

Multiscale Study of Hypersonic Vehicles: From Turbulence to Ceramics

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Webinar with DSIAC
December 13, 2023

About Me



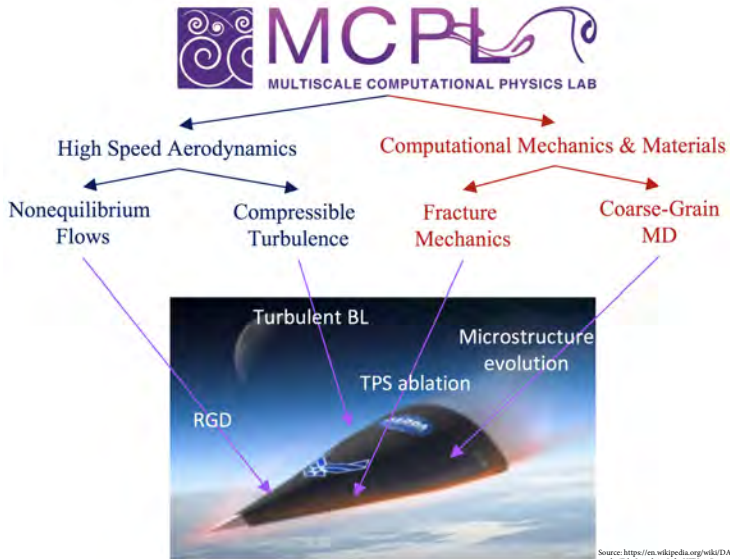
Current Position

- Associate Professor of Mechanical and Aerospace Engineering
- Undergraduate Director of Aerospace Engineering

Selected Honors & Awards

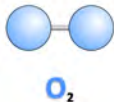
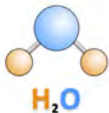
- Fellow of ASME, 2022
- Associate Fellow of AIAA, 2022
- Outstanding Young Engineer Award, AIAA Wichita Section, 2018
- Young Investigator Award, AFOSR, 2017

Research at MCPL



Source: https://en.wikipedia.org/wiki/DARPA_Falcon_Project/media/File:Speed_is_Life_HTV-2_Reentry_New.jpg

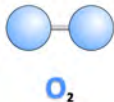
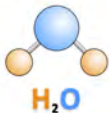
Rotation or Not?



Source: <https://www.flickr.com/photos/cseeman/27442272417>

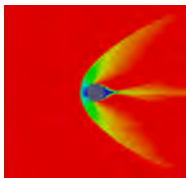
Boltzmann Equation and Navier-Stokes Equations are for **Monatomic Gas** or **Volumeless Point Mass**.

Rotation or Not?



Source: <https://www.flickr.com/photos/cseeman/27442272417>

Boltzmann Equation and Navier-Stokes Equations are for **Monatomic Gas** or **Volumeless Point Mass**.

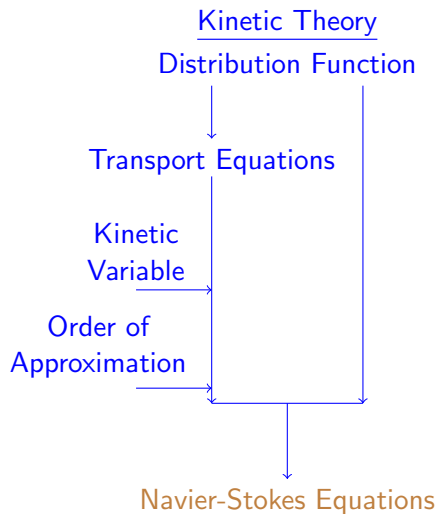


Source: James Chen, University at Buffalo

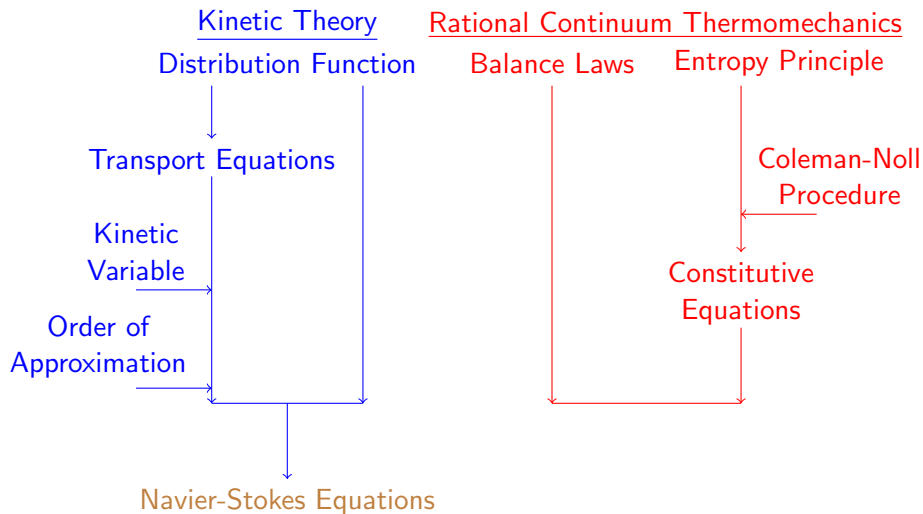
Continuum Theory for Flow with Inner Structures ?

- 1 Real fluids - **Polyatomic molecules**
- 2 High Mach or rarefied flow - **Rotation and/or vibration nonequilibrium**
- 3 Turbulence - **Eddies**

