Some Mathematical Problems in Nonequilibrium Fluid Dynamics and Nonstrictly Hyperbolic Conservation Laws

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Talk outline

- Research goals
- Introduction of nonequilibrium fluid dynamics and MHD
- Derivation of hydrodynamic equations from the Boltzmann equation (problem I)
- Model of molecular interaction between gas particle and surface atoms (problem II)
- Nonstrictly hyperbolic conservation laws (problem III)
- Summary

Research goals

- Fundamental questions:

  Possibility of developing **mesoscopic** mathematical models capable of describing high non-equilibrium flows such as rarefied and microscale gas flows

  Are non-classical shock waves physical?

- Research goals:

  Answering fundamental questions and validation study

  Deriving governing equation and boundary conditions

  -> the basic building block for an **efficient** CFD code

  Providing physical insight and economy of thoughts

- Practical issues**:**

  How to solve the moment equations

  How to develop a numerical scheme capable of describing the non-classical shock waves without explicit treatment of the viscous and dispersive inner profiles

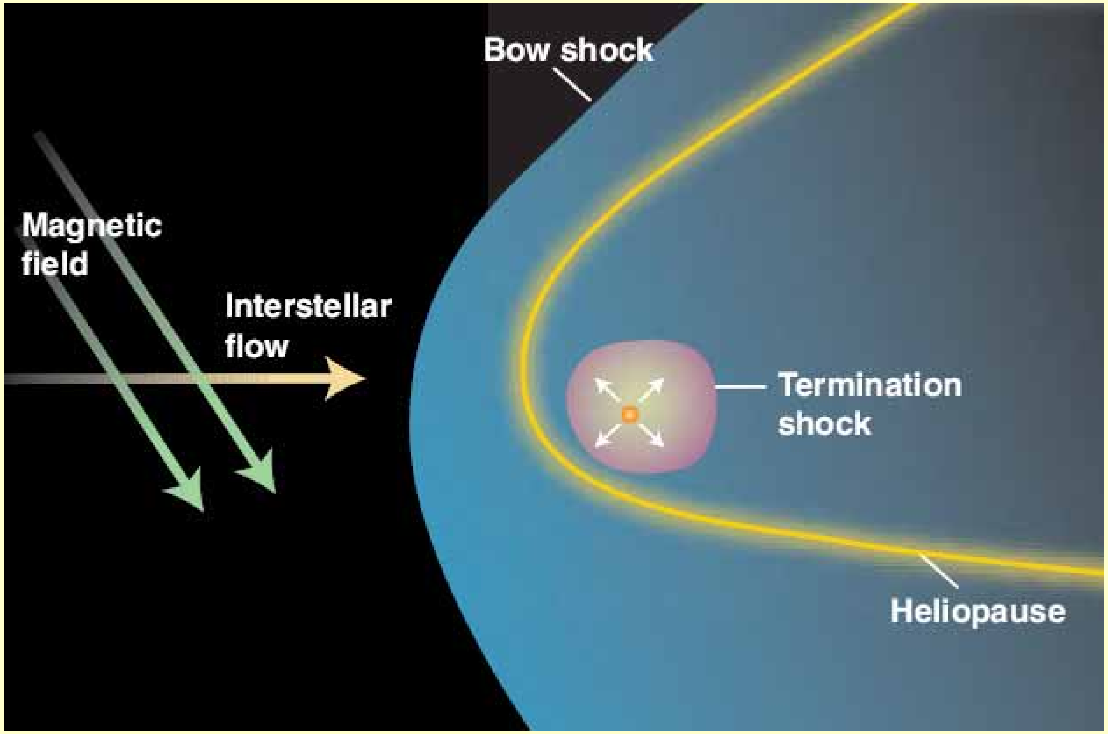
Introduction of nonequilibrium fluid dynamics and MHD

- Nonequilibrium fluid dynamics: Any problem beyond the realm of linear theory (Navier-Stokes; near thermal equilibrium)

  Rarefied gas (vacuum devices, space plasma), hypersonic flow (space shuttle), micro and nanoscale flow (MEMS), charge transport in semiconductor

- MHD: Magneto-hydrodynamics (Navier-Stokes + Maxwell)

  Space plasma, fusion



Strategy for nonequilibrium fluid dynamics

- **Capability**: recover the Navier-Stokes model and extend to the transition regimes [Kn and Kn*M~O(1)]
- **Constraints** on the new model: efficiency, robustness, and mathematical consistency
- **Issues**:

