Pushing the Limits of Continuum Fluid Mechanics and Going beyond the Navier-Stokes-Fourier

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Introduction to Gyeongsang National University

9 Provinces in South Korea
One of the major national universities
Located in Gyeongnam province (manufacturing industrial belt)
Overview of GNU

- 3 campus, 11 colleges, 67 divisions and departments
- 23,000 students
- 730 full-time faculty members
- Founded in 1948
- Aerospace program (9 faculty; 180 undergraduates; 120 graduates)
Research areas of Aerospace Comp. Modeling Lab

Impact on the field

- Rarefied micro/nanoscale gases
- CFD
- MHD space plasmas
- Applied aerodynamics
- Aircraft survivability
- Aircraft icing

No. of papers

JCP, JFM, PoF

Amount of fund

$$$$$

Basic
Idea intensive

Application
Labor intensive
Research goal:

Develop a unified computational model for rarefied and micro- & nano-scale gases upon which others can build efficient CFD codes

http://acml.gnu.ac.kr  ⇔  <Open knowledge>
Part I.

Fundamentals
Introduction to rarefied and micro/nanoscale gases

Compression-dominated
High $M$, low $Kn$

Intermediate Experimental Vehicle

Gas flows around hypersonic vehicles and plume flows
Continuous shift of continuum, transition, and free-molecular regimes
Coexistence of various regimes

Need of unified framework

Shear-dominated
Low $M$, high $Kn$

Micro and nanoscale cylinder

Gas (liquid) flow + MN solid devices
Molecular interaction between gas (liquid) particles and solid atoms
Gas (liquid) flows in thermal (trans., rot.) nonequilibrium regimes
Electrokinetics, surface tension etc.
Approaches for modeling rarefied and micro/nanoscale gases

**Molecular approach**
- DSMC (Direct Simulation Monte Carlo) (Bird)
- Linearized Boltzmann equation (Cercignani, Sone)
- Lattice-Boltzmann method

**Continuum approach**
- Chapman-Enskog: Burnett (1935) etc.
- **Moment method**: Grad (1949), Eu (1992), regularized-13 (2005)
- **Constitutive equations**: the only ingredient in the conservation laws in which the microscopic nature of gas molecules is taken into account.

**Hybrid approach**
- DSMC-continuum coupling (Nie 2004, Schwartzentruber 2007)
- Seamless multi-scale method: viscous stress calculated by MD (Weinan 2009)
Modeling micro and nanomechanics of fluids and rarefied gases

**Top-down:** the classical linear (fluid mechanics) theories can account for virtually everything about materials (fluids).

\[
\frac{D}{Dt} \begin{bmatrix} 1/ \rho \\ u \\ E_t \end{bmatrix} + \nabla \cdot \begin{bmatrix} u \\ pI + \Pi \\ (pI + \Pi) \cdot u + Q \end{bmatrix} = 0
\]

\[\Pi = -\eta[\nabla u]^2, \quad Q = -k\nabla T\]

Navier \quad Fourier

Linear uncoupled constitutive relations

**Bottom-up:** only a molecular-statistical theory of the structure of fluids can provide understanding of their true behavior.

A critical observation: an efficient way of including the molecular nature of gases is to develop nonlinear coupled constitutive relations but to retain the conservation laws.
Linear uncoupled Navier-Fourier equations

Navier (1822) \( \rho \frac{Du}{Dt} + \nabla p + \nabla \cdot \Pi = 0, \quad \rho \frac{D E_t}{Dt} + \nabla \cdot p u + \nabla \cdot [\Pi \cdot u + Q] = 0 \)

Fourier (1822) 
\[
\Pi = -\eta \left[ \nabla u \right]^2, \quad Q = -k \nabla T
\]

\[
\begin{bmatrix}
\Pi_{xx} & \Pi_{xy} \\
\Pi_{yx} & \Pi_{yy}
\end{bmatrix}
\leftarrow
-2\eta
\begin{bmatrix}
u_x - (u_x + v_y)/3 & (u_y + v_x)/2 \\
(v_x + u_y)/2 & v_y - (u_x + v_y)/3
\end{bmatrix}
\]

\( u_x \) case (compression and expansion) \( u_y \) case (velocity shear only)

\[
-2\eta
\begin{bmatrix}
2u_x/3 & 0 \\
0 & -u_x/3
\end{bmatrix}
\]