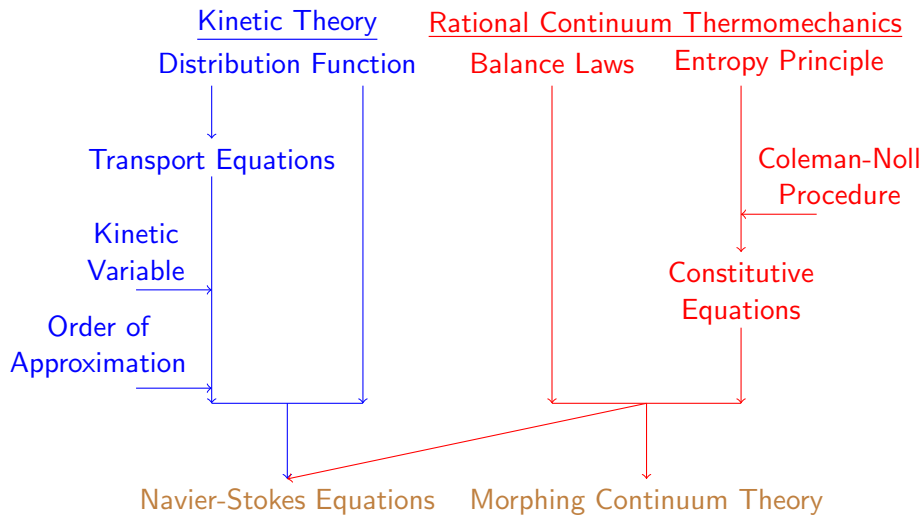
Roadmap to Continuum Theory



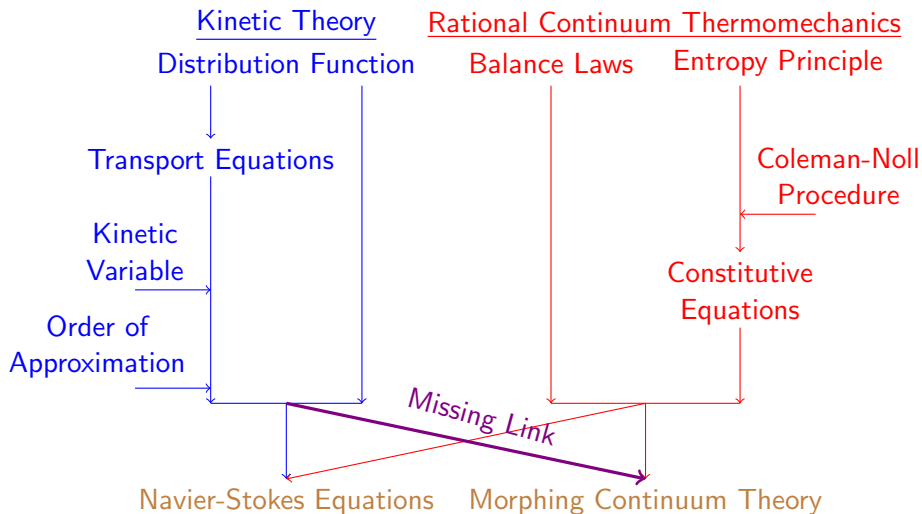
Roadmap to Continuum Theory



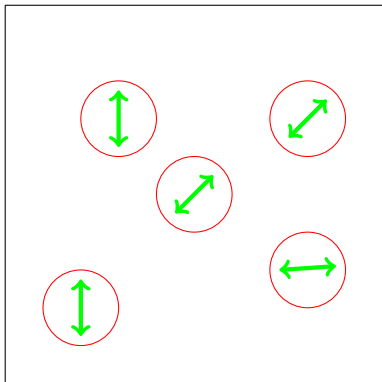
Roadmap to Continuum Theory



Roadmap to Continuum Theory



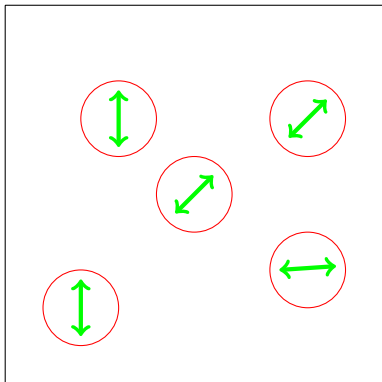
Advanced Kinetic Theory - Boltzmann-Curtiss Equations



$$\begin{aligned}\bar{f}(\mathbf{x}, \mathbf{p}, \phi, \mathbf{M}, t) &= \int f(\mathbf{x}, \mathbf{p}, \phi, \mathbf{M}, E_{\text{vib}}, t) dE_{\text{vib}} d\tau, \\ \left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \frac{\partial}{\partial \mathbf{x}} + \frac{\mathbf{M}}{I} \frac{\partial}{\partial \phi} \right) \bar{f} &= \sum_{\beta} \mathbf{z}_{\beta} \\ \frac{\partial}{\partial t} n\chi + \frac{\partial}{\partial x_i} n\chi v_i - n v_i \frac{\partial \chi}{\partial x_i} &+ \frac{\partial}{\partial \phi_i} n\chi \omega_i - n \omega_i \frac{\partial \chi}{\partial \phi_i} = 0\end{aligned}$$

(Curtiss, 1992)

Advanced Kinetic Theory - Boltzmann-Curtiss Equations



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

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

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

(Curtiss, 1992)

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

Boltzmann-Curtiss Distribution

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

Boltzmann's H-Theorem

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

Boltzmann-Curtiss Distribution

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

Boltzmann's H-Theorem

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

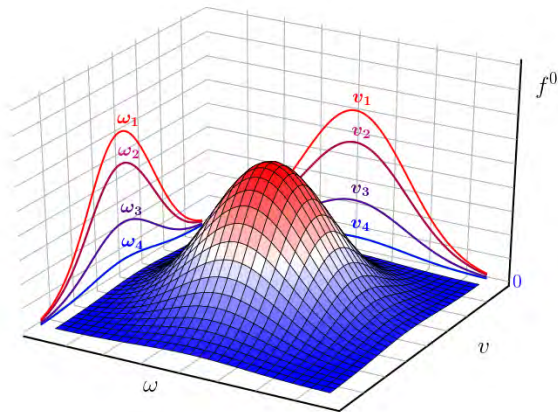
Method of the Most Probable Distribution (Schrödinger, 1989)

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

Chen, 2017; Wonnell and Chen, 2019

Maxwell-Boltzmann vs. Boltzmann-Curtiss Distribution

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



Source: <https://doi.org/10.1115/1.4045761>

From Kinetic Variables to Transport Equations

B-C Equation

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

Kinetic Variables

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

B-C Distribution and Transport Equations

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

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

Kinetic Variables in Advanced Kinetic Theory

Mass, $\chi_1 = m$

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

Linear Momentum, $\chi_2 = m v_i^* = m(v_i + e_{ijk} \omega_j r_k)$

$$\frac{\partial}{\partial t} (\rho U_j) + \frac{\partial}{\partial x_i} (\rho U_i U_j) = -\frac{\partial}{\partial x_i} (\rho \langle v'_i v'_j \rangle + \rho e_{jmn} r_n \langle v'_i \omega'_m \rangle)$$

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

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

Internal Energy, $\chi_4 = \frac{1}{2} (\langle v'_m v'_m \rangle + \langle r_m r_n \omega'_m \omega'_n \rangle)$

$$\begin{aligned} & \frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_i} (\rho e U_i) \\ &= -\frac{\partial}{\partial x_i} \left(\frac{1}{2} \rho (\langle v'_m v'_m v'_i \rangle + i_{mn} \langle \omega'_m \omega'_n v'_i \rangle) \right) + \rho \langle v_i \frac{\partial e}{\partial x_i} \rangle \end{aligned}$$

First-order Approximation

B-C Equation

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \frac{\partial}{\partial \mathbf{x}} + \frac{\mathbf{M}}{I} \frac{\partial}{\partial \phi}\right) \bar{f} = \left(\frac{\partial \bar{f}}{\partial t}\right)_{\text{collision}}$$

BGK Approach

$$\left(\frac{\partial \bar{f}}{\partial t}\right)_{\text{collision}} \Rightarrow -\frac{\bar{f} - \bar{f}^0}{\tau} = -\frac{\mathbf{g}}{\tau}$$

Comparison with Morphing Continuum Theory

The classical Boltzmann's equation with a distribution linearly deviates from the Boltzmann distribution (first-order approximation), leads to the celebrated Navier-Stokes equations. Will the B-C equation with a distribution linearly deviated from the B-C distribution give the MCT governing equations?

Wonnell and Chen, 2019

Linear Momentum

Morphing Continuum Theory

$$\begin{aligned} \frac{\partial}{\partial t}(\rho v_j^{\text{MCT}}) + \frac{\partial}{\partial x_i}(\rho v_i^{\text{MCT}} v_j^{\text{MCT}}) = & -\frac{\partial p}{\partial x_j} + (\lambda + \mu) \frac{\partial^2 v_i^{\text{MCT}}}{\partial x_i \partial x_j} \\ & + (\mu + \kappa) \frac{\partial^2 v_j^{\text{MCT}}}{\partial x_i \partial x_i} + \kappa e_{jlm} \frac{\partial \omega_m^{\text{MCT}}}{\partial x_l} \end{aligned}$$

Advanced Kinetic Theory

$$\begin{aligned} \frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = & -\frac{\partial p}{\partial x_j} + \frac{2n\tau\theta}{3} \frac{\partial^2 U_i}{\partial x_i \partial x_j} \\ & + n\tau\theta \frac{\partial^2 U_j}{\partial x_i \partial x_i} + n\tau\theta e_{jlm} \frac{\partial W_m}{\partial x_l} \end{aligned}$$

Angular Momentum

Morphing Continuum Theory

$$\frac{\partial}{\partial t}(\rho j \omega_j^{\text{MCT}}) + \frac{\partial}{\partial x_i}(\rho j v_i^{\text{MCT}} \omega_j^{\text{MCT}}) = (\alpha + \beta) \frac{\partial^2 \omega_i^{\text{MCT}}}{\partial x_i \partial x_j} + \gamma \frac{\partial^2 \omega_j^{\text{MCT}}}{\partial x_i \partial x_i} + \kappa (e_{jlm} \frac{\partial v_m^{\text{MCT}}}{\partial x_l} - 2\omega_j^{\text{MCT}})$$

Advanced Kinetic Theory

$$\frac{\partial}{\partial t}(\rho j W_j) + \frac{\partial}{\partial x_i}(\rho j U_i W_j) = n j \tau \theta \frac{\partial^2 W_j}{\partial x_i \partial x_i} + \nu_r (e_{jlm} \frac{\partial U_m}{\partial x_l} - 2W_j)$$