  Equation types—hyperbolic or parabolic

  Boundary—definition of independent variables

  Balanced treatment of each effects (convective, kinematic, and dissipative)
- **Consider a simple problem (benchmark problem)**

  Focus on the big picture

Preliminary information for fluid dynamics

Boltzmann equation in phase space: $f(\mathbf{v},\mathbf{r},t)$ where $\mathbf{v}=\mathbf{u}+\mathbf{c}$

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right)f(\mathbf{v},\mathbf{r},t)=C[f],\ \text{where}\ C[f]\equiv\int d\mathbf{v}\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\sin\theta\int_0^{\infty}dbbg_{12}\left[f_1^*f_2^*-f_1f_2\right]$$

Reduction of information

Statistical average:

density $\rho=\langle mf(\mathbf{v},\mathbf{r},t)\rangle$, where $\langle A\rangle=\int d\mathbf{v}Af$

mean velocity $\mathbf{u}=\langle m\mathbf{v}f(\mathbf{v},\mathbf{r},t)\rangle$,

$\ldots$

stress tensor $\mathbf{P}=\langle m\mathbf{cc}f(\mathbf{v},\mathbf{r},t)\rangle$

Navier-Stokes-Fourier in thermodynamic space: $(\rho,\mathbf{u},T)$

$$\rho\frac{D}{Dt}\begin{bmatrix}1/\rho\\ \mathbf{u}\\ E_t\end{bmatrix}+\nabla\cdot\begin{bmatrix}\mathbf{u}\\ p\mathbf{I}+\mathbf{\Pi}\\ (p\mathbf{I}+\mathbf{\Pi})\cdot\mathbf{u}+\mathbf{Q}\end{bmatrix}=\mathbf{0}\ \text{where}\ \mathbf{\Pi}=-2\eta[\nabla\mathbf{u}]^{(2)}\ \text{and}\ \mathbf{Q}=-\lambda\nabla\ln T$$

The moment method (Maxwell and Grad)

By differentiating **stress tensor** $\mathbf{P} = \langle m\mathbf{cc}f(\mathbf{v},\mathbf{r},t)\rangle$ with time and combining with the Boltzmann equation $(\partial_t + \mathbf{v}\cdot\nabla) f(\mathbf{v},\mathbf{r},t) = C[f]$,

we obtain the constitutive equations.

$\mathbf{P}_t = -\langle m\mathbf{cc}(\mathbf{v}\cdot\nabla f)\rangle + \mathbf{\Lambda}^{(P)}$ where $\mathbf{\Lambda}^{(P)} \equiv \langle m\mathbf{cc}C[f]\rangle$ and $\mathbf{P} \equiv p\mathbf{I} + \mathbf{\Pi}$

$$\rho\frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right) + \nabla\cdot\boldsymbol{\psi}^{(\Pi)} = -2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} - 2p[\nabla\mathbf{u}]^{(2)} + \mathbf{\Lambda}^{(\Pi)}\left(\equiv\langle m[\mathbf{cc}]^{(2)}C[f]\rangle\right)$$

substantial derivative of non-conserved variable

+ flux of high order flux = kinematic term + **dissipation term (Boltzmann collision)**

Mathematically, $\mathbf{\Pi}$ = function of conserved variables and their gradients

➡ No approximations; main parameter $\Pi / p \sim \mathrm{Kn}\cdot M$ (not Kn alone)

No explicit C[f(**v**,**r**,t)] except for the dissipation term; not pure hyperbolic

$$\rho\frac{D}{Dt}\begin{bmatrix} [1, \rho\mathbf{u}, \rho E_t]^T / \rho \\ \mathbf{\Pi}/\rho \\ \mathbf{Q}/\rho \end{bmatrix} + \nabla\cdot\begin{bmatrix} [\mathbf{u}, \mathbf{P}, \mathbf{P}\cdot\mathbf{u} + \mathbf{Q}]^T \\ \mathbf{\Psi}^{(\Pi)} \\ \mathbf{\Psi}^{(Q)} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{Z}^{(\Pi)} + \mathbf{\Lambda}^{(\Pi)} \\ \mathbf{Z}^{(Q)} + \mathbf{\Lambda}^{(Q)} \end{bmatrix}$$

Eu's modified moment method

- **Grad's moment method (1949)**

$$\rho \frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right) + \nabla \cdot \boldsymbol{\psi}^{(\Pi)} = -2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)} \underline{-2p\left[\nabla\mathbf{u}\right]^{(2)} + \mathbf{\Lambda}^{(\Pi)}} \left(\equiv \left\langle m[\mathbf{cc}]^{(2)} C[f]\right\rangle \overset{Grad}{=} -\boxed{\frac{\mathbf{\Pi}}{\eta / p}}\right)$$

