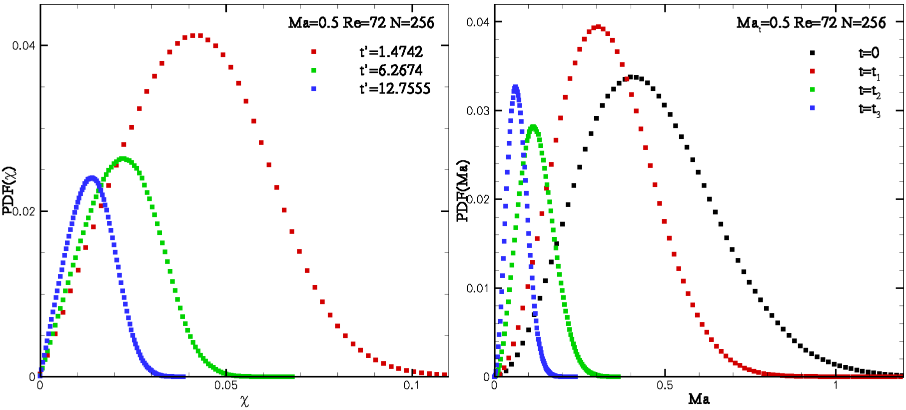


Statistics of shocklet strength and Ma: $Ma_t = 0.1$

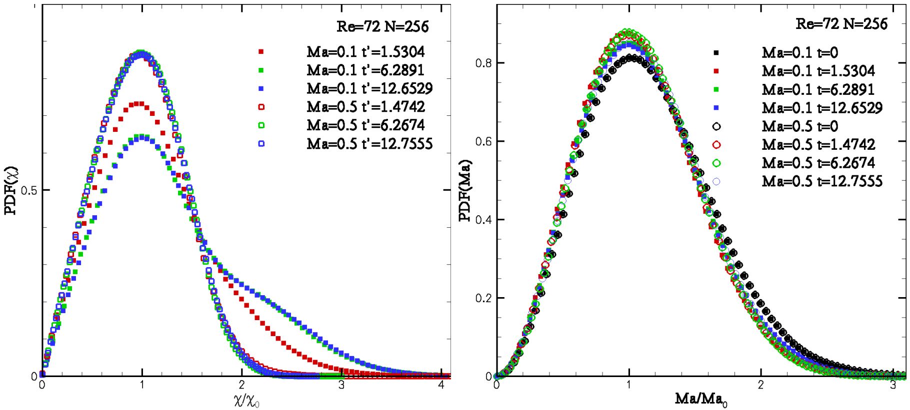




Statistics of shocklet strength and Ma: $\mathrm{Ma_t} = 0.5$



Statistics of shocklet strength and Ma: Scaling



Rescale the PDF's of χ and Ma:

1)Their maxima are always located at 1

2) PDFs satisfy the normalization condition

$$\int_0^{+\infty} P(x)dx = 1, \quad x = \chi \text{ or } \text{ Ma}.$$

Summary

1. With initial Re_λ fixed, increase of initial $\mathrm{Ma_t}$ leads to the increase of ε at the *initial* stage.
2. Change of $\mathrm{Ma_t}$ has no effect on $K(t)$ and the asymptotics of $\varepsilon(t)$.
3. At the lower $\mathrm{Ma_t}$ (=0.1), intermittency persists; while at higher $\mathrm{Ma_t}$ (=0.5), intermittency quickly dies, *i.e.*, $P(\delta u(r), t)$ becomes Gaussian independent of the separation distance r.
4. The PDF's of both shock strength χ, $P(\chi, t)$, and the local Mach number Ma, $P(\mathrm{Ma}, t)$ all appear to follow some scaling laws.

On-going work:

1. Multi-temperature non-equilibrium.
2. Multi-species.