A Kinetic Description of Morphing Continuum Theory and Its Applications

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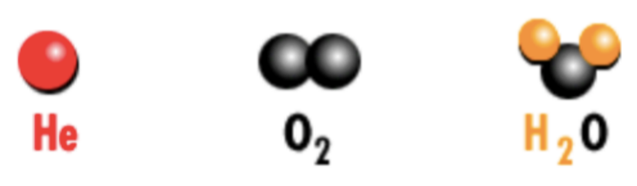
March 8, 2016

Outline

- Introduction and Motivation
- Morphing Continuum Theory - Kinematics
- Morphing Continuum Theory - Balance Law
- Morphing Continuum Theory - Constitutive Equations
- Morphing Continuum Theory - Pathway to N-S Equations
- Advanced Kinetic Theory - Morphing Continuum
- Advanced Kinetic Theory - Boltzmann-Curtiss Distribution
- Advanced Kinetic Theory - Transport Equations
- Numerical Example - Couette Flow with Slip
- Numerical Example - Zero-pressure Gradient Flat Plate
- Numerical Example - Stand-off Distance Growth

Monatomic Gases vs Polyatomic Gases



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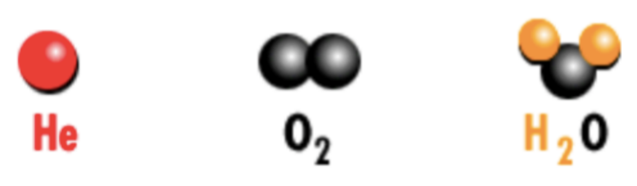

Boltzmann Equations and Classical Continuum Theromechanics are for Monatomic Gases

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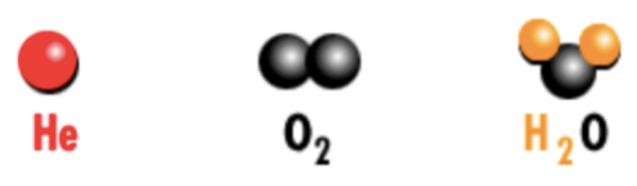

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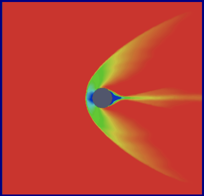
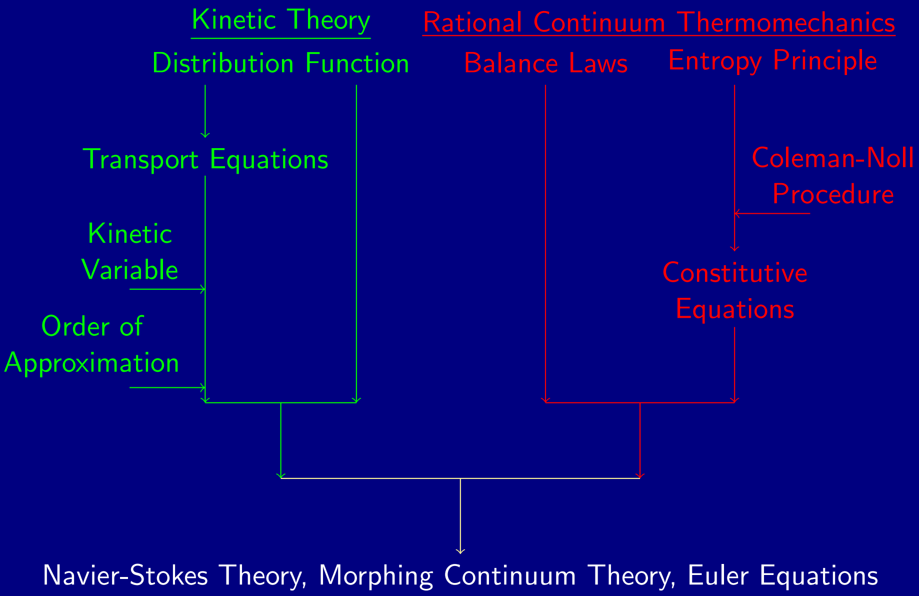


Continuum Theory for Gas Flow ?

1. Real gases - Polyatomic
2. High Mach and Rarefied Flow - Nonequilibrium
3. Turbulence - Multiscale

Roadmap to Continuum Theory

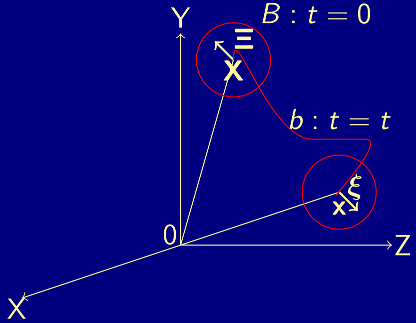


MCT - Kinematics

Motion

$$x_k^{\text{MCT}}(X_K^{\text{MCT}}, t) \qquad X_K^{\text{MCT}}(x_k^{\text{MCT}}, t)$$

$$\xi_k^{\text{MCT}} = \chi_{kK}^{\text{MCT}} \Xi_K^{\text{MCT}} \qquad \Xi_K^{\text{MCT}} = \bar{\chi}_{Kk}^{\text{MCT}} \xi_k^{\text{MCT}}$$



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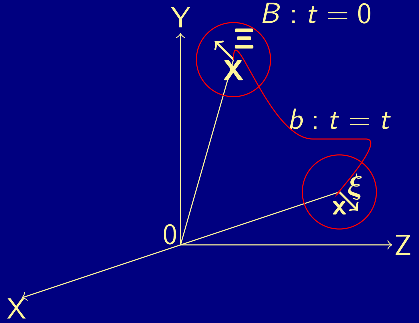

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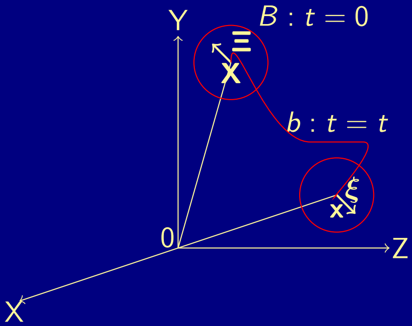
Deformation Rate Tensors

$$a_{kl} = v_{l,k}^{\text{MCT}} + e_{lkm}\omega_m^{\text{MCT}}$$

$$b_{kl} = \omega_{k,l}^{\text{MCT}}$$

MCT - Kinematics



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Deformation Rate Tensors

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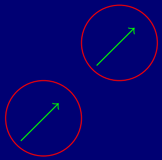
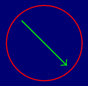
Vorticity