Relaxation (BGK) approximation for C[f] and f in a polynomial form

Closure relation: high order moment $\boldsymbol{\psi}^{(\Pi)}$ ~ heat flux

➡ Mathematical singularity for high Kn*M

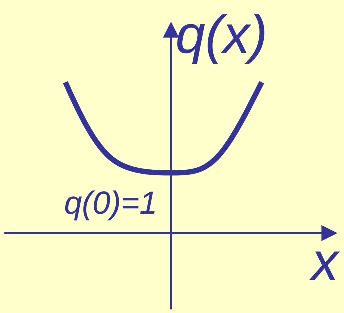
- **Eu's modified moment method (1980, 1992, 1998, 2002)**

$$\rho \frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right) + \nabla \cdot \boldsymbol{\psi}^{(\Pi)} = -2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)} \underline{-2p\left[\nabla\mathbf{u}\right]^{(2)} + \mathbf{\Lambda}^{(\Pi)}} \left(\equiv \left\langle m[\mathbf{cc}]^{(2)} C[f]\right\rangle \overset{Eu}{=} -\boxed{\frac{\mathbf{\Pi}}{\eta / p} q(\kappa)}\right)$$

f in an exponential form

Cumulant expansion for C[f]

$$\boxed{q(\kappa) \equiv \frac{\sinh \kappa}{\kappa}} \text{ where } \kappa = \frac{(mk_B T)^{1/4}}{\sqrt{2}\, pd}\left(\frac{\mathbf{\Pi}:\mathbf{\Pi}}{2\eta} + \frac{\mathbf{Q}\cdot\mathbf{Q}}{\lambda}\right)^{1/2}$$



➡ Mathematical singularity is removed

Differential -> algebraic equations -> resolve the boundary problem

Problem I: Nonlinear algebraic equations

$$0 = -2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} - 2p[\nabla\mathbf{u}]^{(2)} - \frac{\mathbf{\Pi}}{\eta/p}q(\kappa)$$

$$0 = -\mathbf{\Pi}\cdot\nabla T - p\nabla\ln T - \frac{\mathbf{Q}}{\lambda/p}q(\kappa)$$

$$\text{where } q(\kappa) \equiv \frac{\sinh\kappa}{\kappa} \text{ and } \kappa = \frac{(mk_B T)^{1/4}}{\sqrt{2}pd}\left(\frac{\mathbf{\Pi}:\mathbf{\Pi}}{2\eta} + \frac{\mathbf{Q}\cdot\mathbf{Q}}{\lambda}\right)^{1/2}$$

$$\hat{\mathbf{\Pi}}q(\hat{R}) = \hat{\mathbf{\Pi}}_0 + [\hat{\mathbf{\Pi}}\cdot\nabla\hat{\mathbf{u}}]^{(2)}$$

$$\hat{\mathbf{Q}}q(\hat{R}) = \hat{\mathbf{Q}}_0(1+\hat{\mathbf{\Pi}}) \quad \text{where } \hat{R}^2 = \hat{\mathbf{\Pi}}:\hat{\mathbf{\Pi}} + \hat{\mathbf{Q}}\cdot\hat{\mathbf{Q}}$$

In Navier-Stokes,

$$\hat{\mathbf{\Pi}}_0 = \frac{-2\eta[\nabla\mathbf{u}]^{(2)}}{p}, \quad \hat{\mathbf{Q}}_0 = \frac{-\lambda\nabla\ln T}{p\sqrt{C_p T/2\,\mathrm{Pr}}}$$

- **Unknowns: shear stress tensor and heat flux vector**

  Knowns: conserved quantities and their gradients in position

Problem I: Solution method

$$\hat{\mathbf{\Pi}} q(\hat{R}) = \hat{\mathbf{\Pi}}_0 + \left[\hat{\mathbf{\Pi}} \cdot \nabla \hat{\mathbf{u}}\right]^{(2)}$$

$$\hat{\mathbf{Q}} q(\hat{R}) = \hat{\mathbf{Q}}_0 \left(1 + \hat{\mathbf{\Pi}}\right) \qquad \text{where } \hat{R}^2 = \hat{\mathbf{\Pi}} : \hat{\mathbf{\Pi}} + \hat{\mathbf{Q}} \cdot \hat{\mathbf{Q}}$$