Pathway to Navier-Stokes Equations

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial p}{\partial x_j} + \frac{2n\tau\theta}{3} \frac{\partial^2 U_i}{\partial x_i \partial x_j} + n\tau\theta \frac{\partial^2 U_j}{\partial x_i \partial x_i} + n\tau\theta e_{jlm} \frac{\partial W_m}{\partial x_l}$$

Pathway to Navier-Stokes Equations

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial p}{\partial x_j} + \frac{2n\tau\theta}{3} \frac{\partial^2 U_i}{\partial x_i \partial x_j} + n\tau\theta \frac{\partial^2 U_j}{\partial x_i \partial x_i} + n\tau\theta e_{jlm} \frac{\partial W_m}{\partial x_l}$$

Angular Motion Equivalence

$$\vec{W} = \frac{1}{2} \nabla \times \vec{U}$$

Pathway to Navier-Stokes Equations

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial p}{\partial x_j} + \frac{2n\tau\theta}{3} \frac{\partial^2 U_i}{\partial x_i \partial x_j} + n\tau\theta \frac{\partial^2 U_j}{\partial x_i \partial x_i} + n\tau\theta e_{jlm} \frac{\partial W_m}{\partial x_l}$$

Angular Motion Equivalence

$$\vec{W} = \frac{1}{2} \nabla \times \vec{U}$$

Navier-Stokes Equations Type II

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial p}{\partial x_j} + \frac{7n\tau\theta}{6} \frac{\partial^2 U_i}{\partial x_i \partial x_j} + \frac{n\tau\theta}{2} \frac{\partial^2 U_j}{\partial x_i \partial x_i}$$

Navier-Stokes Equations Type I & II

Navier-Stokes Equations Type II - reduced from MCT

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial p}{\partial x_j} + \frac{7n\tau\theta}{6} \frac{\partial^2 U_i}{\partial x_i \partial x_j} + \frac{n\tau\theta}{2} \frac{\partial^2 U_j}{\partial x_i \partial x_i}$$

Navier-Stokes Equations Type I - classical framework

$$\frac{\partial}{\partial t}(\rho U_j) + \frac{\partial}{\partial x_i}(\rho U_i U_j) = -\frac{\partial p}{\partial x_j} + \frac{n\tau\theta}{3} \frac{\partial^2 U_i}{\partial x_i \partial x_j} + n\tau\theta \frac{\partial^2 U_j}{\partial x_i \partial x_i}$$

A Map between Kinetic Theory and Continuum Theory

Boltzmann-Curtiss Equation

$$\frac{\partial}{\partial \phi_i} = 0$$

No angular dependence

Boltzmann Equation

A Map between Kinetic Theory and Continuum Theory

Boltzmann-Curtiss Equation

$$\frac{\partial}{\partial \phi_i} = 0$$

No angular dependence

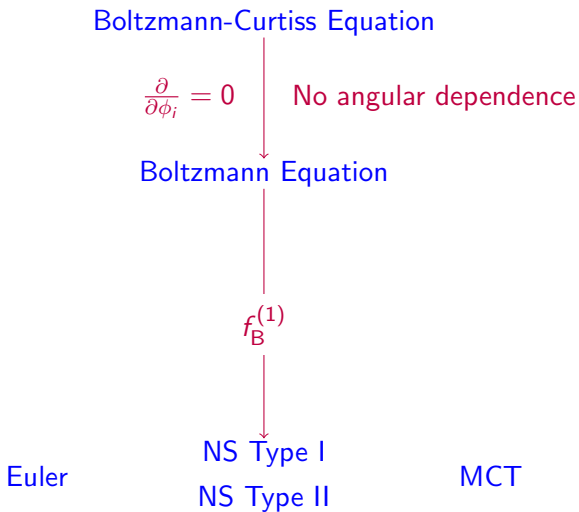
Boltzmann Equation

Euler

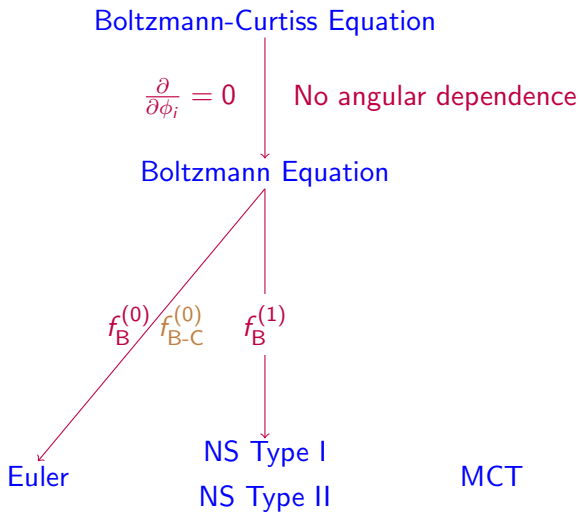
NS Type I
NS Type II

MCT

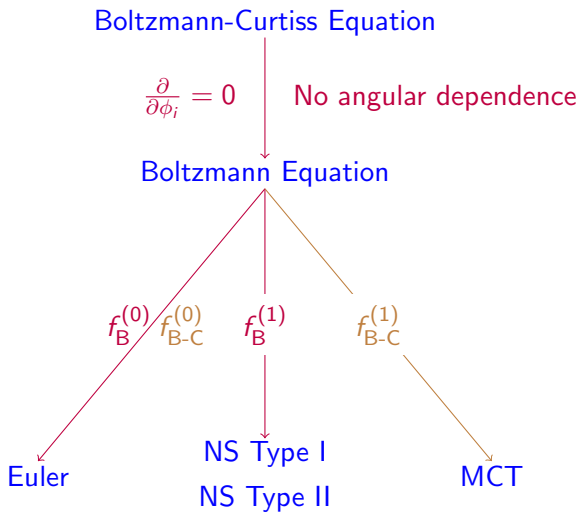
A Map between Kinetic Theory and Continuum Theory



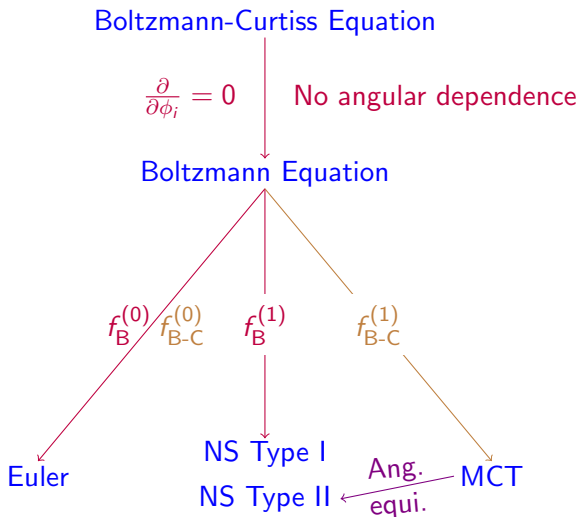
A Map between Kinetic Theory and Continuum Theory



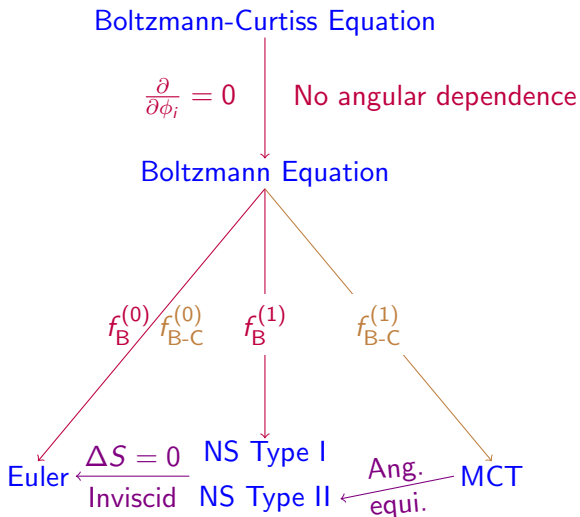
A Map between Kinetic Theory and Continuum Theory