Not like \((u_x)^2\) \hspace{1cm} \text{Newtonian or linear}

\[
-2\eta
\begin{bmatrix}
0 & u_y/2 \\
u_y/2 & 0
\end{bmatrix}
\]

Uncoupled

\[
\begin{bmatrix}
Q_x \\
Q_y
\end{bmatrix}
\leftarrow
-k
\begin{bmatrix}
T_x \\
T_y
\end{bmatrix}
\]

Not like \((T_x)^2\)
Physics of rarefied and micro/nanoscale gases

\[ Kn = M/Re \]

Increase of thermal non-equilibrium

Re-entry trajectory

\[ M^2 / Re = O(1) \]

\[ M^2 / Re = O(10^{-1}) \]

\[ \Pi / p \sim Kn \cdot M \]

Main parameter

Two terms: \( Kn \)

Three terms: \( M, Kn \) (not \( Kn \) alone!)

\( \nabla f(r, v) = C[f, f_2] \)

\( \rho u \cdot \nabla u + \nabla \cdot p I + \nabla \cdot \Pi = 0 \)
Modelling of nonequilibrium gas system

Molecular (Probabilistic) \[ f(t, r; v) \]

Phase Space \[ \left( \frac{\partial}{\partial t} + v \cdot \nabla + a \cdot \nabla_v \right) f(t, r; v) = C[f, f_2] \]

Boltzmann (1844-1906)

\[ f = \rho \theta \]

\[ \beta = \frac{1}{k_B T} \]

Statistical average

\[ \rho = \langle m f(t, r; v) \rangle \]

\[ \rho u = \langle mv f(t, r; v) \rangle \]

\[ \langle \cdots \rangle = \iiint \cdot \cdot \cdot d v_x d v_y d v_z \]

\[ (\rho, u, T, \Pi, Q, \cdots)(t, r) \]

Continuum (Hydrodynamic)

\[ \frac{D u}{Dt} + \nabla \cdot (p I + \Pi) = \rho a \]

Thermodynamic Space Conservation Laws

(Constitutive Relation)

Not far from LTE

Navier-Stokes-Fourier
A modified moment method [Eu, 1992]

\[ \rho \equiv \langle mf(t, r; v) \rangle, \quad \rho u \equiv \langle mvf(t, r; v) \rangle, \quad \left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \mathbf{a} \cdot \nabla_v \right) f(t, r; v) = C[f, f_2] \]

Differentiating the statistical definition \( \rho \equiv \langle mf(t, r; v) \rangle \) with time and then combining with the Boltzmann equation

\[ \frac{\partial}{\partial t} \rho = \frac{\partial}{\partial t} \langle mf(t, r; v) \rangle = \langle m \frac{\partial f}{\partial t} \rangle = \langle mC[f, f_2] \rangle - \langle mv \cdot \nabla f \rangle \]

\[ \frac{\partial \rho}{\partial t} + \langle mv \cdot \nabla f \rangle = \langle mC[f, f_2] \rangle = 0 \]

\[ \frac{\partial \rho}{\partial t} + \langle m \nabla \cdot (fv) \rangle - \langle mf \nabla \cdot v \rangle = \frac{\partial \rho}{\partial t} + \langle m \nabla \cdot (fv) \rangle = 0 \]

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \langle mf v \rangle = 0 \]

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \]
The modified moment method (continued)

Moment equations in vector form

\[ \rho \frac{D}{Dt} \begin{bmatrix} 1/ \rho \\ u \\ E_t \end{bmatrix} + \nabla \cdot \begin{bmatrix} u \\ pI \\ pu \end{bmatrix} + \nabla \cdot \begin{bmatrix} 0 \\ \Pi \\ \Pi \cdot u + Q \end{bmatrix} = \begin{bmatrix} 0 \\ \rho a \\ \rho a \cdot u \end{bmatrix} \]

Unsteady Convection Higher-order
\[ \frac{\partial}{\partial t} \begin{bmatrix} \Pi \\ Q \end{bmatrix} + u \cdot \nabla \begin{bmatrix} \Pi \\ Q \end{bmatrix} = -\nabla \cdot \psi^{(\Pi)} - \nabla \cdot \psi^{(Q)} + \psi^{(P)} : \nabla u \]