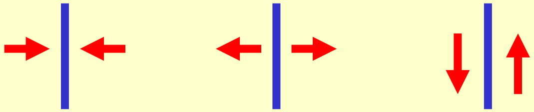
$$\begin{pmatrix} \hat{\Pi}_{xx} & \hat{\Pi}_{xy} & \hat{\Pi}_{xz} \\ \hat{\Pi}_{yx} & \hat{\Pi}_{yy} & \hat{\Pi}_{yz} \\ \hat{\Pi}_{zx} & \hat{\Pi}_{zy} & \hat{\Pi}_{zz} \end{pmatrix}, \begin{pmatrix} \mathrm{Q}_x \\ \mathrm{Q}_y \\ \mathrm{Q}_z \end{pmatrix} = \mathrm{fn}\left(p, T, \nabla u, \nabla v, \nabla w, \nabla T\right)$$

- **Method of iterations**

$$\left(\hat{\mathbf{\Pi}}, \hat{\mathbf{Q}}\right) = f\left(\hat{\mathbf{\Pi}}, \hat{\mathbf{Q}}\right) \quad \Rightarrow \quad \left(\hat{\mathbf{\Pi}}_{n+1}, \hat{\mathbf{Q}}_{n+1}\right) = f\left(\hat{\mathbf{\Pi}}_n, \hat{\mathbf{Q}}_n\right)$$

In Navier-Stokes, $\hat{\mathbf{\Pi}}_0$ and $\hat{\mathbf{Q}}_0$

When the kinematic terms are neglected, $\hat{\mathbf{\Pi}}_1 = \dfrac{\sinh^{-1}(R_0)}{R_0} \hat{\mathbf{\Pi}}_0$ and $\hat{\mathbf{Q}}_1 = \dfrac{\sinh^{-1}(R_0)}{R_0} \hat{\mathbf{Q}}_0$

- **Well-posed in one-dimensional case:** 

- **Challenge: how about in general three-dimensional case?**
  well-posedness and efficient numerical algorithm

Boundary condition based on Langmuir adsorption isotherm

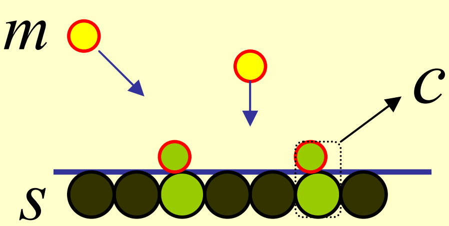
N : number of sites (s) per unit area of the surface interacting with gas molecules (m)

$N\alpha$: number of sites which are covered

$N(1-\alpha)$: number of sites which are not covered

Let us assume that m and s form the complex c. Then the equilibrium constant K becomes

$$K = \frac{C_c}{C_m C_s} = \frac{N\alpha}{\left[p / k_B T_w\right] N(1-\alpha)},$$



that is,

$$\boxed{\alpha = \frac{\beta p}{1+\beta p}} \quad \text{where} \quad \beta = \frac{K}{k_B T_w}.$$

$m + s \Rightarrow c$

Slip Boundary Conditions

- **Langmuir slip condition (Dirichlet type)**

$$u = \alpha u_w + (1-\alpha)u_r, \quad T = \alpha T_w + (1-\alpha)T_r \text{ where } \alpha = \frac{p/4\omega Kn}{1+p/4\omega Kn}$$

$$\omega = \omega_0(\nu)\left(\frac{T_w}{T_r}\right)^{1+2/(\nu-1)} \exp\left(-\frac{D_e}{k_B T_w}\right) = fn(\nu, T_w, D_e)$$

D_e : Heat of adsorption [$O(10^{-1} \sim 10)$ kcal/mol]

- **Maxwell slip condition (Neumann type)**

$$u = u_w + \varsigma \Pi_w = u_w + \sigma_v \ell \left(\frac{\partial u}{\partial n}\right)_w, \quad T = T_w + \sigma_T \frac{1}{\Pr}\frac{2\gamma}{\gamma+1}\ell\left(\frac{\partial T}{\partial n}\right)_w$$

Cf. We can prove $\omega \sim \sigma_v \left(\equiv (2-\theta)/\theta\right)$ in the case of microchannel flow.