Gyration



MCT - Balance Laws

Conservation of Mass

$$\frac{\partial \rho}{\partial t} + (\rho v_i^{\mathsf{MCT}})_{,i} = 0$$

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$m_{lk,l} + e_{ijk} t_{ij} + \rho i_{km}(l_m - \dot{\omega}_m^{\mathrm{MCT}}) = 0$

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Conservation of Energy

$$\rho \dot{e} - t_{kl} a_{kl} - m_{kl} b_{lk} + q_{k,k} = 0$$

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Clausius-Duhem Inequality (Entropy Principle)

$$\rho(\dot{\psi} + \eta \dot{\theta}) + t_{kl} a_{kl} + m_{kl} b_{lk} - \frac{q_k}{\theta} \theta_{,k} \geq 0$$

MCT - Constitutive Equations

Coleman-Noll Procedure

$$\rho(\dot{\psi} + \eta\dot{\theta}) + t_{kl}a_{kl} + m_{kl}b_{lk} - \frac{q_k}{\theta}\theta_{,k} \geq 0$$

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Onsager's Reciprocal Relations

$$\mathbf{J}(\mathbf{Z}^R; \mathbf{Z}^D) \cdot \mathbf{Z}^D \geq 0$$

$$\mathbf{J} = \frac{\partial\Psi(\mathbf{Z}^R, \mathbf{Z}^D)}{\partial\mathbf{Z}^D} + \mathbf{U}$$

$$\Psi = \frac{1}{2}\lambda a_{mm}a_{mm} + \frac{1}{2}\mu a_{mn}a_{mn} + \frac{1}{2}(\mu + \kappa)a_{mn}a_{nm} + \frac{1}{2}\alpha b_{mm}b_{mm} + \frac{1}{2}\beta b_{mn}b_{nm} + \frac{1}{2}\gamma b_{mn}b_{nm} + \frac{1}{2}K\frac{\theta_{,m}}{\theta}\frac{\theta_{,m}}{\theta} + \alpha_T\frac{\theta_{,m}}{\theta}e_{mnp}b_{pn}$$

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Linear Constitutive Equations

$$t_{kl} = -p\delta_{kl} + \lambda v^{\mathrm{MCT}}_{m,m}\delta_{kl} + (\mu+\kappa)(v^{\mathrm{MCT}}_{l,k} + e_{lkm}\omega^{\mathrm{MCT}}_m) + \mu(v^{\mathrm{MCT}}_{k,l} + e_{klm}\omega^{\mathrm{MCT}}_m)$$

$$m_{kl} = \alpha_T e_{klm}\frac{\theta_{,m}}{\theta} + \alpha\omega^{\mathrm{MCT}}_{m,m}\delta_{kl} + \beta\omega^{\mathrm{MCT}}_{k,l} + \gamma\omega^{\mathrm{MCT}}_{l,k}$$

$$q_m = \alpha_T e_{klm}\omega^{\mathrm{MCT}}_{k,l} + K\frac{\theta_{,m}}{\theta}$$

MCT - Constitutive Equations

Linear Thermodynamic Matrix

$$\begin{bmatrix} t_{(kl)} \\ t_{[kl]} \\ m_{(kl)} \\ m_{[kl]} \\ q_m \end{bmatrix} = \begin{bmatrix} \lambda\delta_{kl} + 2\mu + \kappa & 0 & 0 & 0 & 0 \\ 0 & \kappa & 0 & 0 & 0 \\ 0 & 0 & \alpha\delta_{kl} + \beta + \gamma & 0 & 0 \\ 0 & 0 & 0 & \beta - \gamma & \alpha_T e_{klm} \\ 0 & 0 & 0 & \alpha_T e_{klm} & K \end{bmatrix} \begin{bmatrix} a_{(kl)} \\ a_{[kl]} \\ b_{(kl)} \\ b_{[kl]} \\ \frac{\theta_{,m}}{\theta} \end{bmatrix}$$

1. Thermodynamic Fluxes v.s. Thermodynamic Forces

MCT - Constitutive Equations

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1. Thermodynamic Fluxes v.s. Thermodynamic Forces
2. Symmetry of the thermodynamic matrix - Onsager's Reciprocal Relations (1968 Nobel Prize in Chemistry)

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1. Thermodynamic Fluxes v.s. Thermodynamic Forces
2. Symmetry of the thermodynamic matrix - Onsager's Reciprocal Relations (1968 Nobel Prize in Chemistry)
3. Nonlinear Onsager Theory of Irreversibility (Edelen, 1972; Chen, 2013)

MCT Governing Equations

Conservation of Linear Momentum

$$\frac{\partial}{\partial t}(\rho v_j^{\mathrm{MCT}}) + \frac{\partial}{\partial x_i}(\rho v_j^{\mathrm{MCT}} v_i^{\mathrm{MCT}}) = - p_{,j} + (\lambda + \mu) v_{m,mj}^{\mathrm{MCT}} + (\mu + \kappa) v_{j,mm}^{\mathrm{MCT}} + \kappa e_{jki} \omega_{i,k}^{\mathrm{MCT}}$$

Conservation of Angular Momentum

$$\frac{\partial}{\partial t}(\rho i_{jk} \omega_k^{\mathrm{MCT}}) + \frac{\partial}{\partial x_i}(\rho i_{jk} \omega_k^{\mathrm{MCT}} v_i^{\mathrm{MCT}}) = (\alpha + \beta) \omega_{m,mj}^{\mathrm{MCT}} + \gamma \omega_{j,mm}^{\mathrm{MCT}} + \kappa (e_{jki} v_{i,k}^{\mathrm{MCT}} - 2\omega_j^{\mathrm{MCT}})$$

MCT - Pathway to NS Equations

How to determine swirling motion?

$$\boldsymbol{\omega}^{\mathsf{MCT}} = \frac{1}{2}\nabla \times \mathbf{v}^{\mathsf{MCT}}$$