A Map between Kinetic Theory and Continuum Theory



A Map between Kinetic Theory and Continuum Theory



Morphing Continuum Theory for Incompressible Fluids

Conservation of Mass

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

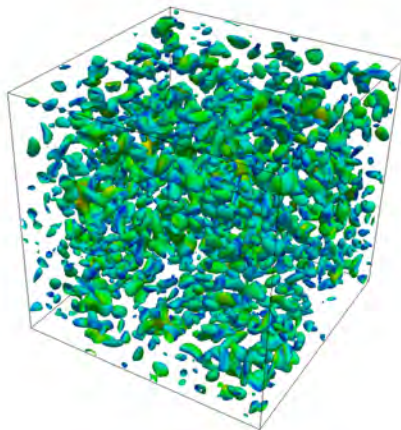
Balance Law of Linear Momentum

$$\frac{\partial}{\partial t} (U_j) + U_i \frac{\partial}{\partial x_i} (U_j) = \frac{1}{\rho} \frac{\partial p}{\partial x_j} + \frac{\mu + \kappa}{\rho} \frac{\partial^2 U_j}{\partial x_i \partial x_i} + \frac{\kappa}{\rho} e_{jkl} \frac{\partial W_l}{\partial x_k}$$

Balance Law of Angular Momentum

$$\frac{\partial}{\partial t} (W_m) + U_i \frac{\partial}{\partial x_i} (W_m) = \frac{\gamma}{\rho_j} \frac{\partial W_j}{\partial x_i \partial x_i} + \frac{\kappa}{\rho_j} (e_{jkl} \frac{\partial U_l}{\partial x_k} - 2W_j)$$

Homogeneous Isotropic Turbulence



Source: James Chen, University at Buffalo

Linear Momentum Equations

Balance Law of Linear Momentum

$$\frac{d\langle U_j \rangle}{dt} = \frac{1}{\rho} \left\langle \frac{\partial p}{\partial x_j} \right\rangle + \frac{\mu + \kappa}{\rho} \left\langle \frac{\partial^2 U_j}{\partial x_i \partial x_i} \right\rangle + \frac{\kappa}{\rho} \left\langle e_{jkl} \frac{\partial U_l}{\partial x_k} \right\rangle$$

$$\frac{d\langle U_j \rangle}{dt} = \frac{1}{\rho} \left\langle \frac{\partial p}{\partial x_j} \right\rangle + \frac{\mu + \kappa}{\rho} \left\langle \frac{\partial^2 U_j}{\partial x_i \partial x_i} \right\rangle + \frac{\kappa}{\rho} \left\langle e_{jkl} \frac{\partial U_l}{\partial x_k} \right\rangle$$

$$\frac{d\langle U_j \rangle}{dt} = 0$$

Angular Momentum Equations

Balance Law of Angular Momentum

$$\frac{d}{dt} \langle W_j \rangle = \frac{\gamma}{\rho_j} \left\langle \frac{\partial^2 W_j}{\partial x_i \partial x_i} \right\rangle + \frac{\kappa}{\rho_j} \left(\left\langle e_{jkl} \frac{\partial U_l}{\partial x_k} \right\rangle - 2 \langle W_j \rangle \right)$$

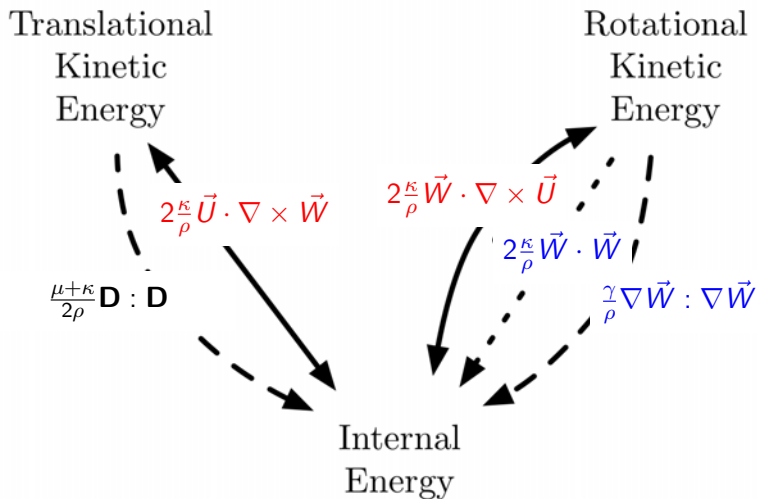
$$\frac{d}{dt} \langle W_j \rangle = \frac{\gamma}{\rho_j} \left\langle \frac{\partial^2 W_j}{\partial x_i \partial x_i} \right\rangle + \frac{\kappa}{\rho_j} \left(\left\langle e_{jkl} \frac{\partial U_l}{\partial x_k} \right\rangle - 2 \langle W_j \rangle \right)$$

$$\frac{d}{dt} \langle W_j \rangle = -\frac{2\kappa}{\rho_j} \langle W_j \rangle$$

$$\langle W_j \rangle = C e^{-\tau_w t} \quad \tau_w = \frac{2\kappa}{\rho_j}: \text{turbulence relaxation time}$$

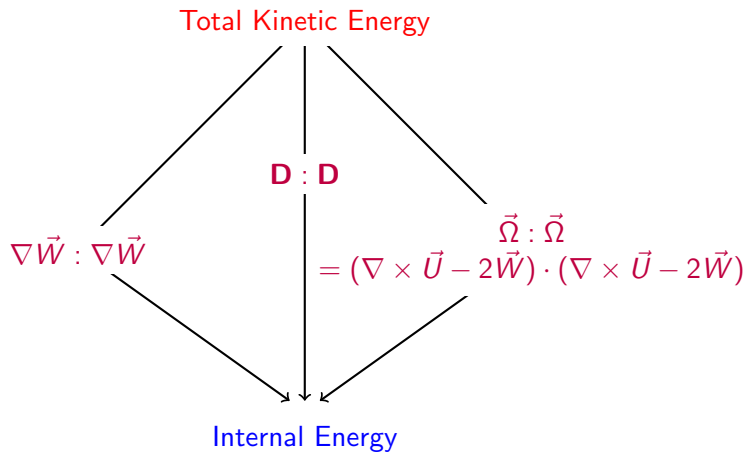
Wonnell and Chen, 2019; Chen, 2003 (Science)

Energy Equation

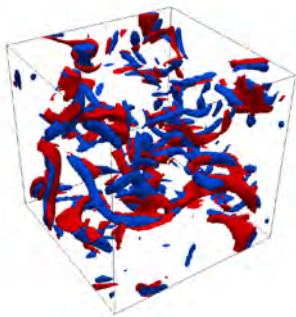


Total Energy Cascade

Energy Transfer & Absolute Rotation

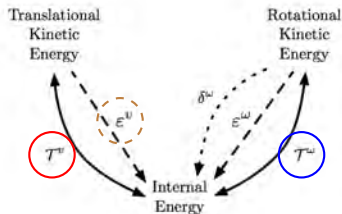


Homogeneous Isotropic Turbulence - Energy Transfer



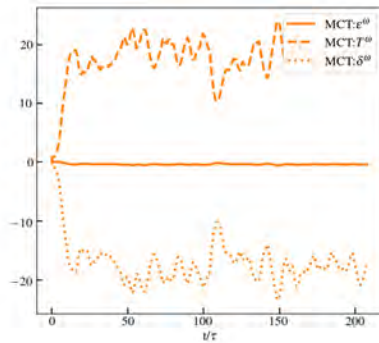
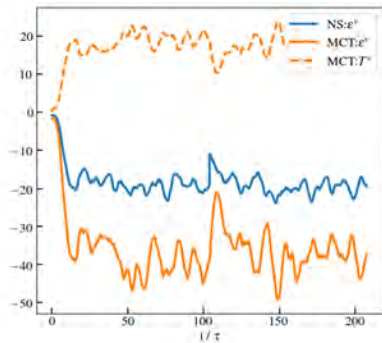
Source: James Chen, University at Buffalo