As a result, **a physical meaning can be assigned to** $\sigma_{v,T}$.

$$\sigma_{v,T} \sim \omega = \omega_0(\nu)\left(\frac{T_w}{T_r}\right)^{1+2/(\nu-1)} \exp\left(-\frac{D_e}{k_B T_w}\right)$$

Pressure-driven compressible flow in a long micro-channel

- Navier - Stokes (isothermal and low Mach : $p \sim \rho$)

$$\begin{pmatrix} \rho \\ \rho \mathbf{u} \end{pmatrix}_t + \nabla \cdot \begin{pmatrix} \rho \mathbf{u} \\ \rho \mathbf{u}\mathbf{u} + p\mathbf{I} \end{pmatrix} + \nabla \cdot \begin{pmatrix} 0 \\ \mathbf{\Pi}_0 \end{pmatrix} = 0$$

- Expand $(\mathbf{u}, p)$ in powers of $\varepsilon \equiv$ Height / Length

$$\frac{\partial (pu)}{\partial x} + \frac{\partial (pv)}{\partial y} = 0$$

$$\frac{dp}{dx} = \frac{\partial^2 u}{\partial y^2}$$

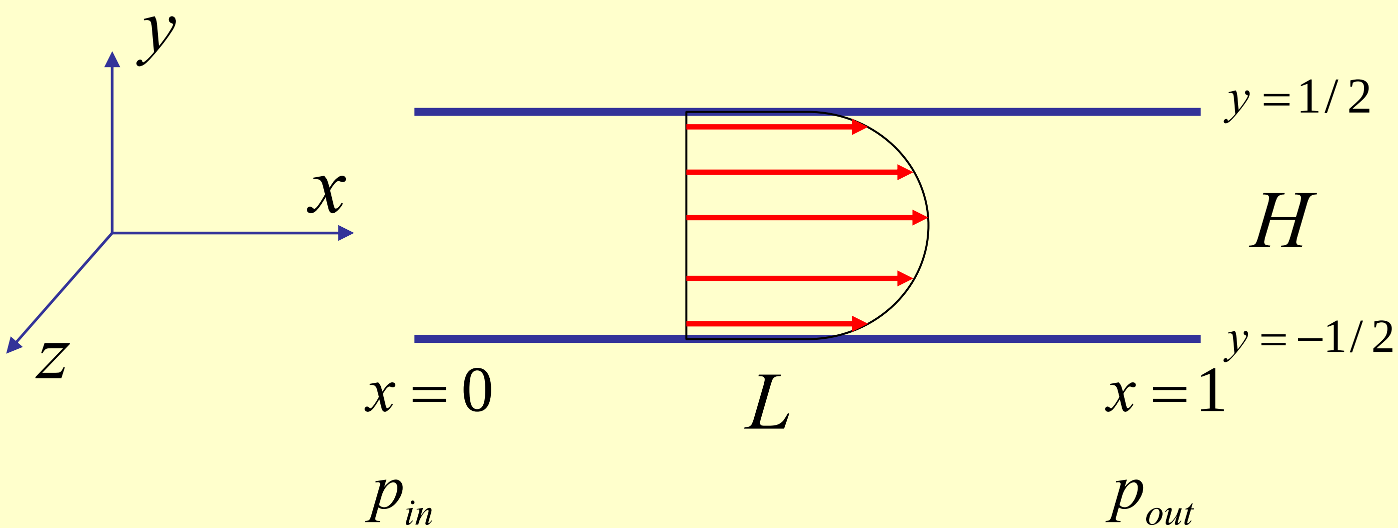
with slip b. c. ⇨

$$p(x)$$

$$u(x, y)$$

$$v(x, y)$$

Problem II: O. D. E. of pressure distribution



- O. D. E. of pressure distribution along the channel

$$\mathit{local}\ \text{b.c.}\ u = \frac{u(x, y=0)}{1+\bar{\beta} p} \quad \Rightarrow \quad \left(p^2\right)'' = -\frac{3}{\bar{\beta}} p''$$

$\Rightarrow\ p(x)$ well-defined for all $\bar{\beta}$ and p_{inlet}

Problem II: O. D. E. of pressure distribution with special b. c.

- O. D. E. of pressure distribution along the channel

$$\mathit{global}\ \text{b. c.}\ u = \frac{u(x=1, y=0)}{1+\bar{\beta}p}$$

$$\Rightarrow \quad \left(p^2\right)'' = -\frac{3}{\bar{\beta}} \frac{\left(1+\bar{\beta}\right)}{\left(1+\bar{\beta}p\right)^2} \boxed{p'_{x=1}} p'$$

$$\Rightarrow \quad p(x)\ \text{well-defined only for}\ \bar{\beta} > \left\{\left[1+6p_{\text{inlet}}(p_{\text{inlet}}-1)\right]^{1/2} - 1\right\} / 2p_{\text{inlet}}$$

- Conjecture: Higher order b. c. may show the range of their validity within the formulation whereas the calculations in the first-order approximation in general do not show in themselves the range of their validity.