MCT - Pathway to NS Equations

How to determine swirling motion?

$$\omega^{\mathrm{MCT}} = \frac{1}{2}\nabla \times \mathbf{v}^{\mathrm{MCT}}$$

Linear Momentum → Navier-Stokes Equations

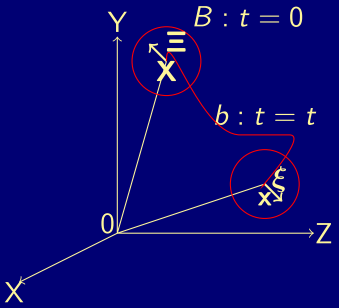
$$\frac{\partial}{\partial t}(\rho v_j^{\mathrm{MCT}}) + \frac{\partial}{\partial x_i}(\rho v_j^{\mathrm{MCT}} v_i^{\mathrm{MCT}}) = + (\mu^* + \lambda) v_{m,mj}^{\mathrm{MCT}} + \mu^* v_{j,mm}^{\mathrm{MCT}}$$

Angular Momentum → Vorticity Equations

$$\frac{\partial}{\partial t}(\rho i_{jk}(e_{pqk} v_{q,p}^{\mathrm{MCT}})) + \frac{\partial}{\partial x_i}(\rho(i_{jk} e_{pqk} v_{q,p}^{\mathrm{MCT}}) v_i^{\mathrm{MCT}}) = \gamma(e_{pqk} v_{q,p}^{\mathrm{MCT}})_{,mm}$$

Advanced Kinetic Theory for Morphing Continuum

Morphing Continuum Theory



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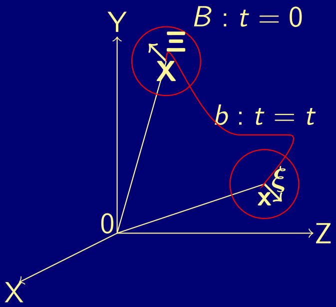
$$q_m = \alpha_T e_{klm}\omega^{MCT}_{k,l} + K\frac{\theta_{,m}}{\theta}$$

Advanced Kinetic Theory for Morphing Continuum

Morphing Continuum Theory



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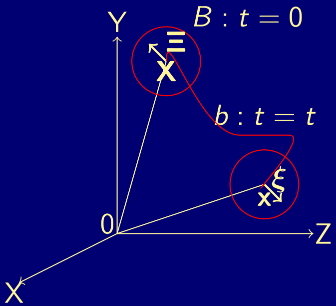
Eringen, 1966; Chen et. al., 2011; Hansen, 2013

Advanced Kinetic Theory for Morphing Continuum

Morphing Continuum Theory



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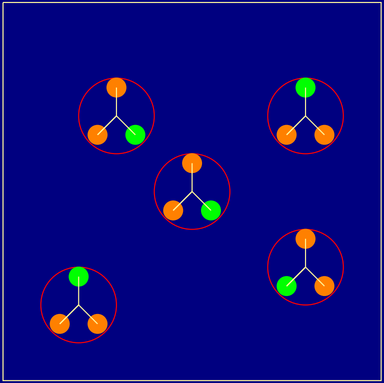
$q_m = \alpha_T e_{klm}\omega_{k,l}^{MCT} + K\frac{\theta_{,m}}{\theta}$

Eringen, 1966; Chen et. al., 2011; Hansen, 2013

1. What kind of system can Morphing Continuum describe?
2. How do we determine the physical meanins of the material constants in Rational Continuum Thermomechanics?
3. Can we use the rotation to represent the motions of polyatomic gases?

Advanced Kinetic Theory - Boltzmann-Curtiss Equations



$$\bar{f}(\mathbf{x}, \mathbf{p}, \phi, \mathbf{M}, t) = \int f(\mathbf{x}, \mathbf{p}, \phi, \mathbf{M}, E_{\text{vib}} t) dE_{\text{vib}} d\tau,$$

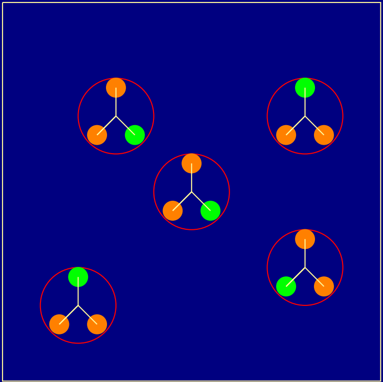
$$(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m}\frac{\partial}{\partial \mathbf{x}} + \frac{\mathbf{M}}{I}\frac{\partial}{\partial \phi})\bar{f} = \sum_{\beta} \mathbf{Z}_{\beta}$$

$$\frac{\partial}{\partial t} n\chi + \frac{\partial}{\partial x_i} n\chi v_i - n v_i \frac{\partial \chi}{\partial x_i} + \frac{\partial}{\partial \phi_i} n\chi\omega_i - n\omega_i \frac{\partial \chi}{\partial \phi_i} = 0$$

$$\Rightarrow \frac{\partial}{\partial t} n\chi + \frac{\partial}{\partial x_i} n\chi v_i - n v_i \frac{\partial \chi}{\partial x_i} = 0$$

(Curtiss, 1992)

Advanced Kinetic Theory - Boltzmann-Curtiss Equations



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(Curtiss, 1992)

$$\bar{f}(\mathbf{x}, \mathbf{v}, \omega) = \left(\frac{\sqrt{mI}}{2\pi k\theta}\right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\omega^2}{2k\theta}\right]$$

Boltzmann-Curtiss Distribution

$$\bar{f}(\mathbf{x}, \mathbf{v}, \omega) = \left(\frac{\sqrt{mI}}{2\pi k\theta} \right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\omega^2}{2k\theta} \right]$$