Kinematic Force Thermo. driving Dissipation
\[ -\begin{bmatrix} 2[\Pi \cdot \nabla u]^{(2)} \\ C_p \Pi \cdot \nabla T + Q \cdot \nabla u + \frac{Du}{Dt} \cdot \Pi \end{bmatrix} + \begin{bmatrix} 0 \\ a \cdot \Pi \end{bmatrix} -\begin{bmatrix} 2p[\nabla u]^{(2)} \\ C_p p \nabla T \end{bmatrix} + \Lambda^{(\Pi)} + \Lambda^{(Q)} \]

\[ \Pi = \langle m[cc]^{(2)} f \rangle, \quad Q = \langle mc^2 cf / 2 \rangle, \]
\[ \psi^{(\Pi)} = \langle m[cc]^{(2)} cf \rangle, \quad \psi^{(P)} = \langle mccef \rangle, \quad \psi^{(Q)} = \langle mc^2 cef / 2 \rangle \]
\[ \Lambda^{(\Pi)} = \langle m[cc]^{(2)} C[f, f_2] \rangle, \quad \Lambda^{(Q)} = \langle mc^2 e / 2C[f, f_2] \rangle \]
A physically motivated closure

By noting the relative importance of various terms, for example,

\[
\left| \nabla \cdot \psi^{(\Pi)} \right| < \left| \Pi \cdot \nabla u \right|^{(2)} , \left| p \left[ \nabla u \right]^{(2)} \right|
\]

Kinematic Thermo. driving

one may neglect the higher-order term as an approximation.

\[
\nabla \cdot \psi^{(\Pi)} \approx 0,
\]

\[
\nabla \cdot \psi^{(Q)} + \psi^{(P)} : \nabla u \approx 0
\]

Then we have a nonlinear coupled algebraic constitutive relation (NCCR)

\[
0 = - \left[ 2 \left[ \Pi \cdot \nabla u \right]^{(2)} \right] + \left[ 0 \right] - \left[ 2 p \left[ \nabla u \right]^{(2)} \right] + \left[ \Lambda^{(\Pi)} \right]
\]

\[
\begin{bmatrix}
\text{Kinematic} \\
\text{Force} \\
\text{Thermo. driving} \\
\text{Dissipation}
\end{bmatrix}
\]
A computational framework based on
NCCR

Edge based finite volume formulation in general coordinates (JCP 2004)

\[
\frac{\partial}{\partial t} \int_V U dV + \int_S F \cdot n dS = 0
\]

\[
U_{i,j}^{n+1} = U_{i,j}^n - \frac{\Delta t}{A_{i,j}} \sum_{k=1}^{N} R_k^{-1} F_k^n \Delta L_k
\]

\[
\Pi = f_\Pi (\Pi_{\text{NSF}}, Q_{\text{NSF}}, p, T), \quad Q = f_Q (\Pi_{\text{NSF}}, Q_{\text{NSF}}, p, T)
\]
NCCR property in compression-expansion and velocity shear case

\[-2\eta \left[ \nabla \mathbf{u} \right]^2 \frac{\partial p}{\partial \eta} \]

\[-k \nabla T \]

Thermodynamic driving force

Algebraic NCCR

\[ \Pi \]

Shear stress

Heat flux

\[ \Pi / p \]

\[ \Pi_{xx} / p \]

Nonlinear (non-Newtonian)

Expansion

Compression

Coupled

\[ \Pi_{xx, xy} / p \]

Shear stress (Navier–Stokes)

Shear stress (monatomic NCCR)

Normal stress (Navier–Stokes)

Normal stress (monatomic NCCR)

\[ -\eta du / dx / p \]

\[ -\eta du / dy / p \]
Non-Fourier law by the coupling of force and shear stress

\[ \hat{Q}_y = \frac{3}{3 + 2\hat{\Pi}_{xy0}^2} \left( \hat{Q}_{y0} + a\hat{\Pi}_{xy0} \right); \quad a \text{ is force} \]

\[ \hat{\Pi}_{xy} \equiv \hat{\Pi}_{xy} / p \]

\[ \hat{Q}_{x,y} \equiv Q_{x,y} / \left( p \sqrt{C_p T / (2 \text{Pr})} \right) \]

Non-Fourier behavior!

Fourier law

\[ \hat{Q}_y = \hat{Q}_{y0} \]
Part II.

