GIAN Course on

Rarefied & Microscale Gases and Viscoelastic Fluids: a Unified Framework

Lecture 1
Introduction of the Course and History of Rarefied & Microscale Gasdynamics (RMG)

Feb. 23rd ~ March 2nd, 2017

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Content

I. Introduction of the course and lecturers

II. Rationale (why unified?)

III. Emphasis and style

IV. History of RMG

V. Applications of RMG and challenges

I. Introduction of the course and lecturers

- ## Lecturers

Prof. Rho Shin Myong is a Professor of the Department of Aerospace and Software Engineering at the Gyeongsang National University in Jinju, South Korea. He is also the director of Next-Generation Mechanical and Aerospace Creative Engineers Education Program (Brain Korea 21 PLUS National Program) and the chair of the Graduate School of Mechanical and Aerospace Engineering. He is a guest professor of Northwestern Polytechnical University (Xian, China).

He received a Ph.D. degree from the Department of Aerospace Engineering in the University of Michigan in 1996. Prior to the present position, he worked at the NASA Goddard Space Flight Center from 1997 to 1999 as a NRC research associate. In 2014, he was elected to the associate fellow of American Institute of Aeronautics and Astronautics. He is an associate editor of the Communications in Computational Physics (Cambridge) and an editorial board member of the International Journal of Computational Fluid Dynamics (Taylor & Francis). He also serves as a scientific committee member for several international conferences including International Conference on Mathematical Modeling in Physical Sciences. He made fundamental contributions to the theory of rarefied and microscale gases and development of constitutive equation based on the so-called balanced closure, Langmuir slip model, and innovative computational methods. He also made a seminal contribution to theory of shock waves in gases and MHD including intermediate shocks, compound waves, numerical schemes for non-strictly hyperbolic problem applicable to all fields of continuum mechanics associated with rotational symmetry of Newton's law.

Dr. Rakesh K. Mathpal is Assistant Professor in the Department of Aerospace Engineering of the Indian Institute of Technology, Kanpur. He received his Ph.D. from the Pennsylvania State University, US in 2011, and subsequently joined IIT Kanpur in 2012. His research interests include rarefied gas dynamics, hypersonics, molecular dynamics, microfluidics, thermal protection system design and heat transfer analysis.

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Deparment of Mechanical Engineering
Indian Institute of Technology Bombay

Prof. Shripad P. Mahulikar
Department of Aerospace Engineering
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Prof. Amit Agrawal
Department of Mechanical Engineering
Indian Institute of Technology Bombay

I. Introduction of the course and lecturers

- **Rarefied & Microscale Gases (RMG) and Viscoelastic Fluids: a Unified Framework**
  - Rarefied: low density state
  - Microscale: small scale in micro and nano
  - Viscoelastic: complex fluids like macromolecular polymers (soft matter)

  visco- (fluidic) + elastic (amorphous solid) → continuum mechanics

↓ (Always) combining

kinetic molecular + macroscopic continuum

- **Fundamental physics of RMG**

  in form of Non-Navier (1822) + Non-Fourier (1822) constitutive laws +

boundary conditions + Non-Newtonian + non-Hookean (1660) constitutive laws

I. Introduction of the course and lecturers

- **R. S. Myong**
  - Research is in essence a personal journey in the sea of knowledge.
  - Myong's journey:

  Aerodynamics (BS) → CFD, Aeroacoustics (MS) → MHD, Applied Math, CFD (PhD) → RMG, Applied Aerodynamics, Icing/Lightning, Survivability, etc.