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Boltzmann's H-Theorem

$$H(t) = \int_0^\infty f(E,t)[log(\frac{f(E,t)}{\sqrt{E}}) - 1]dE$$

Boltzmann-Curtiss Distribution

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Boltzmann's H-Theorem

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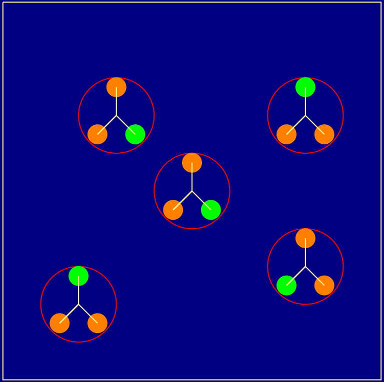
McDowell's Approach (McDowell, 1999)

$$W = \frac{N!}{\sum_{i=0}^{m} n_i!} \qquad S = k \ln W$$

Boltzmann-Curtiss Distribution - Microstates



- N distinguishable polyatomic molecules
- Let ϵ_i denote the i-th nondegenerate energy level having n_i molecules, where $i = 0, 1, 2, 3, ..., m$.
- Constant temperature

Number of Microstates, W

$$W = \frac{N!}{\prod_{i=0}^{m} n_i!} \qquad \sum_{i=0}^{m} n_i = N.$$

Boltzmann-Curtiss Distribution - Boltzmann Principle

$$S = k \ln W = k \ln\left(\frac{N!}{\prod_{i=0}^{m} n_i!}\right) = k[\ln(N!) - \sum_{i=0}^{m} \ln(n_i!)].$$

Boltzmann-Curtiss Distribution - Boltzmann Principle

$$S = k \ln W = k \ln(\frac{N!}{\prod_{i=0}^{m} n_i!}) = k[\ln(N!) - \sum_{i=0}^{m} \ln(n_i!)].$$

Entropy Change

The change of entropy, $\triangle S$, between the two different states (before and after the energy injection, $\triangle \epsilon$) can be found as ...

$$\begin{aligned}\triangle S &= k \sum_{i=0}^{m} \{\ln(n_i!) - \ln[(n_i + \triangle n_i)!]\} \\ &= k \sum_{i=0}^{m} \triangle n_i [\ln(n_i) - \ln(n_i + \triangle n_i)] + O(\triangle n_i^2) \\ &\approx k \sum_{i=0}^{m} \triangle n_i \ln(\frac{n_i}{n_i + \triangle n_i})\end{aligned}$$

Boltzmann-Curtiss Distribution - Total Energy

Thermodynamics

- constant temperature
- $dS = \frac{dU}{\theta}$
- $\triangle U = \triangle \epsilon = \frac{1}{2}(m\triangle v^2 + I\triangle\omega^2)$

$$\triangle S = \int dS = \int \frac{dU}{\theta}$$
$$= \frac{1}{\theta}\int dU = \frac{1}{\theta}\triangle U$$

Boltzmann-Curtiss Distribution - Total Energy

Thermodynamics

- constant temperature
- $dS = \frac{dU}{\theta}$
- $\triangle U = \triangle\epsilon = \frac{1}{2}(m\triangle v^2 + I\triangle\omega^2)$

$$\triangle S = \int dS = \int \frac{dU}{\theta} = \frac{1}{\theta}\int dU = \frac{1}{\theta}\triangle U$$

$$\triangle S = \frac{1}{\theta}\triangle\epsilon = \frac{1}{2\theta}(m\triangle v^2 + I\triangle\omega^2)$$

Boltzmann-Curtiss Distribution - The Last Step

Bolzmann Principle

$$\triangle S \approx k \sum_{i=0}^{m} \triangle n_i \ln(\frac{n_i}{n_i + \triangle n_i})$$

Total Energy

$$\triangle S = \frac{1}{\theta} \triangle \epsilon = \frac{1}{2\theta}(m \triangle v^2 + I \triangle \omega^2)$$

Boltzmann-Curtiss Distribution

$$k \sum_{i=0}^{m} \triangle n_i \ln\left(\frac{n_i}{n_i + \triangle n_i}\right) = \frac{1}{2\theta}(m \triangle v^2 + I \triangle \omega^2),$$

$$\sum_{i=0}^{m} \left(\frac{n_i + \triangle n_i}{n_i}\right)^{\triangle n_i} = \exp[-\frac{m \triangle v^2 + I \triangle \omega^2}{2k\theta}].$$

Boltzmann-Curtiss Distribution - The Last Step

Bolzmann Principle

$$\triangle S \approx k \sum_{i=0}^{m} \triangle n_i \ln(\frac{n_i}{n_i + \triangle n_i})$$

Total Energy

$$\triangle S = \frac{1}{\theta}\triangle\epsilon = \frac{1}{2\theta}(m\triangle v^2 + I\triangle\omega^2)$$

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$$\bar{f}(\mathbf{x}, \mathbf{v}, \omega) = \left(\frac{\sqrt{mI}}{2\pi k\theta}\right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\omega^2}{2k\theta}\right]$$

From Kinetic Variables to Transport Equations

B-C Equation

$$(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m}\frac{\partial}{\partial \mathbf{x}} + \frac{\mathbf{M}}{I}\frac{\partial}{\partial \phi})\bar{f} = \sum_{\beta} \mathbf{Z}_{\beta},$$

Kinetic Variables

1. Mass
2. Linear Momentum
3. Angular Momentum
4. Internal Energy

B-C Distribution and Transport Equations

$$\bar{f}(\mathbf{x}, \mathbf{v}, \boldsymbol{\omega}) = \left(\frac{\sqrt{mI}}{2\pi k\theta}\right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\boldsymbol{\omega}^2}{2k\theta}\right]$$

$$\frac{\partial}{\partial t}n\chi + \frac{\partial}{\partial x_i}n\chi v_i - nv_i\frac{\partial \chi}{\partial x_i} = 0$$

Kinetic Variables in Advanced Kinetic Theory

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$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}(\rho U_i) = 0$

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Angular Momentum, $\chi_3 = m r_j r_m \omega_m$

$$\frac{\partial}{\partial t}(\rho i_{jm} W_m) + \frac{\partial}{\partial x_i}(\rho i_{jm} W_m U_i) = -\frac{\partial}{\partial x_i}(\rho i_{jm} < \omega_m' v_i' >)$$

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Internal Energy, $\chi_4 = \frac{1}{2} < v_m' v_m' >$

$$\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_i}(\rho e U_i)$$
$$= -\frac{\partial}{\partial x_i}(\frac{1}{2}\rho(< v_m' v_m' v_i' > + i_{mn} < \omega_m' \omega_n' v_i' >)) + \rho < v_i \frac{\partial e}{\partial x_i} >$$

Zero-order Approximation

Classical Boltzmann's Formulation for Monatomic Gases

If the system of monatomic gases is at the Boltzmann's distribution, the Boltzmann equations reduces to the Euler's equations, i.e. Navier-Stokes equations without dissipations.