Validation
Validation I: Celebrated shock structure

Major stumbling blocks for theoreticians for a long time

“... is found that the solution breaks down completely, and no solution exists for stronger shocks (specifically, at Mach number $M=1.65$)…” (H. Grad 1952)

It was solved by B. C. Eu in 1997 (Phys. Rev. E)

How his theory works is explained here.

Graveyard of theoreticians
Validation I (continued)

Unsteady Convection Higher-order

\[ \frac{\partial \Pi}{\partial t} + (u \cdot \nabla) \Pi = -\nabla \cdot \psi^{(\Pi)} - 2[\Pi \cdot \nabla u]^{(2)} - 2p[\nabla u]^{(2)} + \Lambda^{(\Pi)} \]

Comment: In steady-state case, one has to deal with 5 terms, which is really difficult juggling. Even in simple 3 ball juggling, there can be as many as 17 methods.

Key finding: Gases are *compressed rapidly* across the shock wave and so accurate treatment of *dissipation* term will be critical.

What B. C. Eu did: Assume the distribution function \( f \) in exponential form (not in usual polynomial form) and then apply the cumulant expansion method: the celebrated Eu’s *hyperbolic sine* factor.
Validation I (continued)

Essential terms are three in the right-hand side

\[ 0 + 0 = 0 - 2 \left( \Pi \cdot \nabla \mathbf{u} \right)^{(2)} - 2 p \left( \nabla \mathbf{u} \right)^{(2)} + \Lambda^{(\Pi)} \]

Kinematic Thermo. driving Dissipation

\[ \Lambda^{(\Pi)} = -\frac{\Pi}{\eta / p} q(\kappa), \quad q(\kappa) \equiv \frac{\sinh \kappa}{\kappa} \]

where \( \kappa = \left( \frac{m k_B T}{2 \eta} \right)^{1/4} \left( \frac{\Pi : \Pi + Q \cdot Q}{kT} \right)^{1/2} \)

Cf. \( q(\kappa) = 1; \) BGK or relaxation approx.

\[ C[f, f_2] \approx \frac{f^{\text{equil}} - f}{\tau} \]

Comment: No 1st-order term in the series expansion of \( q(\kappa) \) explains why the NSF approximation is so successful.

Cf. Drag polar in aerodynamics
Validation I (continued)

Before

\[
\frac{\Pi_{xx}}{p}
\]

Singularity

expansion

compression

With

\[
q(\kappa) = \frac{\sinh \kappa}{\kappa}
\]

After

singularity removed!

expansion

compression

Navier-Stokes

Grad

2nd-Burnett

3rd-Burnett

\[ -\eta \frac{du}{dx}/p \]

\[ \frac{\Pi_{xx}}{p} \]

\[ \frac{\partial u}{\partial x}/p \]

\[ \frac{\partial p}{\partial x}/p \]

\[ \frac{\partial \Pi_{xx}}{\partial x}/p \]

\[ \frac{\partial u}{\partial x} \cdot \frac{\partial p}{\partial x}/p \]

\[ \frac{\partial \Pi_{xx}}{\partial x}/p \]
Shock density thickness for a diatomic gas versus the Mach number (o: experimental data)

Normalized temperature contours (NSF vs NCCR) in multi-species flowfield around a reentry vehicle (M=23.47, Kn=0.2238; courtesy of J. H. Ahn)
Validation II: 1-d force-driven compressible Poiseuille gas flow (velocity shear dominated; PoF 2011)

\[ \varepsilon_{\text{wall}} = \frac{ah}{RT_{\text{wall}}} : \text{Richardson no.}, \quad Kn = \sqrt{\frac{\pi \eta_{\text{wall}} RT_{\text{wall}}}{2 p_{\text{reservoir}} h}} : \text{Knudsen no.} \]
Different role of $q(\kappa)$ term in velocity shear

With

\[ q(\kappa) = 1 \]

\[ q(\kappa) \equiv \frac{\sinh \kappa}{\kappa} \]

\[
\left( \frac{\Pi_{xy}}{p} \right)^2 = -\frac{3}{2} \left( 1 + \frac{\Pi_{yy}}{p} \right) \frac{\Pi_{yy}}{p}
\]

Local kinematic stress constraint

BGK or relaxation is fairly good approximation, in stark contrast with the shock structure case!
Validation II: Fully *analytical* solution \((\text{Kn}=0.1, \varepsilon_{hw} = 0.6)\)

\[
\frac{p(S^*)}{p(0)} = 1 + \tan^2 S^*
\]