- **Research goal**

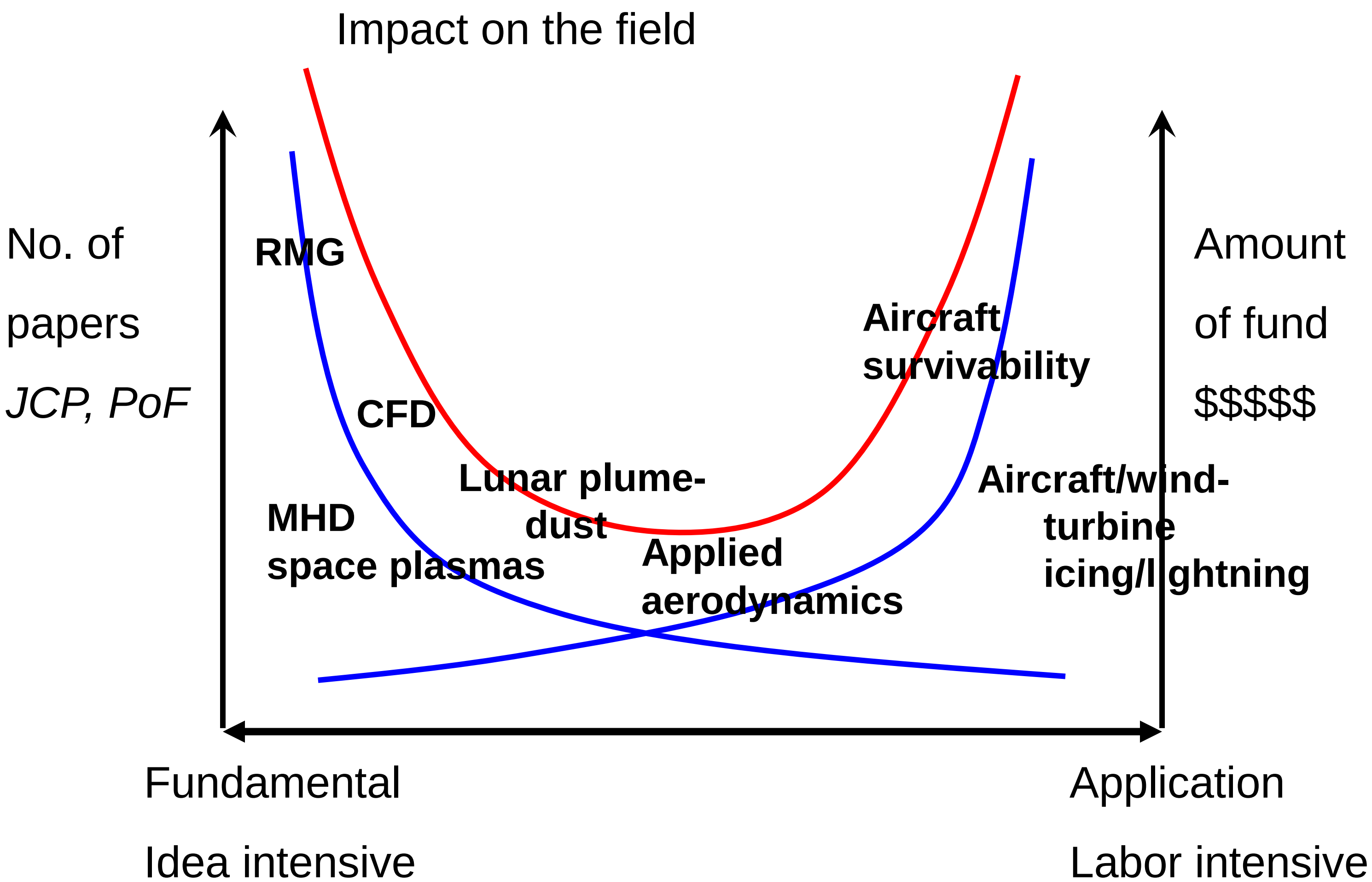
  Develop unified theoretical & computational models for RGM, upon which others can build their own research including efficient CFD codes

  http://acml.gnu.ac.kr

  <Open knowledge>

I. Introduction of the course and lecturers

Research Topics



II. Rationale (why unified?)

- **A bold proposition**
  - Any materials undergoing internal motion basically have two parts in molecular level:

    1) Movement (kinematic nature)

    2) Interaction (or collision) (dissipative nature; related to 2^{nd}-law of thermodynamics)
  - Therefore, a unified theory based on the kinetic molecular description, in particular, via the probabilistic Boltzmann theory, may be possible.
- **Cases**
  - Binary collision among gas particles
  - Interaction between a polymer macromolecule and solution
  - ???