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What if the system is at Boltzmann-Curtiss Distribution?

$$\bar{f}(\mathbf{x}, \mathbf{v}, \omega) \approx \bar{f}^0(\mathbf{x}, \mathbf{v}, \omega) = \left(\frac{\sqrt{mI}}{2\pi k\theta}\right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\omega^2}{2k\theta}\right]$$

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Comparison with Morphing Continuum Theory

Are the Boltzmann-Curtiss equations the same as the MCT equations without dissipations while the system is at the equilibrium?

Linear Momentum

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial}{\partial x_i}(\rho < v_i' v_j' > + \rho e_{jmn} r_n < v_i' \omega_m' >)$$

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Boltzmann Stress, $t_{ij}^{\text{Boltzmann},0}$

$$t_{ij}^{\text{Boltzmann},0} = \iint \rho v_i v_j \left(\frac{\sqrt{mI}}{2\pi k\theta}\right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\boldsymbol{\omega}^2}{2k\theta}\right] d^3\mathbf{v} d^3\boldsymbol{\omega} = \rho n k\theta \delta_{ij}$$

Linear Momentum

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Curtiss Stress, $t_{ij}^{\text{Curtiss},0}$

$$t_{ij}^{\text{Curtiss},0} = e_{jmn} r_n \iint \rho v_i' \omega_m' \left(\frac{\sqrt{mI}}{2\pi k\theta}\right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\boldsymbol{\omega}^2}{2k\theta}\right] d^3\mathbf{v} d^3\boldsymbol{\omega} = 0,$$

Linear Momentum

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial}{\partial x_i}(\rho < v_i' v_j' > + \rho e_{jmn} r_n < v_i' \omega_m' >)$$

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$$t_{ij}^{\text{Curtiss},0} = e_{jmn} r_n \iint \rho v_i' \omega_m' \left(\frac{\sqrt{mI}}{2\pi k\theta}\right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\omega^2}{2k\theta}\right] d^3\mathbf{v} d^3\boldsymbol{\omega} = 0,$$

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial}{\partial x_i}(\rho n k\theta)$$

Angular Momentum

$$\frac{\partial}{\partial t}(\rho i_{jm} W_m) + \frac{\partial}{\partial x_i}(\rho i_{jm} W_m U_i) = -\frac{\partial}{\partial x_i}(\rho i_{jm} < \omega'_m v'_i >)$$

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Moment Stress

$$m^0_{ij} = \iint \rho i_{jm} \omega'_m v'_i \left(\frac{\sqrt{mI}}{2\pi k\theta} \right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\boldsymbol{\omega}^2}{2k\theta} \right] d^3\mathbf{v} d^3\boldsymbol{\omega} = 0$$

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$$\frac{\partial}{\partial t}(\rho i_{jm} W_m) + \frac{\partial}{\partial x_i}(\rho i_{jm} W_m U_i) = 0$$

Internal Energy

$$\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_i}(\rho e U_i)$$
$$= -\frac{\partial}{\partial x_i}\left(\frac{1}{2}\rho(< v'_m v'_m v'_i > + i_{mn} < \omega'_m \omega'_n v'_i >)\right) + \rho < v_i \frac{\partial e}{\partial x_i} >$$

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Heat Flux

$$q_i^0 = \iint \frac{\rho}{2}(v'_m v'_m v'_i + i_{mn}\omega'_m \omega'_n v'_i) \left(\frac{\sqrt{mI}}{2\pi k\theta}\right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\boldsymbol{\omega}^2}{2k\theta}\right] d^3\mathbf{v} d^3\boldsymbol{\omega}$$
$$= 0$$

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$$= 0$$

Mechanical Energy

$$\rho < v_i \frac{\partial e}{\partial x_i} > = (t_{ij}^{\text{Curtiss}} + t_{ij}^{\text{Boltzmann}})\left(\frac{\partial v_j}{\partial x_i} + e_{jim}\omega_m\right) + m_{ij}\frac{\partial \omega_j}{\partial x_i} = \rho n k \theta v_{m,m}$$

Internal Energy

$$\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_i}(\rho e U_i)$$
$$= -\frac{\partial}{\partial x_i}\left(\frac{1}{2}\rho(< v'_m v'_m v'_i > + i_{mn} < \omega'_m \omega'_n v'_i >)\right) + \rho < v_i \frac{\partial e}{\partial x_i} >$$

Heat Flux

$$q_i^0 = \iint \frac{\rho}{2}(v'_m v'_m v'_i + i_{mn}\omega'_m \omega'_n v'_i)\left(\frac{\sqrt{ml}}{2\pi k\theta}\right)^3 \exp\left[-\frac{m\mathbf{v}^2 + I\boldsymbol{\omega}^2}{2k\theta}\right] d^3\mathbf{v} d^3\boldsymbol{\omega}$$
$$= 0$$

Mechanical Energy

$$\rho < v_i \frac{\partial e}{\partial x_i} > = (t_{ij}^{\text{Curtiss}} + t_{ij}^{\text{Boltzmann}})(\frac{\partial v_j}{\partial x_i} + e_{jim}\omega_m) + m_{ij}\frac{\partial \omega_j}{\partial x_i} = \rho n k\theta v_{m,m}$$

$$\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_i}(\rho e U_i) = \rho n k\theta v_{m,m}$$

MCT v.s. AKT

Advanced Kinetic Theory

1. $\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}(\rho U_i) = 0$
2. $\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial}{\partial x_i}(\rho n k \theta)$
3. $\frac{\partial}{\partial t}(\rho i_{jm} W_m) + \frac{\partial}{\partial x_i}(\rho i_{jm} W_m U_i) = 0$
4. $\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_i}(\rho e U_i) = \rho n k \theta v_{m,m}$

Morphing Continuum Theory

1. $\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_i}(\rho v_i^{\mathrm{MCT}}) = 0$
2. $\frac{\partial}{\partial t}(\rho v_j^{\mathrm{MCT}}) + \frac{\partial}{\partial x_i}(\rho v_j^{\mathrm{MCT}} v_i^{\mathrm{MCT}}) = -\frac{\partial p}{\partial x_i}$
3. $\frac{\partial}{\partial t}(\rho i_{jk} \omega_k^{\mathrm{MCT}}) + \frac{\partial}{\partial x_i}(\rho i_{jk} \omega_k^{\mathrm{MCT}} v_i^{\mathrm{MCT}}) = 0$
4. $\frac{\partial}{\partial t}(\rho e) + \frac{\partial}{\partial x_i}(\rho e v_i^{\mathrm{MCT}}) = p v_{m,m}$

MCT v.s. AKT

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Now, we know...