Magneto-hydrodynamics: NS+Maxwell

- **1-D MHD equations of hydrodynamic description of a plasma**

$$\begin{pmatrix} \rho \\ \rho\mathbf{u} \\ \mathbf{B}_\perp \\ E \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho\mathbf{u}u + (p + \mathbf{B}_\perp \cdot \mathbf{B}_\perp / 2)\mathbf{I} - B_x\mathbf{B}_\perp \\ \mathbf{B}_\perp u - B_x\mathbf{v} \\ (E + p + \mathbf{B}_\perp \cdot \mathbf{B}_\perp / 2)u - B_x(\mathbf{B}_\perp \cdot \mathbf{v}) \end{pmatrix}_x = \begin{pmatrix} 0 \\ D_1\mathbf{u} \\ D_2\mathbf{B}_\perp \\ \Sigma + \kappa T \end{pmatrix}_{xx}$$

$$\text{where } 2\Sigma = \mu(\mathbf{u}\cdot\mathbf{u}) + \nu(\mathbf{v}\cdot\mathbf{v}) + \eta(\mathbf{B}_\perp \cdot \mathbf{B}_\perp), \quad D_1 = \begin{pmatrix} \mu & 0 & 0 \\ 0 & \nu & 0 \\ 0 & 0 & \nu \end{pmatrix}, \quad D_2 = \begin{pmatrix} \eta & -\chi \\ \chi & \eta \end{pmatrix}$$

Invariance of $U_t + F_x = 0$ under $x, t \leftrightarrow \alpha x, \alpha t$

$\Rightarrow$ two limits $\alpha \to 0$, $\alpha \to \infty$

- **Riemann problem: neglecting the viscous terms**

  Large-time asymptotics of a general resistive solution

  Instantaneous response to discontinuities

  Basic building block of Godunov-type numerical methods

MHD Singularities: Nonstrictly hyperbolic conservation laws

- **MHD waves (s-slow, f-fast, A-Alfvén)**

$$-c_f, -c_A, -c_s, 0, c_s, c_A, c_f; \quad c_s \le c_A \le c_f$$

$$c_A = |B_x| / \sqrt{\rho}, \; 2c_{f,s}^2 = a^2 + \frac{\mathbf{B}\cdot\mathbf{B}}{\rho} \pm \sqrt{\left(a^2 + \frac{\mathbf{B}\cdot\mathbf{B}}{\rho}\right)^2 - 4a^2 c_A^2}, \; a^2 = \frac{\gamma p}{\rho}$$

- **Singularities -> nonstrictly hyperbolic**

A. Rotational degeneracy $(\mathbf{B}_\perp \cdot \mathbf{B}_\perp = 0)$

$$c_s = c_A, \; c_f = a \text{ for } a > c_A; \; c_f = c_A, \; c_s = a \text{ for } a < c_A$$

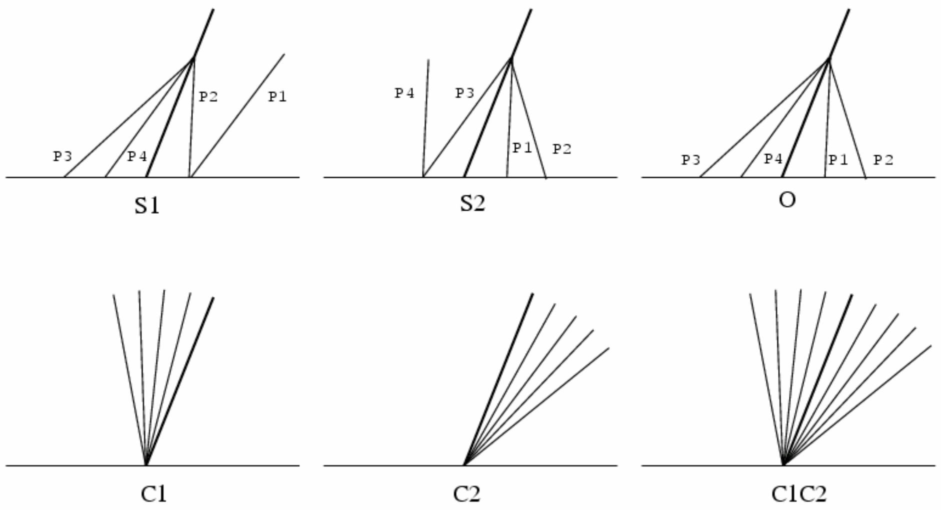
B. Triple umbilic point $(\mathbf{B}_\perp \cdot \mathbf{B}_\perp = 0 \text{ and } c_A = a)$