III. Emphasis and style

- **Emphasis in this lecture**
  - Clear demonstration of knowns (full analytic approach, focusing on simple benchmark problems) and always practical (design) application in mind
  - Mesoscale and fundamental (focusing on theory)
  - Qualitative & holistic over quantitative & fragmental (putting many multi-faceted abnormal behaviors in proper context, rather than one-time snap-shot agreement)
  - Verification & validation (V & V) of computational simulation of RMG
  - Alien spirit is needed because we try to explore the unknown territory
- **Style**
  - Open & on-going research (preprints)
  - Sharing failure and struggle (rather than making conclusive); for example, harsh review comments and rejections from journals (personal collections)
  - Hands-on theoretical derivation and computer programming

III. Emphasis and style

- **Alien spirit** (P. Phillips, The “alien spirit” of relativity, *Physics Today*, March, 2016.)
  - Try to step outside the established line of reasoning because we venture into the unexplored territory beyond the safe-ground protected/validated by the classical linear laws like Navier, Fourier, and Hookean
  - Need to feel comfortable with being different (minority)
  - Textbooks will not help very much, since they basically focus on codified set of solved problems. Research, on the other hand, demands the inevitable confrontation with the unknowns.
  - Scrutinize everything we learned from textbooks; in particular, underlying assumptions
- **Big questions**

  What are the essences of RMG? What is the ultimate origin of the Knudsen minimum? Knowledges based on the linear laws can be extrapolated to RMG?

III. Emphasis and style

- **Why V & V in RMG are difficult?**
  - Too many computational models (governing equation, boundary condition)

    Cf. Only one in near-equilibrium: Linear uncoupled NSF + no-slip
  - DSMC is not immune, since it is also subject to the boundary condition and post-processing employed.
  - Lack of experimental data (how to measure exotic properties such as temperature jump? And experimental observations often relying on the application of classical first-order models. But, recently, there are active experimental works in EU Micro Gas Network (S. Colin etc.)
  - Lack of theories:
    - No consensus what the proper master kinetic equations would be for describing diatomic gases like simple nitrogen in thermal non-equilibrium
    - No rigorous gas-surface molecular interaction theory

III. Emphasis and style (18 papers by Myong)

- **MHD (2)**

- **Myong, R. S**., and Roe, P. L., “Shock waves and rarefaction waves in magnetohydrodynamics: I. A model system,” *Journal of Plasma Physics*, Vol. 58, pp. 485-519, 1997. **[JPP 97a]**
- **Myong, R. S**., and Roe, P. L., “Shock waves and rarefaction waves in magnetohydrodynamics: II. The MHD system,” *Journal of Plasma Physics*, Vol. 58, pp. 521-552, 1997. **[JPP 97b]**

- **RMG (14)**

- **Myong, R. S.**, “Thermodynamically-consistent hydrodynamic computational models for high-Knudsen-number gas flows,” *Physics of Fluids*, Vol. 11, No. 9, pp. 2788-2802, 1999. **[PoF 99]**
- **Myong, R. S.**, “A computational method for Eu's generalized hydrodynamic equations of rarefied and microscale gasdynamics,” *Journal of Computational Physics*, Vol. 168, No. 1, pp. 47-72, 2001. **[JCP 01]**
- **Myong, R. S.**, “A generalized hydrodynamic computational model for rarefied and microscale diatomic gas flows,” *Journal of Computational Physics*, Vol. 195, No. 2, pp. 655-676, 2004. **[JCP 04]**
- **Myong, R. S.**, “Gaseous slip model based on the Langmuir adsorption isotherm,” *Physics of Fluids*, Vol. 16, No. 1, pp. 104-117, 2004. **[PoF 04]**
- **Myong, R. S.**, Reese, J. M., and Lockerby, D. A., “The effect of gaseous slip on microscale heat transfer: An extended Graetz problem,” *International Journal of Heat and Mass Transfer*, Vol. 49, pp. 2502-2513, 2006. **[IJHMT 06]**