System of Polyatomic Gases at Equilibrium $\Longrightarrow$ MCT without Dissipation

Numerical Methods for Morphing Continuum

1. Continuity: $\dot{\rho} + \rho v_{l,l} = 0$
2. Linear Momentum:
   $\rho \dot{v}_k = -p_{,k} + (\lambda + \mu) v_{m,mk} + (\mu + \kappa) v_{k,mm} + \kappa e_{kij} \omega_{j,i} + \rho g_k$
3. Angular Momentum:
   $\rho i_{km} \dot{\omega}_m = (\alpha + \beta) \omega_{m,mk} + \gamma \omega_{k,mm} + \kappa (e_{kij} v_{j,i} - 2\omega_k) + \rho l_k$
4. Internal Energy: $\rho \dot{e} = t_{ij} (v_{j,i} + e_{jim} \omega_m) + m_{ij} \omega_{j,i} - q_{k,k}$

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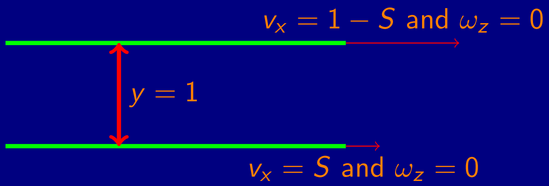
Numerical Solver; $\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} + \mathbf{S} = 0$

- Finite Difference Method: Unsteady 2-D incompressbile case for structured grids (Chen, et. al., 2011)
- Spectral Difference Method: High Order Unsteady 2-D compressible case for unstructured grids (Chen, et. al., 2012)
- Finite Volume Method: Unsteady 2-D subroutine in Fluent (Wonnell and Chen, 2015)
- Finite Volume Method: Unsteady 3-D compressible case for unstructured grids (Ongoing efforts)

Numerical Example - Couette Flow with Slip Velocity



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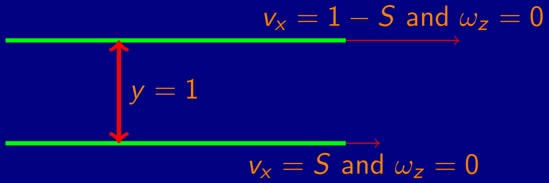
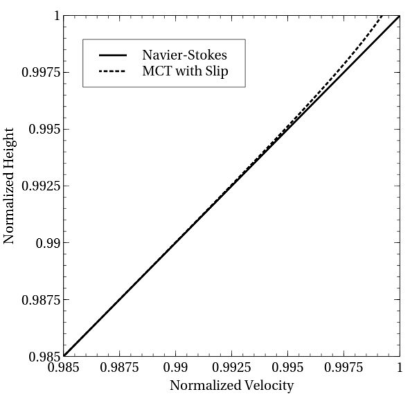


Analytical Solution

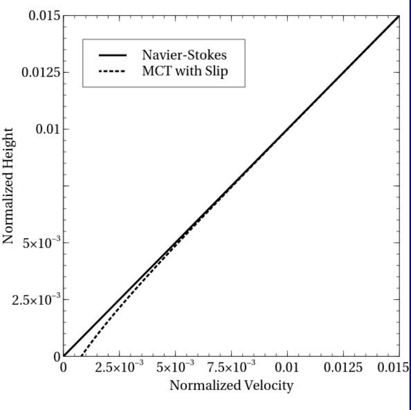
$$v_x = -\frac{\kappa}{(\mu+\kappa)M}(C_2 e^{My} - C_3 e^{-My}) + \frac{2(\mu+\kappa)}{2\mu+\kappa} C_1 y + C_4$$
$$\omega_z = C_2 e^{My} + C_3 e^{-My} - \frac{\mu+\kappa}{2\mu+\kappa} C_1$$
$$M^2 = \frac{\kappa(2\mu+\kappa)}{\gamma(\mu+\kappa)}$$
$$C_1 = (1-2S)/(\frac{2\kappa}{M(2\mu+\kappa)}\frac{(e^{-M}-1)(1-e^M)}{e^{-M}-e^M} + \frac{2(\mu+\kappa)}{2\mu+\kappa})$$
$$C_2 = \frac{\mu+\kappa}{2\mu+\kappa}\frac{e^{-M}-1}{e^{-M}-e^M} C_1$$
$$C_3 = \frac{\mu+\kappa}{2\mu+\kappa}\frac{1-e^M}{e^{-M}-e^M} C_1$$
$$C_4 = \frac{\kappa}{(\mu+\kappa)M}(C_2 - C_3) + S$$