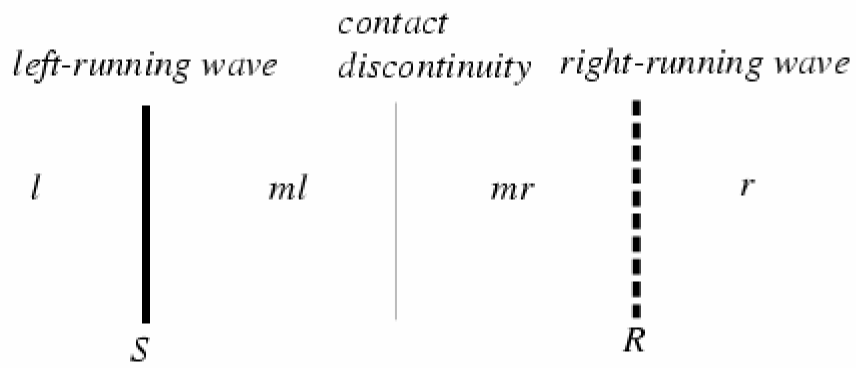
$$c_s = c_A = c_f = a$$

C. Double umbilic point in flatland $(B_y = 0 \text{ and } c_A = a)$

$$c_s = c_f = a$$

Gasdynamics vs MHD



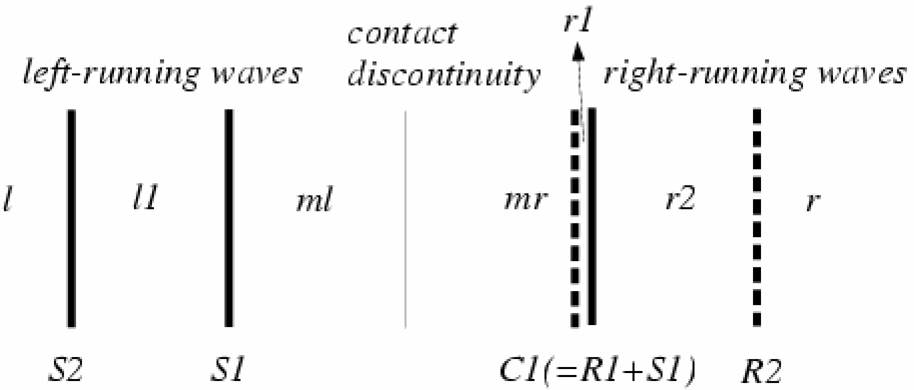


(a)

- A 3×3 model equation

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_t + \begin{pmatrix} cu^2 + v^2 + w^2 \\ 2uv \\ 2uw \end{pmatrix}_x = \begin{pmatrix} \mu & 0 & 0 \\ 0 & \eta & -\chi \\ 0 & \chi & \eta \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix}_{xx}$$

where $c(>2) = \gamma + 1,\ u \sim p,\ v \sim B_y,\ w \sim B_z$

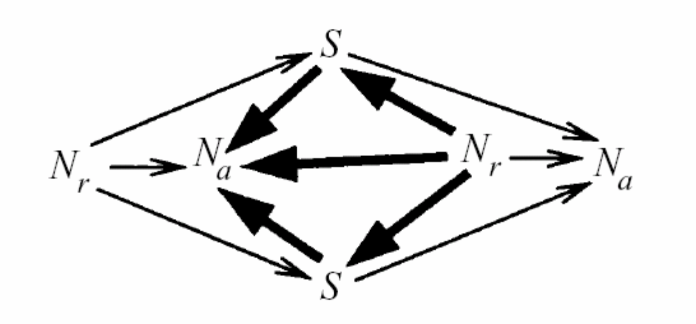


(b)

Problem III: Stability of shock waves in flatland (planar case)

- A 2×2 model equation

$$\begin{pmatrix} u \\ v \end{pmatrix}_t + \begin{pmatrix} cu^2+v^2 \\ 2uv \end{pmatrix}_x = \begin{pmatrix} \mu & 0 \\ 0 & \eta \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}_{xx}$$