III. Emphasis and style (Myong's papers)

- **Myong, R. S.**, "A full analytical solution for the force-driven compressible Poiseuille gas flow based on a nonlinear coupled constitutive relation," *Physics of Fluids*, Vol. 23, No. 1, 012002, 2011. **[PoF 11]**
- **Myong, R. S.**, "Impact of computational physics on multi-scale CFD and related numerical algorithms," *Computers & Fluids*, Vol. 45, No. 1, pp. 64-69, 2011. **[C&F 11]**
- **Myong, R. S.**, "Analytical solutions of shock structure thickness and asymmetry in Navier-Stokes/Fourier framework," *AIAA Journal*, Vol. 52, No. 5, pp. 1075-1080, 2014. **[AIAAJ 14]**
- **Myong, R. S.**, "On the high Mach number shock structure singularity caused by overreach of Maxwellian molecules," *Physics of Fluids*, Vol. 26, No. 5, 056102, 2014. **[PoF 14]**
- Xiao, H., and **Myong, R. S**., "Computational simulations of microscale shock-vortex interaction using a mixed discontinuous Galerkin method," *Computers & Fluids*, Vol. 105, pp. 179-193, 2014. **[C&F 14]**
- Le, N. T. P., Xiao, H., and **Myong, R. S.**, "A triangular discontinuous Galerkin method for non-Newtonian implicit constitutive models of rarefied and microscale gases," *Journal of Computational Physics*, Vol. 273, pp. 160-184, 2014. **[JCP 14]**
- Karchani, A., and **Myong, R. S.**, "Convergence analysis of the direct simulation Monte Carlo based on the physical laws of conservation," *Computers & Fluids*, Vol. 115, pp. 98-114, 2015. **[C&F 15]**

III. Emphasis and style (Myong's papers)

- **Myong, R. S.**, "Theoretical description of the gaseous Knudsen layer in Couette flow based on the second-order constitutive and slip-jump models," *Physics of Fluids*, Vol. 28, No. 1, 012002, 2016. **[PoF 16a]**
- Rana, A., Ravichandran, R., Park, J. H., and **Myong, R. S**., "Microscopic molecular dynamics characterization of the second-order non-Navier-Fourier constitutive laws in the Poiseuille gas flow," *Physics of Fluids*, Vol. 28, No. 8, 082003, 2016. **[PoF 16b]**

▪ Viscoelastic fluids (2)

- **Myong, R. S**., "On singularity of the UCM and Oldroyd-B models in viscoelastic fluids: resolving the high-Weissenberg number problem," *The DFD12 Meeting of The American Physical Society*, San Diego, 2012. **[APSFD 12]**
- **Myong, R. S., "**Origin of the high Weissenberg number singularity in viscoelastic fluids and its removal via a Boltzmann non-Hookean model," *Preprint*, 2017. **[Preprint 17]**

Memo

III. Emphasis and style: acknowledgments

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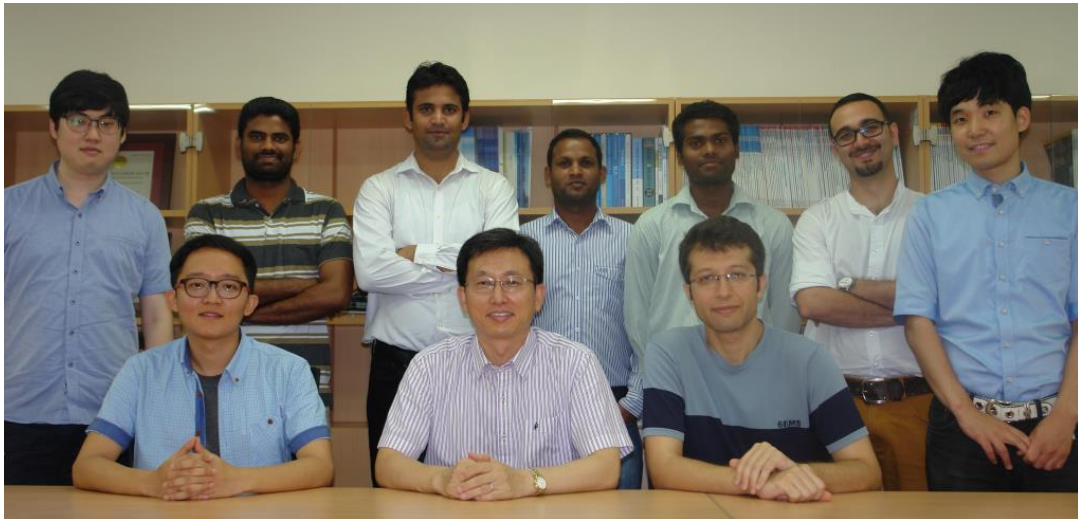


Aerospace Computational Modeling Lab.