Translational energy cascade

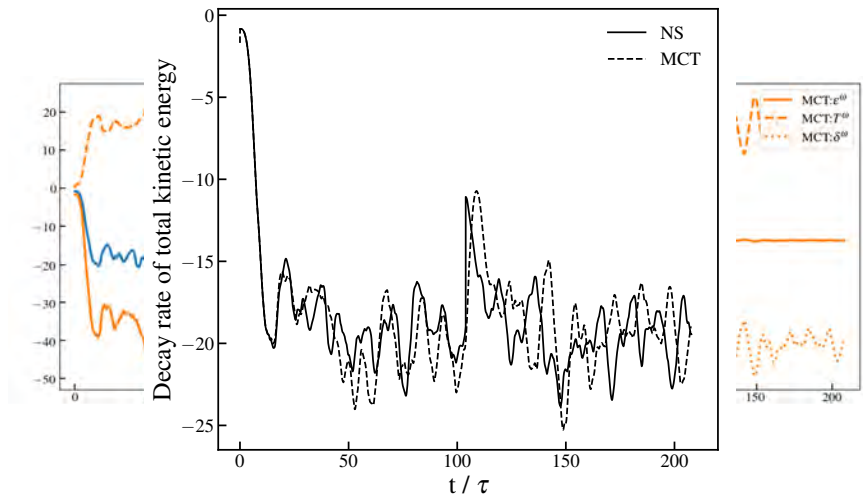


Rotational energy cascade

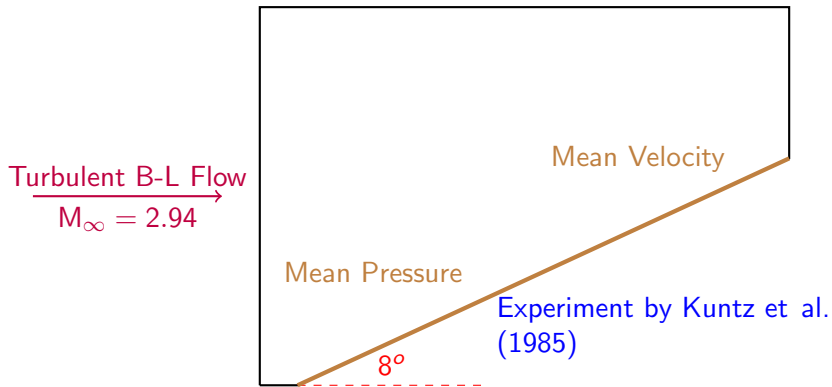
Homogeneous Isotropic Turbulence - MCT vs. NS



Homogeneous Isotropic Turbulence - MCT vs. NS

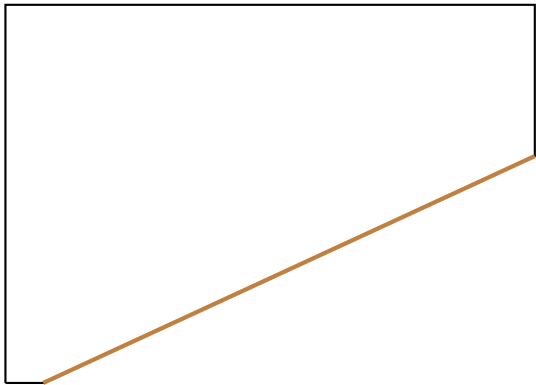


Supersonic Flow Over an 8° Compression Ramp

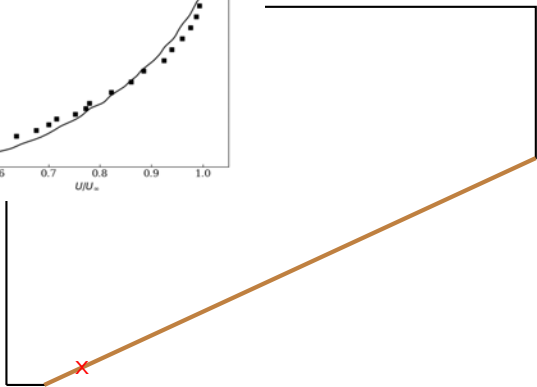
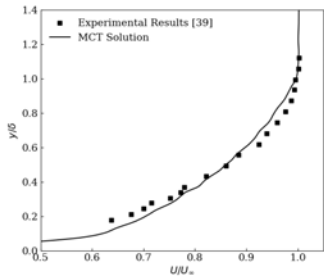


(Cheikh et al., 2018)

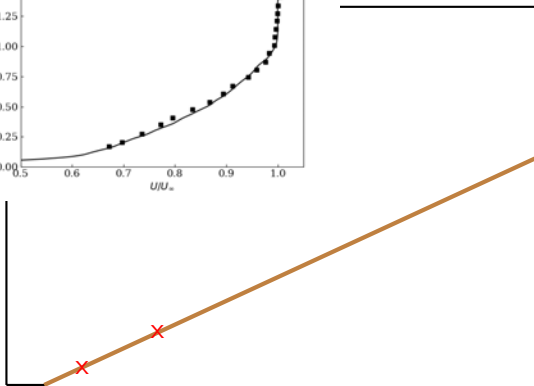
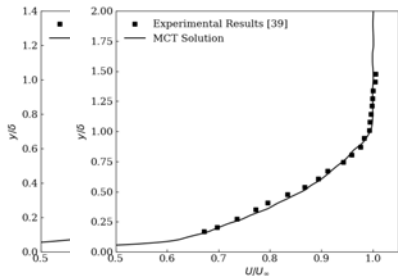
Supersonic Flow - Compression Ramp



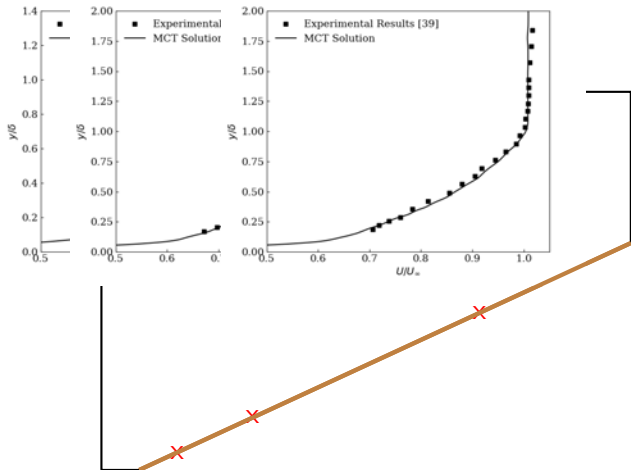
Supersonic Flow - Compression Ramp



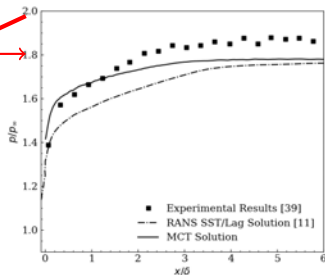
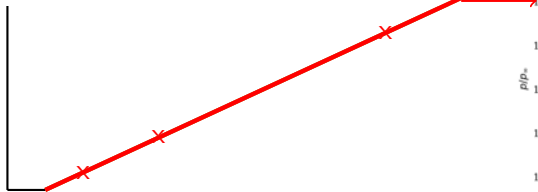
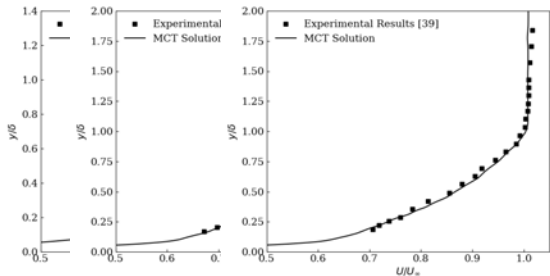
Supersonic Flow - Compression Ramp



Supersonic Flow - Compression Ramp



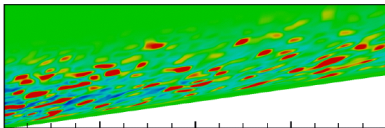
Supersonic Flow - Compression Ramp



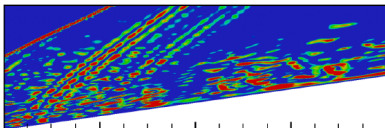
Source: <https://doi.org/10.1103/PhysRevFluids.3.024604>