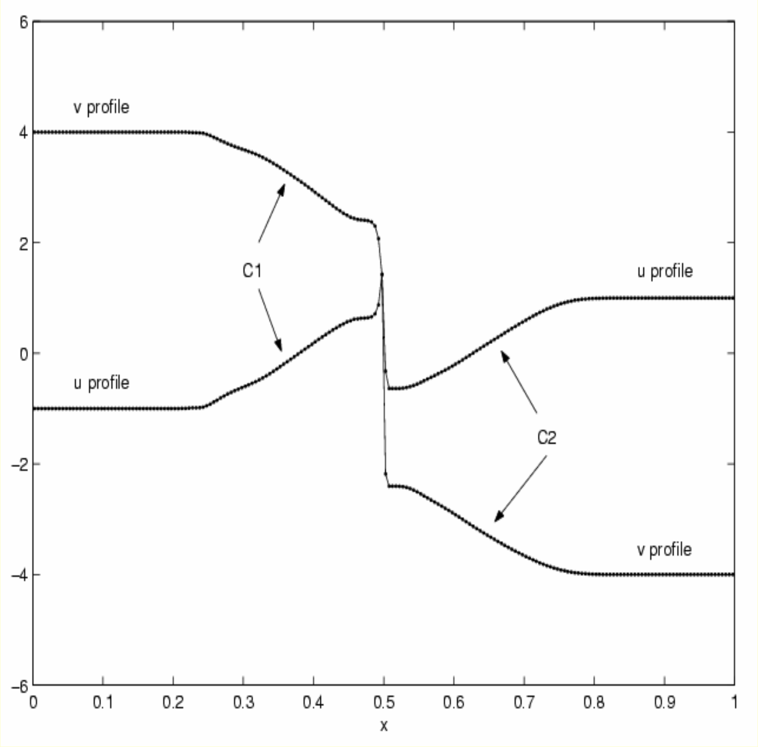


- A viscosity admissibility condition on the global phase portrait of the dynamical system of shock structure was developed: 1) Blow-up of singularities through the Poincaré transform and 2) Poincaré index theorem

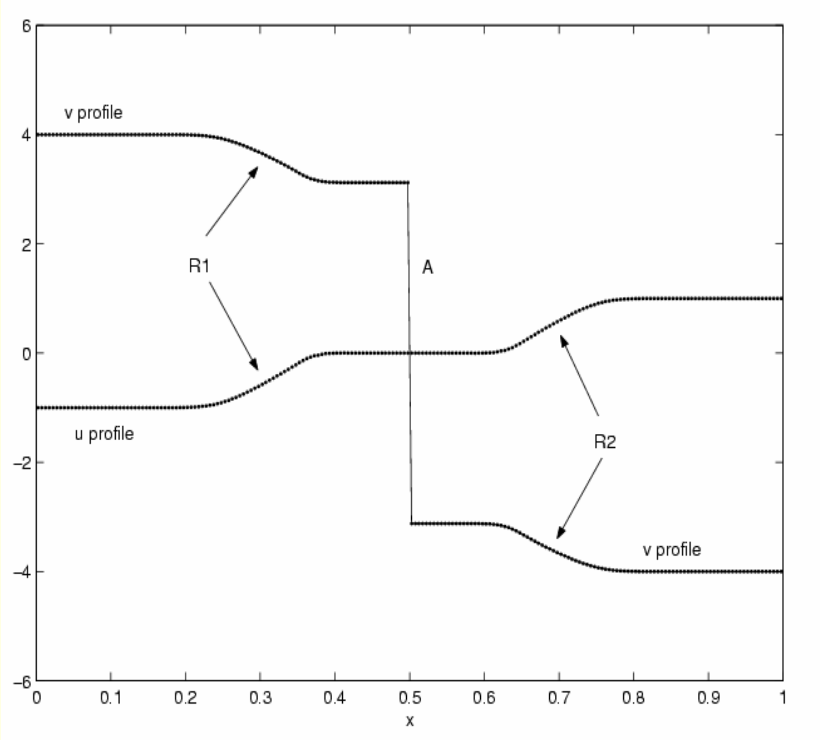
- Challenge: difficulty in developing the stability theory for the non-planar case

Problem III: Further description of challenge

Numerical experiment



Conventional Solver (Two Compound Waves)



Rotational Solver (Slow Rarefaction, Alfvén, Fast Rarefaction Waves)

Implication: It may be extremely difficult to resolve the shock structure correctly since all the numerical schemes have their own numerical dissipation and dispersion.

Concluding remarks

- Many exciting problems are expected in the field of mathematical fluid dynamics as scientific interests go beyond near-equilibrium linear regimes.
- Three unsolved problems in these areas have been described.