http://acml.gnu.ac.kr

IV. History of RMG (with focus on theory)

- **Maxwell, J. C.**, "On the dynamical theory of gases," *Philosophical Transactions of the Royal Society of London*, Vol. 159, pp. 49-88, 1867. **[Maxwell 1867]**
- **Grad**, **H.**, "On the kinetic theory of rarefied gases," *Communications on Pure and Applied Mathematics*, Vol. 2, pp. 331-407, 1949. **[Grad 49]**
- **Grad**, **H.**, "The profile of a steady plane shock wave," *Communications on Pure and Applied Mathematics*, Vol. 5, pp. 257-300, 1952. **[Grad 52]**
- **Eu, B. C**., "A modified moment method and irreversible thermodynamics," *Journal of Chemical Physics*, Vol. 73, pp. 2958-2969, 1980. **[Eu 80]**
- Al-Ghoul, M., and **Eu, B. C.**, "Generalized hydrodynamics and shock waves," *Physical Review E*, Vol. 56, pp. 2981-92, 1997.
- **Eu, B. C.**, *Kinetic Theory and Irreversible Thermodynamics*, Wiley, 1992. **[Eu 92]**
- **Eu, B. C.**, *Generalized Thermodynamics: The Thermodynamics of Irreversible Processes and Generalized Hydrodynamics*, Kluwer, 2002. **[Eu 02]**
- **Eu, B. C**., *Kinetic Theory of Nonequilibrium Ensembles, Irreversible Thermodynamics, and Generalized Hydrodynamics: Volume 1. Nonrelativistic Theories*. Springer, 2016. **[Eu 16]**
- **Jou, D., Casas-Vazques, J., Lebon, G.**, *Extended Irreversible Thermodynamics*, 4th edition, Springer, 2009. **[Jou 09]**
- **Truesdell, C. A., Muncaster, R. G**., *Fundamentals of Maxwell's Kinetic Theory of a Simple Monatomic Gas*, Academic Press, 1980. **[Truesdell 80]**
- **Levermore, C. D**., "Moment Closure Hierarchies for Kinetic Theories." *Journal of Statistical Physics*, Vol. 83, pp. 1021-1065, 1996. [**Levermore 96]**

IV. History of RMG (with focus on theory)

- Navier, Fourier, Maxwell, Boltzmann, Gibbs, Onsager, Prigogine, Muller, Jou, Eu
- Chapman, Enskog, Grad, Truesdel, Cercignani, Ruggeri, Levermore, Villani

Arnold Sommerfeld (1868-1951):
"Thermodynamics is a funny subject. The first time you go through it, you don't understand it at all. The second time you go through it, you think you understand it, except for one or two small points. The third time you go through it, you know you don't understand it, but by that time you are so used to it, it doesn't bother you anymore."

C. A. Truesdell (1952, 1969)
"The rational student must cleave the stinging fog of pseudo-philosophical mysticism which hides this statement [of the second law] in the usual physical treatments."
"I hesitate to use the terms 'first law' and 'second law', because there are almost as many 'first laws' as there are thermodynamicists, and I have been told by these people for so many years that I disobey their laws that now I prefer to exult in my criminal status and non-condemning names to the concrete mathematical axioms I wish to use in my outlaw studies of heat and temperature. The term 'entropy' seems superfluous, also, since it suggest nothing to ordinary persons and only intense headaches to those who have studied thermodynamics but have not given in and joined the professionals."

IV. History of RMG (with focus on theory)

Claude-Louis Navier

Bust of Claude Louis Marie Henri Navier at the École Nationale des Ponts et Chaussées

Born	10 February 1785 Dijon, France
Died	21 August 1836 (aged 51) Paris, France
Nationality	French
Fields	Mathematical physics
Institutions	École Nationale des Ponts et Chaussées École polytechnique French Academy of Science
Alma mater	École Nationale des Ponts et Chaussées
Doctoral advisor	Joseph Fourier
Known for	Navier–Stokes equations