Supersonic Flow - Energy Analysis

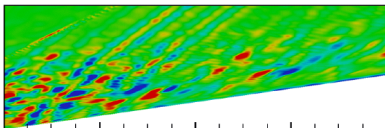
Rotation



Translation



Internal



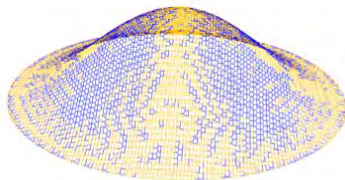
$$\begin{array}{ccc} & \frac{j}{2} \langle \omega_i'' \omega_i'' \rangle & \\ & \swarrow \quad \searrow & \\ \frac{1}{2} \langle v_i'' v_i'' \rangle & \longleftrightarrow & \langle e'' \rangle \end{array}$$

Transonic Flow Over an Axisymmetric Hill

Flow Profile

M_∞	0.6
δ_{inlet}	0.039 m
H_{bump}	0.078 m
Re_H	6709

Hill Surface Pressure Coefficient



- Experiment: Simpson et al. (2002)
- NS-based DNS: Castagna et al. (2014)
- MCT-based DNS: Wonnell, Cheikh, and Chen (2018)

From "Morphing Continuum Simulation of Transonic Flow over Axisymmetric Hill" by Louis B. Wonnell, Mohamad I. Cheikh and James Chen; reprinted by permission of the American Institute of Aeronautics and Astronautics, Inc. Source: <https://doi.org/10.2514/1.1057064>

Transonic Flow - Vortex Visualization and Surface Pressure

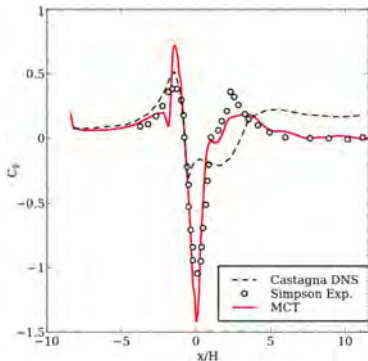
Objective Q-Criterion for Vortex Visualization



$$2I_a = (\nabla \cdot \vec{v})^2 - \nabla \vec{v} : \nabla \vec{v}^T - 2(\nabla \times \vec{v}) \cdot \vec{\omega} + 2\vec{\omega} \cdot \vec{\omega}$$

Source: James Chen, University at Buffalo

Hill Surface Pressure Coefficient



Computation Cost:

MCT: 6M cells

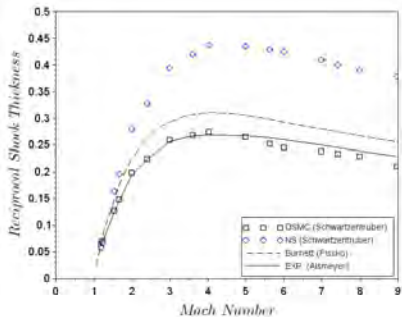
DNS: 54M cells

From "Morphing Continuum Simulation of Transonic Flow over Axisymmetric Hill" by Louis B. Wonnell, Mohamad I. Cheikh and James Chen, reprinted by permission of the American Institute of Aeronautics and Astronautics, Inc. Source: <https://doi.org/10.2514/1.1057064>

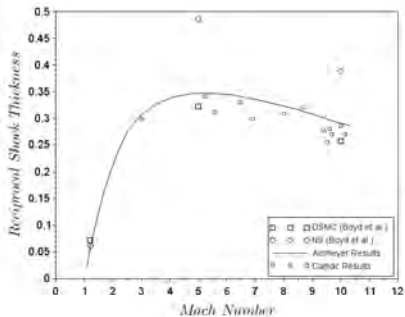
1-D Shock Profile – Argon and Nitrogen

ρ_1	—	ρ_2
T_1	—	T_2
p_1	—	p_2

Argon



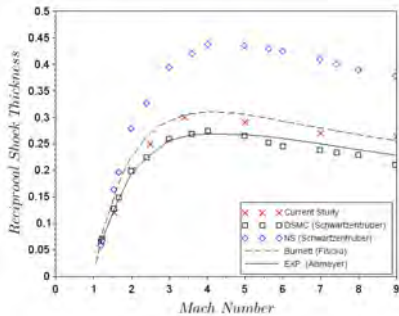
Nitrogen



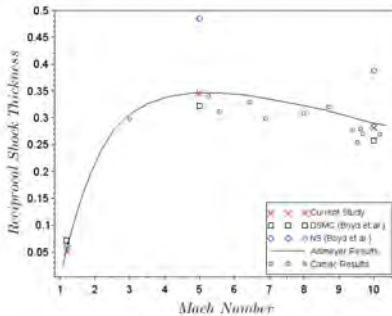
1-D Shock Profile – Argon and Nitrogen



Argon

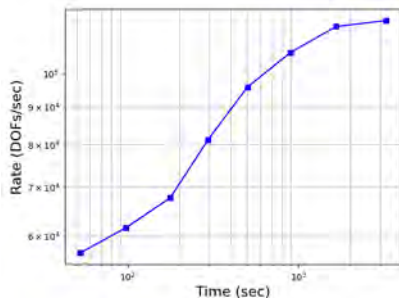
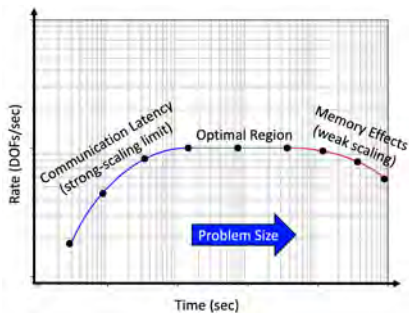


Nitrogen



Source: <https://doi.org/10.1115/1.4045761>

Scalability - Static Scaling



Sementilli, McGurn, and Chen, 2023

- Number of Cores Tested: 32,768 (DoE Quartz)
- Test Case: Multiphase (liquid and gas) Kelvin-Helmholtz instability
- Degrees of Freedom Tested: 48M

Integrated Computational Materials Engineering for Hypersonics



Source: https://en.wikipedia.org/wiki/Atmospheric_entry#/media/File:Apollo_cm.jpg

- Limited data availability for ceramics under hypersonic condition
 - Bayesian-based uncertainty management

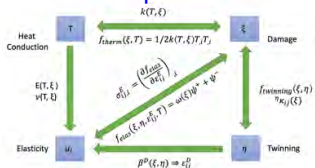
- Insufficient understanding at vehicle/flow interface
 - Artificial Neural Network with Bayesian statistics
 - Physics-based models with exascale simulation