Pressure profile across channel
*(NSF: blue, NCCR: cyan)*

\[
\frac{p(S^*)}{p(0)} = 1
\]

\[
\text{concave}
\]

\[
T(S^*) \frac{1}{T(0)} = \sec^{3/5} S^* \left[ 1 - \frac{\pi \Pr_T}{816} \frac{T_w}{T(0)} \frac{\varepsilon_{hw}^2}{S_w} \frac{F(S^*)}{S^*} \right], \quad S^* \equiv \sqrt[3]{\frac{2}{3}T_w \varepsilon_{hw} S^*}
\]

\[
F(S^*) \equiv 17 \left[ \frac{1}{17 \cos^{17/5} S^*} - \frac{1}{7 \cos^{7/5} S^*} - \left( \frac{1}{17} - \frac{1}{7} \right) \right]
\]

Temperature profile across channel
*(NSF: blue, NCCR: cyan)*
Validation II: comparison with other solutions

Pressure profile across channel

Temperature profile across channel

Capturing all the qualitative features predicted by the DSMC

Cf. DSMC (Bird), Regularized-13 (Struchtrup)
An exotic prediction: heat conduction from **cold** to **hot**

Non-Fourier behavior in NCCR

\[
\hat{Q}_y = \frac{3}{\left(3 + 2\overline{\Pi}^2_{xy_{NSF}}\right)}\left(\hat{Q}_{y_{NSF}} + a\overline{\Pi}_{xy_{NSF}}\right); \ a \text{ is force}
\]

Temperature contours (Courtesy of E. Roohi)

Heat transfer from **Cold** (center) to **hot**

Cf. \( H(t) = \sum_{bins} \Delta v \frac{N_h(v)}{N} \ln \frac{N_h(v)}{N} \) in DSMC

\( N_h(v) \): the number of particles in a histogram bin of width \( \Delta v \)
Another example of exotic prediction: lid-driven cavity 2-D gas flows (no force; DSMC; Kn=0.5)

Lid-driven cavity gases

Non-Fourier behavior in NCCR

Temperature contours
(Courtesy of E. Roohi)

$H$ function contours

Heat transfer from Cold (center) to hot in 2-D
Part III.

New Potential Applications of the Present Framework
Loss of convergence of viscoelastic flow solutions in complex fluids (polymer solutions; rheology)

Viscoelastic fluids are complex fluids that have “memory” (the state-of-stress depends on the flow history)
Visco: friction, irreversibility, loss of memory
Elastic: recoil, internal energy storage

The high-Weissenberg number problem: A 30 year old mystery. ...All methods, without exception, were found to break down at a frustratingly low value of the Weissenberg number around We=1.

(R. Fattal, R. Kupferman 2005)
Analogy of viscoelastic flow and rarefied gases

\[ \text{We} \equiv \frac{\tau}{T} \sim \left( \frac{l}{a} \right) \left( \frac{L}{u} \right) \sim \text{Kn} \cdot M \quad \text{vs} \quad \text{N}_\delta \equiv \frac{\Pi}{p} \sim \text{Kn} \cdot M \]

Upper-convected Maxwell equation derived from the stochastic model of dumbbells

Nonlinear coupled constitutive equation derived from the Boltzmann equation

Key observation: almost complete parallel with the gas dynamic problem -> on-going topic
Occurrence of the singularity in the stationary solution of continuum models of carrier transport in semiconductors

The mathematic singularity problem in the ballistic regime:

...Concerning the second effect, the spike is enhanced by a smaller mesh size, which is an indication of the occurrence of some sort of “singularity” in the stationary solution.

We remark that such phenomena is not a numerical artifact. Indeed, a similar behavior has been observed with different discretization based on kinetic schemes.

(A. M. Anile et al. 2000)
Concluding remarks

• **Pushing the limits of continuum theory:**
  - algebraic nonlinear coupled constitutive relation (NCCR)
  - persistent attack on the key problems—the shock structure problem
  - delicate balancing in juggling terms

• **Going beyond Navier-Stokes-Fourier:**
  - not easy due to no appearance of 1st order term
  - nothing taken for granted such as the possibility of heat transfer from **cold** to **hot**

• **Applicable to other unsolved issues:** defeating the high Weissenberg number problem in computational rheology and the ballistic transport of carriers in semi-conductors.
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