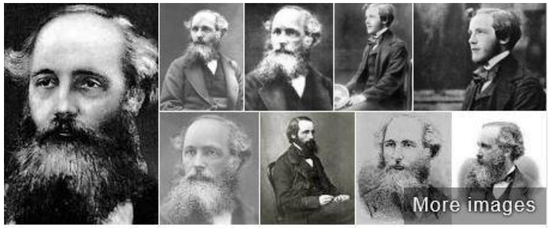
Navier & Fourier conservation laws and constitutive laws (1822)

$$\rho \frac{d\mathbf{u}}{dt} + \nabla p = \nabla \cdot \left(2\eta [\nabla \mathbf{u}]^{(2)} \right)$$

$$\text{Equivalently, } \rho \frac{d\mathbf{u}}{dt} + \nabla \cdot \left(p\mathbf{I} + \mathbf{\Pi} \right) = \mathbf{0}$$

$$\text{and viscous stress } \boxed{\mathbf{\Pi} = -2\eta [\nabla \mathbf{u}]^{(2)}}$$

Maxwell (1867), Boltzmann (1872)



James Clerk Maxwell

Physicist

James Clerk Maxwell FRS FRSE was a Scottish mathematical physicist. His most notable achievement was to formulate the classical theory of electromagnetic radiation, bringing together for the first time ... Wikipedia

Born: June 13, 1831, Edinburgh, United Kingdom

Died: November 5, 1879, Cambridge, United Kingdom

Education: University of Edinburgh, Trinity College, Cambridge, More

Awards: Rumford Medal

Ludwig Boltzmann

Ludwig Boltzmann

Born	Ludwig Eduard Boltzmann February 20, 1844 Vienna, Austrian Empire (present-day Austria)
Died	September 5, 1906 (aged 62) Tybein near Trieste, Austria-Hungary (present-day Duino, Italy) Suicide
Residence	Austria, Germany
Nationality	Austrian
Fields	Physics

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(t, \mathbf{r}, \mathbf{v}) = \boxed{C[f, f_2]}$$

$$C[f, f_2] \sim \int |\mathbf{v} - \mathbf{v}_2| (f^* f_2^* - f f_2) d\mathbf{v}_2$$

IV. History of RMG (with focus on theory)

Grad (1949, 1952)

Communications on
PURE AND APPLIED MATHEMATICS

Polynomial expansion with 3 terms

$$f = f^{(0)}\left[1+\frac{1}{2}\hat{\mathbf{\Pi}}:[\hat{\mathbf{c}}\hat{\mathbf{c}}]^{(2)} - \hat{\mathbf{Q}}\cdot\hat{\mathbf{c}}\left(1-\frac{1}{5}\hat{c}^{2}\right)\right]$$

was inserted into the Maxwell's continuum version of BTE.

COMMUNICATIONS ON PURE AND APPLIED MATHEMATICS, VOL. V, 257–300 (1952)

The Profile of a Steady Plane Shock Wave

By HAROLD GRAD

Harold Grad (born January 23, 1923 in New York City, died November 17, 1986) was an American applied mathematician. His work specialized in the application of statistical mechanics to plasma physics and magnetohydrodynamics.

Contents [hide]

Dr. Harold Grad

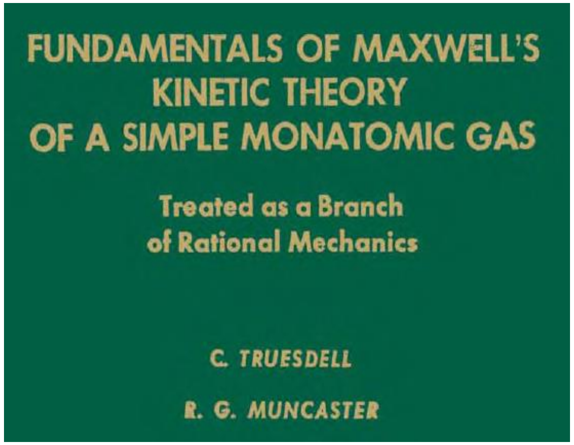
Work [edit]