Source: Getty Images

ICME Framework for Ceramics

Properties

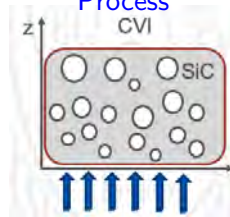


Performance

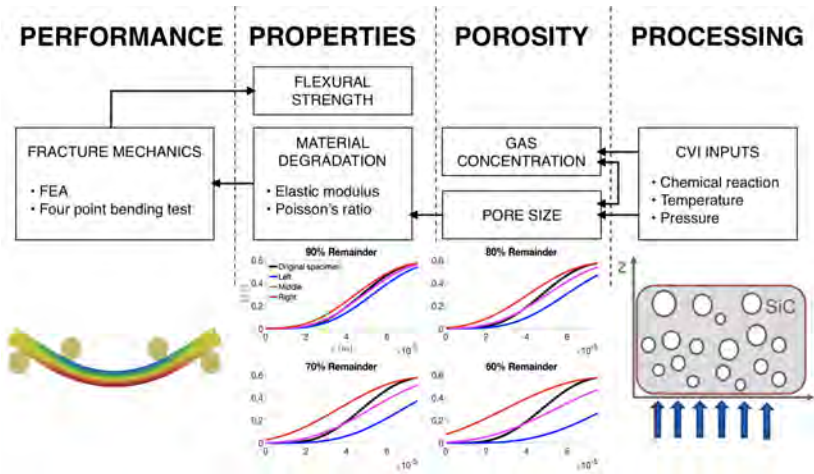


Structure

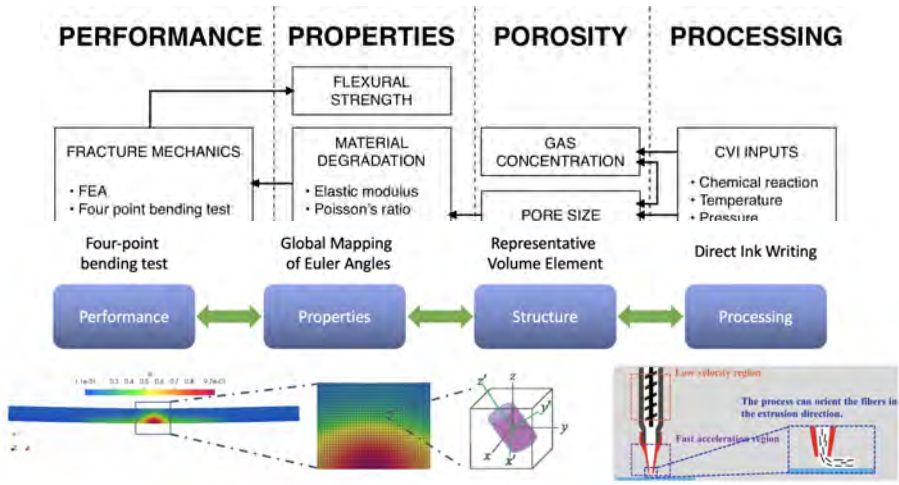
Process



Manufacturing-Driven ICME for CMC in Hypersonics



Manufacturing-Driven ICME for CMC in Hypersonics

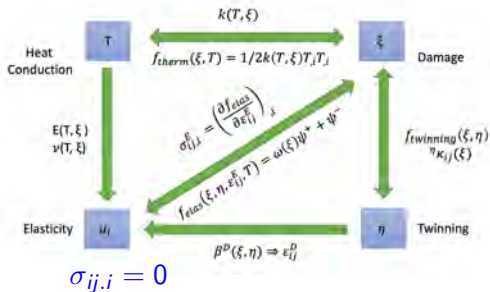


Source: James Chen, University at Buffalo

Four-Way Thermo-Mechanical Coupling

$$\frac{\partial T}{\partial t} = w(\xi)k(T)T_{,ii}$$

$$\frac{\partial \xi}{\partial t} = -L_{\xi} \left(\frac{\partial f_{loc}(\xi, \epsilon, T, \eta)}{\partial \xi} - \kappa \xi_{,ii} \right)$$

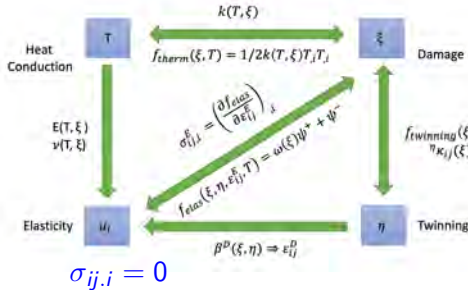


$$\frac{\partial \eta}{\partial t} = -L_{\eta} \left(\frac{\partial f_{loc}(\xi, \epsilon, T, \eta)}{\partial \eta} - \kappa \eta_{,ii} \right)$$

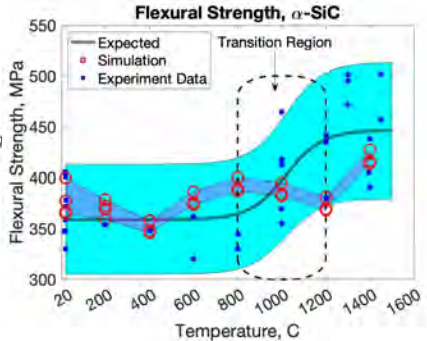
Four-Way Thermo-Mechanical Coupling

$$\frac{\partial T}{\partial t} = w(\xi)k(T)T_{,ii}$$

$$\frac{\partial \xi}{\partial t} = -L_{\xi} \left(\frac{\partial f_{loc}(\xi, \epsilon, T, \eta)}{\partial \xi} - \kappa \xi_{,ii} \right)$$



$$\frac{\partial \eta}{\partial t} = -L_{\eta} \left(\frac{\partial f_{loc}(\xi, \epsilon, T, \eta)}{\partial \eta} - \kappa \eta_{,ii} \right)$$



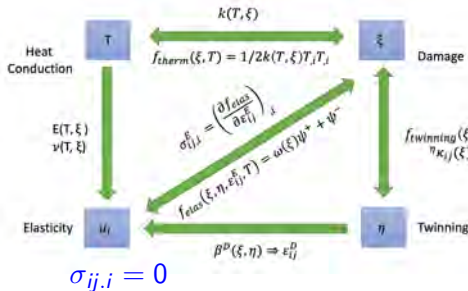
(Sun et al., 2023) Source: <https://doi.org/10.1111/jace.19202>

jace.19202

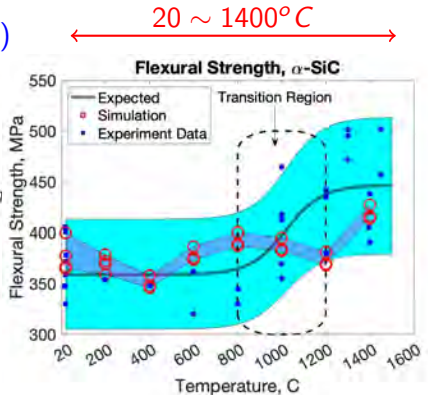
Four-Way Thermo-Mechanical Coupling

$$\frac{\partial T}{\partial t} = w(\xi)k(T)T_{,ii}$$

$$\frac{\partial \xi}{\partial t} = -L_{\xi} \left(\frac{\partial f_{loc}(\xi, \epsilon, T, \eta)}{\partial \xi} - \kappa \xi_{,ii} \right)$$



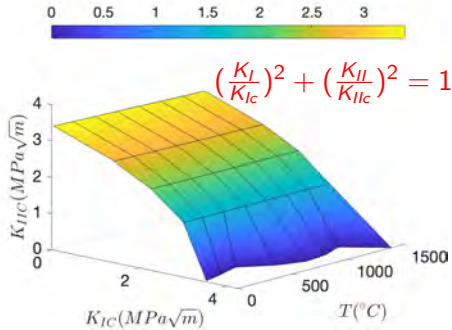
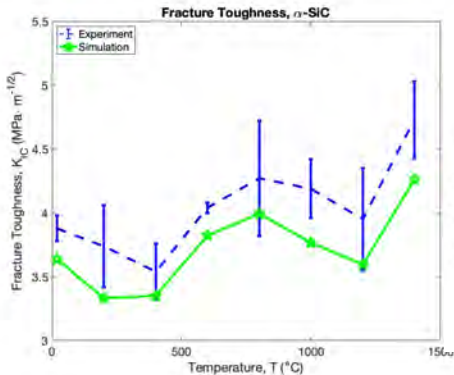
$$\frac{\partial \eta}{\partial t} = -L_{\eta} \left(\frac{\partial f_{loc}(\xi, \epsilon, T, \eta)}{\partial \eta} - \kappa \eta_{,ii} \right)$$



(Sun et al., 2023)

Source: <https://doi.org/10.1111/jace.19202>

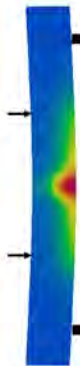
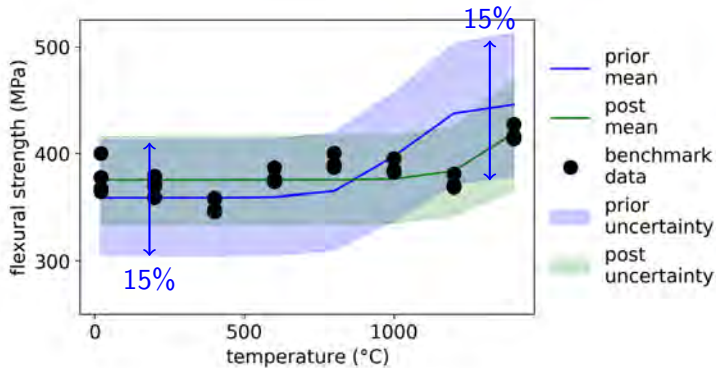
Damage Criteria of α -SiC