Slip Velocity & Knudsen Layer

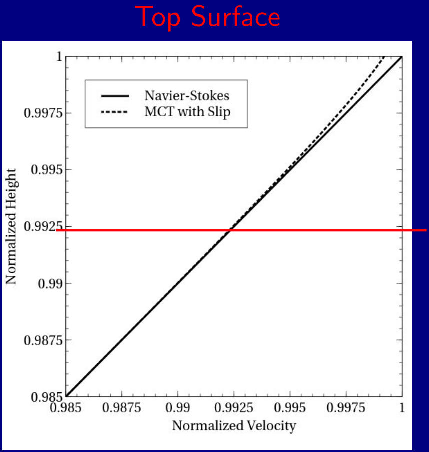
Top Surface

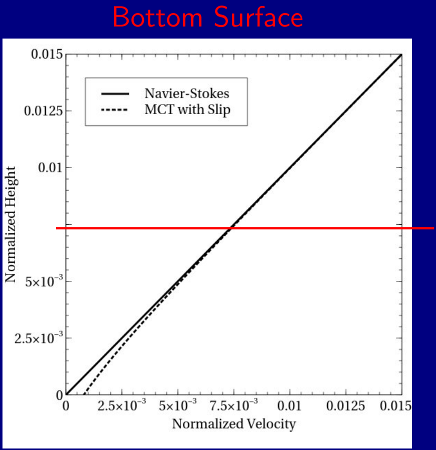


Bottom Surface



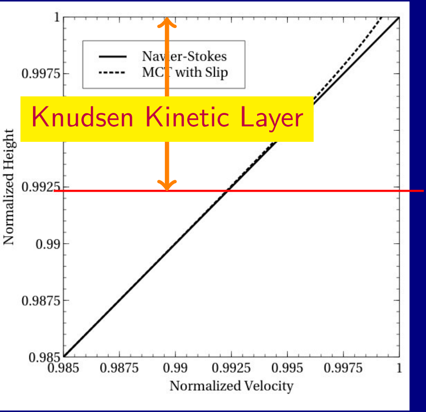
Slip Velocity & Knudsen Layer



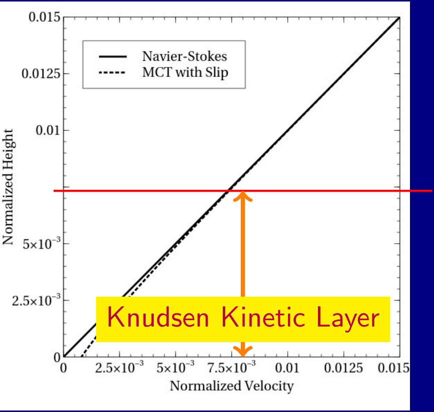


Slip Velocity & Knudsen Layer

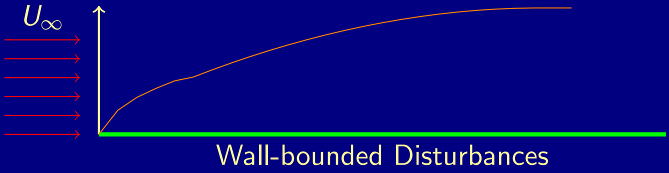
Top Surface



Bottom Surface

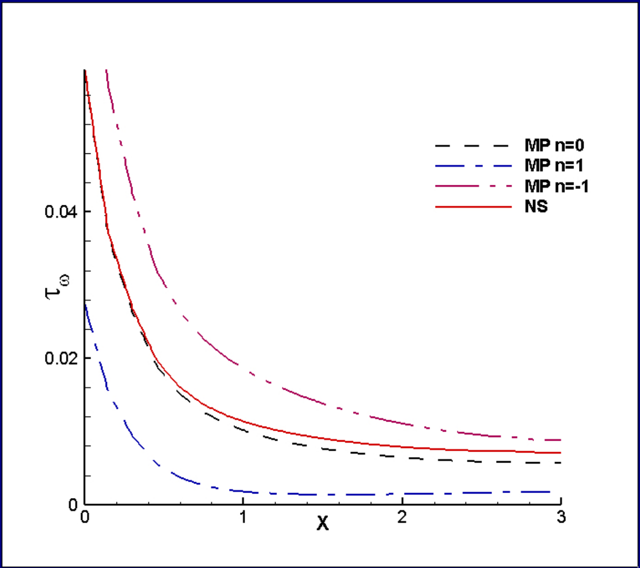


Numerical Example - Zero Pressure Gradient Flat Plate (ZPG)