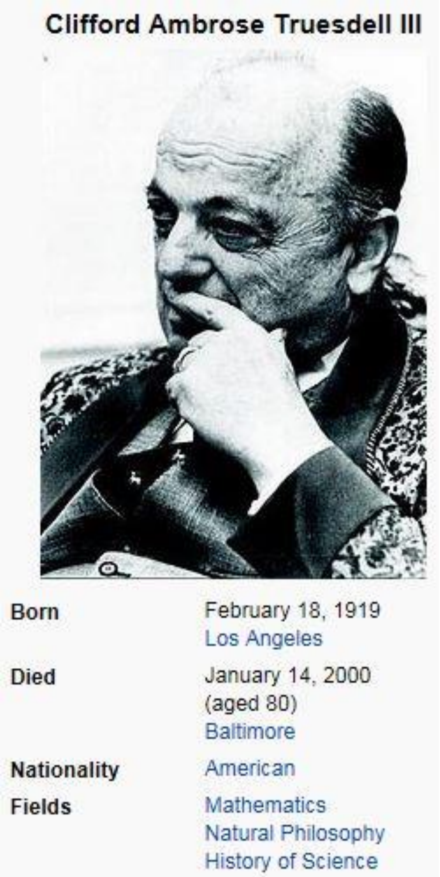
In statistical mechanics he had developed in his thesis new methods for the solution of the Boltzmann equation. Harold Grad was the founder of the Magneto-fluid Dynamics Division of the Courant Institute and served as its head until shortly before his death[1] From 1964 to 1967 and 1974 to 1977 he was a member of the Advisory Committee for Fusion Energy at Oak Ridge National Laboratory.[2]

Grad found a shock structure singularity at M=1.65 in 1952.

IV. History of RMG (with focus on theory)

Truesdel (1956)





It was rigorously proven in the Maxwellian molecule that the linear relation in the collisional term is an exact consequence of the original Boltzmann collision integral by Truesdell ("On the pressures and the flux of energy in a gas according to Maxwell's kinetic theory," II, *J. Rational Mech. Anal*. 5 (1956), 55–128.)

IV. History of RMG (with focus on theory)

B. C. Eu (1980 etc.): Chemist in McGill (Emeritus Prof.)

- Exponential canonical form with no finiteness assumption
- Consideration of entropy production
- Non-polynomial expansion called ‘cumulant expansion’

PHYSICAL REVIEW E VOLUME 56, NUMBER 3 SEPTEMBER 1997

Generalized hydrodynamics and shock waves

Mazen Al-Ghoul and Byung Chan Eu*
Department of Chemistry, McGill University, 801 Sherbrooke Street West, Montreal, Quebec, Canada H3A 2K6
(Received 6 December 1996; revised manuscript received 3 March 1997)

In this paper, the generalized hydrodynamic equations are applied to calculate the shock profiles, shock widths, and calortropy production (energy dissipation) for a Maxwell and variable hard sphere gas.

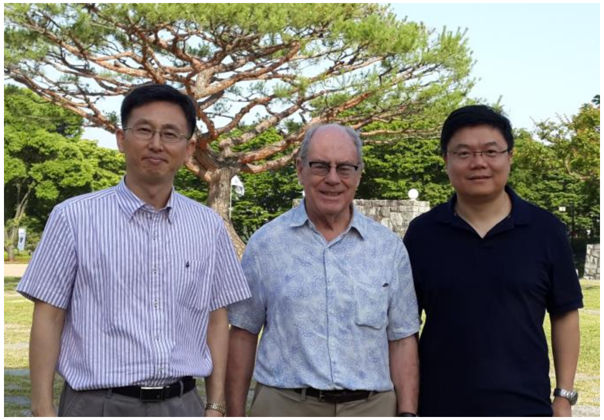
With B. C. Eu (2007)

Our journey in the realm of science is personal in its essence, and one mode of journey, delightful to one, may be an intense discomfort to another. The modes are indeed diverse, and let them be.

The solitary journey in the course of this work has been often lightened by the distant echoes which seem to reverberate from the depth of Old Master Boltzmann’s soul: “Alas, without me for eternity, the sun will rise in the east and will set in the west. Why suffer the pains but for just even a glimpse of Nirvana?”

One still hopes for the day of the ultimate privilege.

In preface of B. C. Eu’s 1997 book ‘Nonequilibrium Statistical Mechanics: Ensemble Method’(Kluwer Academic Publishers)



With P. L. Roe and K. Xu (2015)

V. Applications of RMG and challenges

- **Applications**
  - High-altitude flying vehicles
  - Micro sensors & actuators, micro cooling units for electronic devices
  - Micro power generation & propulsion
  - Information storage devices
  - Devices operating near vacuum condition
  - OLED (organic light emitting diodes) deposition devices
  - Electron transport in semi-conductor
- **Challenges**
  - Unknown problem (deviation from classical physics)
  - Not easily testable (limited information)
  - Theoretical barrier (G.E. and B.C.)
  - Cross-disciplines

Q & A