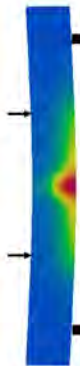
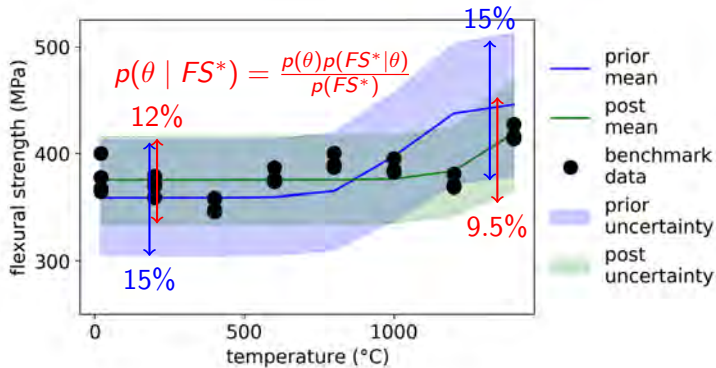
(Sun et al., 2023)

Source: <https://doi.org/10.1111/jace.19202>

Uncertainty Management with Bayesian Update



Uncertainty Management with Bayesian Update

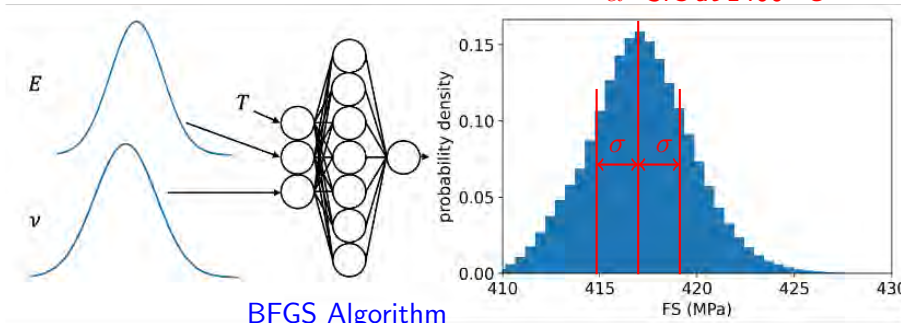


Source: James Chen, University at Buffalo

(Walker, Sun, and Chen, under revision)

Uncertainty-Informed Artificial Neural Network

Forward Uncertainty Sampling

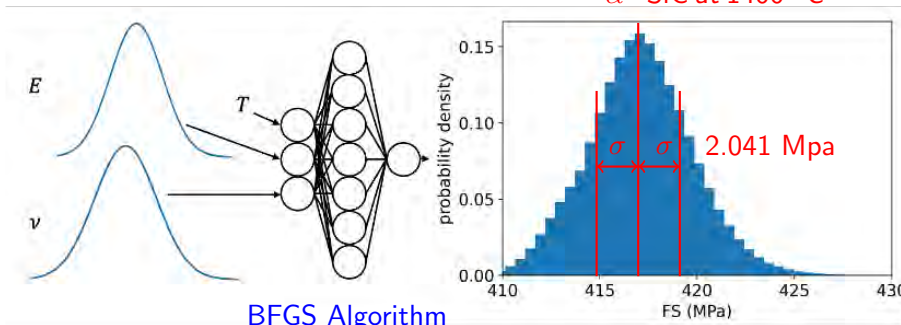


BFGS Algorithm

$$y^k = g^{k+1} - g^k$$

Uncertainty-Informed Artificial Neural Network

Forward Uncertainty Sampling



BFGS Algorithm

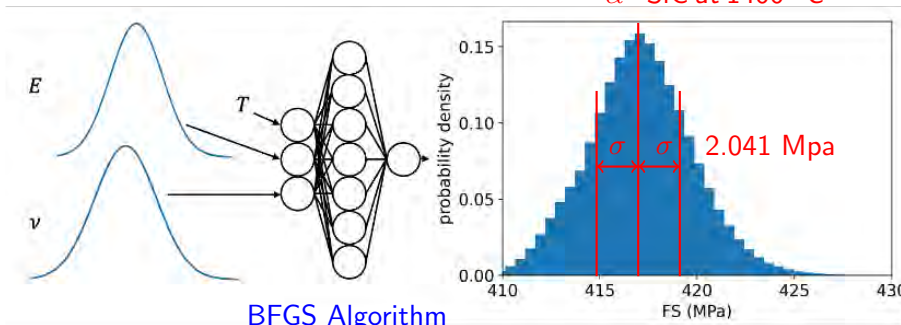
$$y^k = g^{k+1} - g^k$$

417.03 MPa

Source: James Chen, University at Buffalo

Uncertainty-Informed Artificial Neural Network

Forward Uncertainty Sampling



BFGS Algorithm

$$y^k = g^{k+1} - g^k$$

417.03 MPa

416.84 MPa (Physics-based Simulation)

Source: James Chen, University at Buffalo

(Walker, Sun, and Chen, accepted for publication)

Design of Hypersonic Vehicles



High Speed Aerodynamics

Computational Mechanics & Materials

Nonequilibrium
Flows

Compressible
Turbulence

Fracture
Mechanics

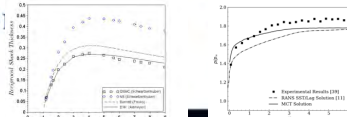
Coarse-Grain
MD



Design of Hypersonic Vehicles



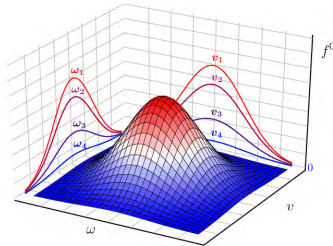
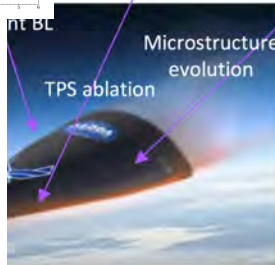
High Speed Aerodynamics



Computational Mechanics & Materials

Fracture
Mechanics

Coarse-Grain
MD

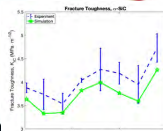
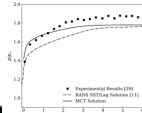
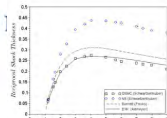


Design of Hypersonic Vehicles

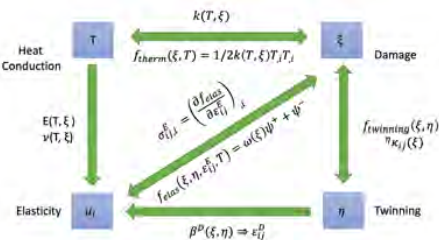
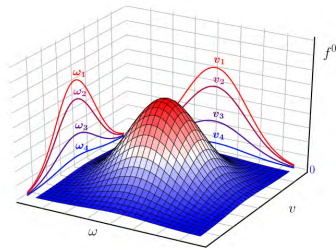


High Speed Aerodynamics

Computational Mechanics & Materials



Coarse-Grain MD



Source: <https://doi.org/10.1115/1.4045761>

Source: https://en.wikipedia.org/wiki/DARPA_Falcon_Project/media/File:Speed_in_Life_HITV-2_Reentry_New.jpg

Acknowledgments

- Dr. Paul DesJardin
- Dr. David Salac
- Dr. Matt McGurn
- Dr. Eric Walker
- Dr. Rozie Zangeneh
- Mae Sementilli
- Jason Sun
- Joe Marziale
- Yu Chen



The relentless pursuit of hypersonic flight

How much new science will it take to design a vehicle that can routinely fly at many times the speed of sound? (I. Leyva)



MCPL THANKS YOU!!!



James Chen; (716) 645-3162; chenjm@buffalo.edu

Source: James Chen, University at Buffalo