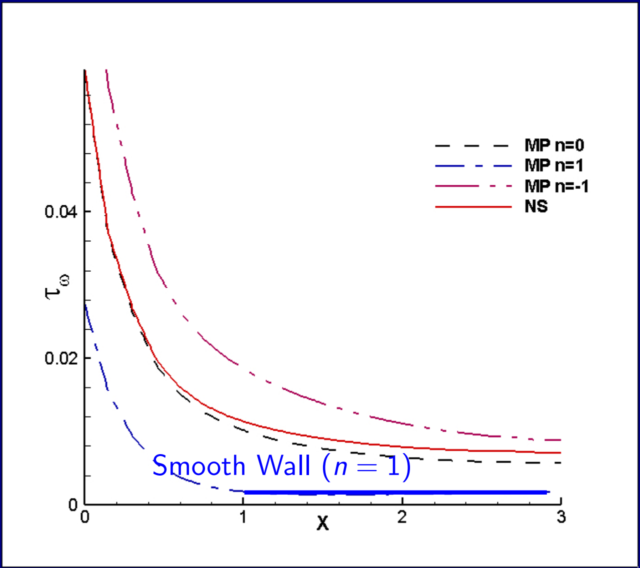


$$\omega_k^{\mathrm{MCT}} = n e_{ijk} v_{j,i}^{\mathrm{MCT}}$$

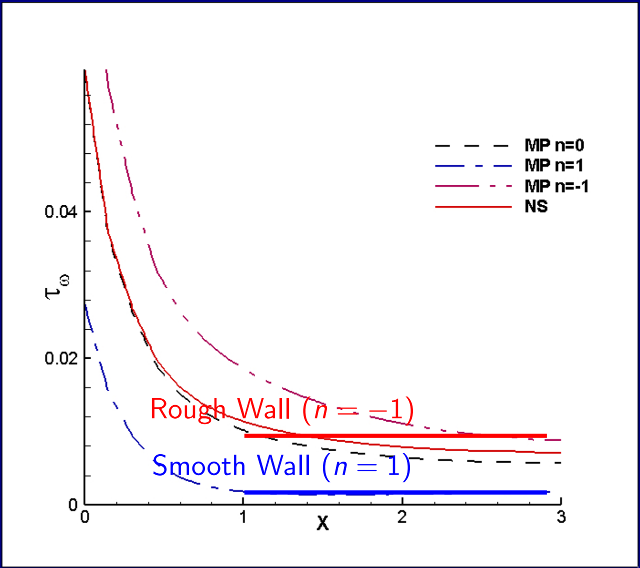
ZPG : Wall Roughness for Microfluids



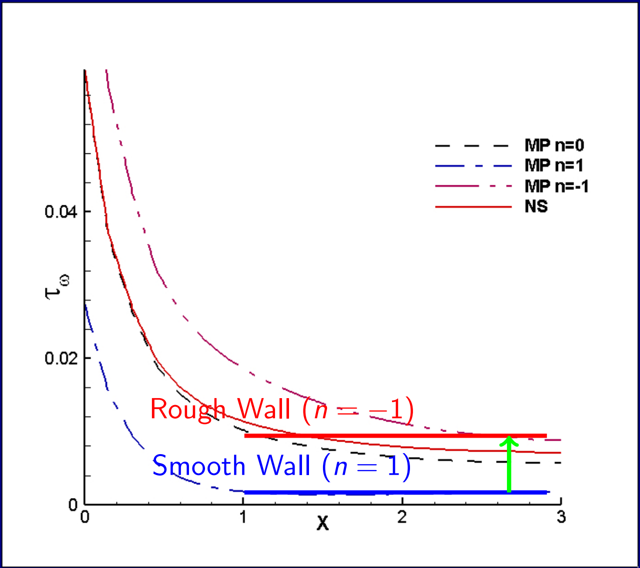
ZPG : Wall Roughness for Microfluids



ZPG : Wall Roughness for Microfluids



ZPG : Wall Roughness for Microfluids

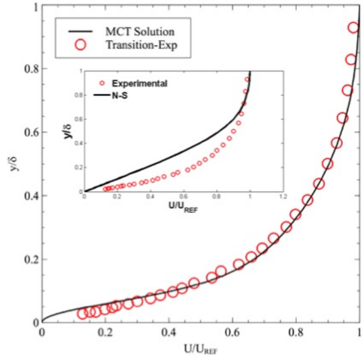


ZPG : Numerical Results (MCT v.s. NS v.s. Experiment)

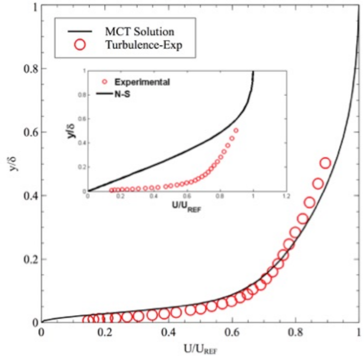
$$\text{Reynolds Number in MCT} = Re_L = \frac{\rho VL}{\mu+\kappa} = 1,000,000$$

$$\text{Disturbances: } \omega_k^{\text{MCT}} = n e_{ijk} v_{j,i}^{\text{MCT}}$$

Transitional Flow

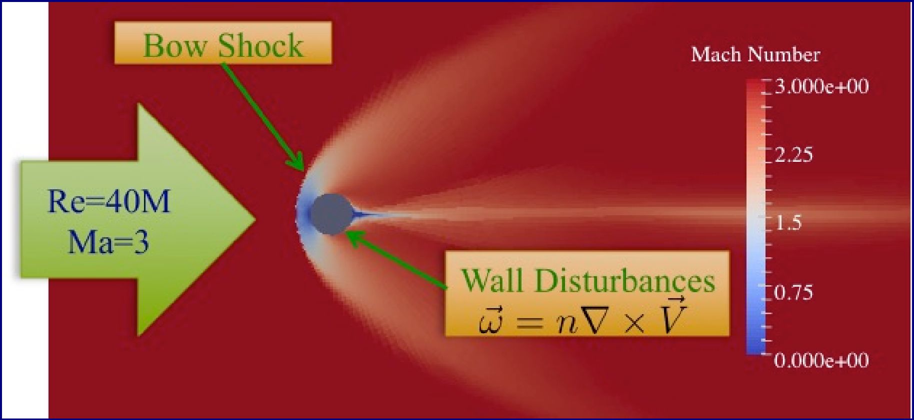


Turbulent Flow

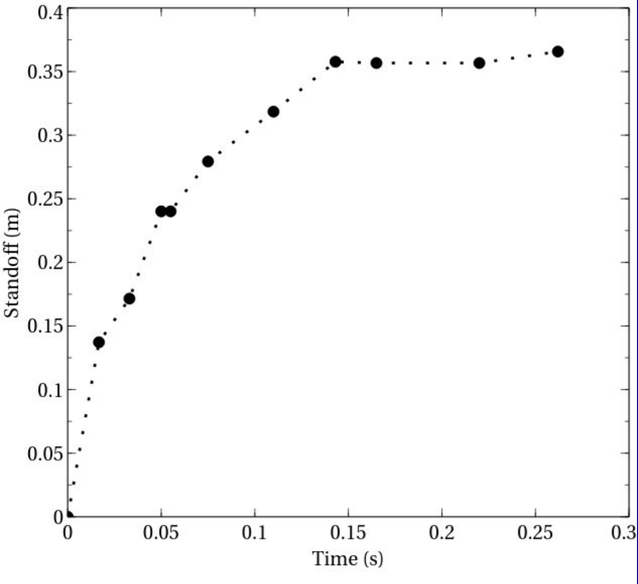


Experiment Source: ERCOFTAC C20 Flat Plate Boundary Layer Case

Numerical Example - Supersonic Flow past a Cylinder



Supersonic Flow - Standoff Distance Growth



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- Theoretical formulation and numerical simulation
- Largest Cluster in Kansas, Beocat ($>$3,500 cores)
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1. First order approximation for Advanced Kinetic Theory
2. LB method or DSMC method for Boltzmann-Curtiss equations
3. High order numerical solutions for Morphing Continuum Theory
4. Multiscale simulation of hypersonic transition
5. Knudsen kinetic layer in high Knudsen number flow
6. Hypersonics for polyatomic gases
7. Non-equilibrium flow of polyatomic gases

Acknowlesgement

- Louis B. Wonnell - PhD Student
- Grant Ferland - Undergrad
- Andrew Walsten - Undergrad
- Leidong Xu - Undergrad
- Emma Schinstock - Undergrad

What is a good theory?

A theory is a good theory if it satisfies two requirements: it must accurately describe a large class of observations on the basis of a model that contains only a few arbitrary elements, and it must make definite predictions about the results of future observations. (S. Hawking in *A Brief History of Time*)

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