GIAN Course on

Rarefied & Microscale Gases and Viscoelastic Fluids: a Unified Framework

Lecture 3

Uniqueness of Mesoscale Modeling of RMG and Various Methods

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I. Degree of non-equilibrium

II. Irreversible processes and thermodynamics

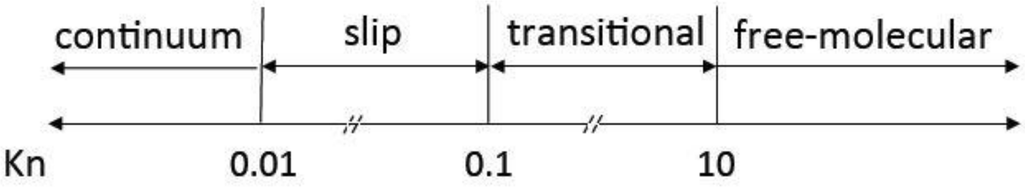
III. Theory and simulation methods

IV. Liquid?

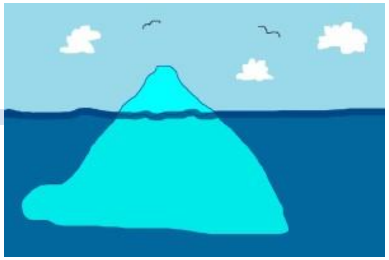
I. Degree of non-equilibrium

- How we can define **‘degree of non-equilibrium’**
  - Essential to understanding the fundamentals of fluid flows in high thermal non-equilibrium
  - Traditionally, the Knudsen number, defined as λ/L= mean-free-path / characteristic length, was considered the sole parameter for classifying the gaseous flow regimes.
  - The ratio of the collision term to the kinematic term in the Boltzmann equation is nothing but the Knudsen number;

$$\mathbf{v}\cdot\nabla f = \frac{1}{Kn} C\left[f, f_2\right]$$



I. Degree of non-equilibrium



- A **misfit** from RMG (tip of the iceberg)
- Microscale gas flows (*M*=0.0002) with high Knudsen number (Kn=0.145) were solved accurately by the linear NSF theory with slip boundary condition, whereas the same linear theory does not produce accurate results in hypersonic (*M*=28.7) rarefied gas flows with low Knudsen number (Kn=0.037).
- This inconsistency can be only resolved by recognizing that, owing to the statistical average procedure, there are **three, instead of two**, terms in the conservation law of momentum: convective, pressure, and viscous terms:

$$\rho \frac{d\mathbf{u}}{dt} + \nabla \cdot \left(\frac{1}{\gamma M^2} p\mathbf{I} + \frac{1}{\mathrm{Re}} \mathbf{\Pi} \right) = 0$$

An exact consequence of Boltzmann equation (regardless of the degree of non-equilibrium).

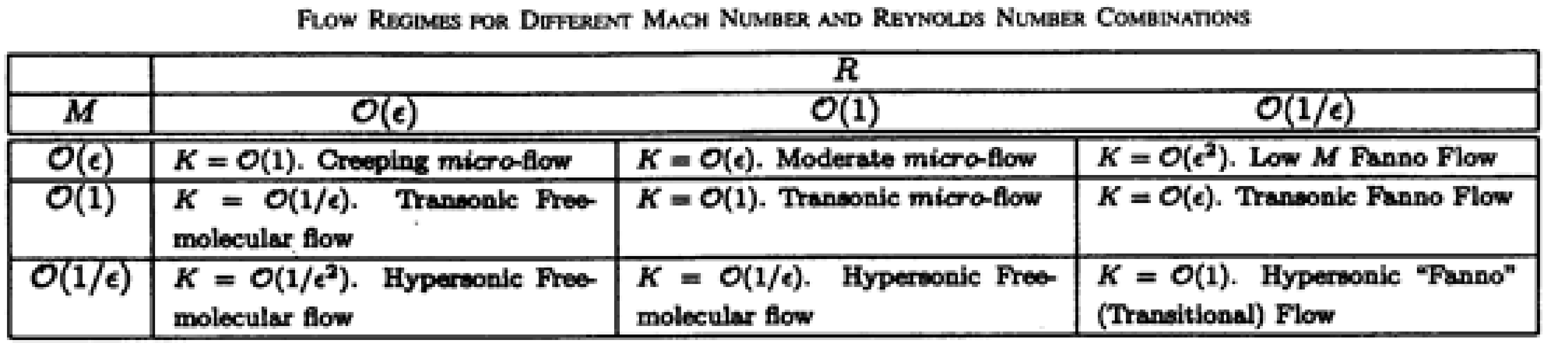
Cf. $\mathbf{v} \cdot \nabla f = \frac{1}{Kn} C[f, f_2]$, $Kn = \frac{M}{\mathrm{Re}}$ (no velocity)

I. Degree of non-equilibrium

- Therefore, **Kn must be replaced by two parameters**
  - (M, Re) or (M, Kn) or (Kn, Re)
  - Indeed, the degree of non-equilibrium should be the ratio of the viscous force to the pressure, since the viscous force is a direct consequence of the thermal non-equilibrium effect.

$$\text{Degree of non-equilibrium} = \frac{\Pi}{p} = \frac{M^2}{\mathrm{Re}} = M \cdot \mathrm{Kn} = N_\delta$$

- **Flow classification based on two parameters (*M*, Re)** (Arkilic et al. 1997)



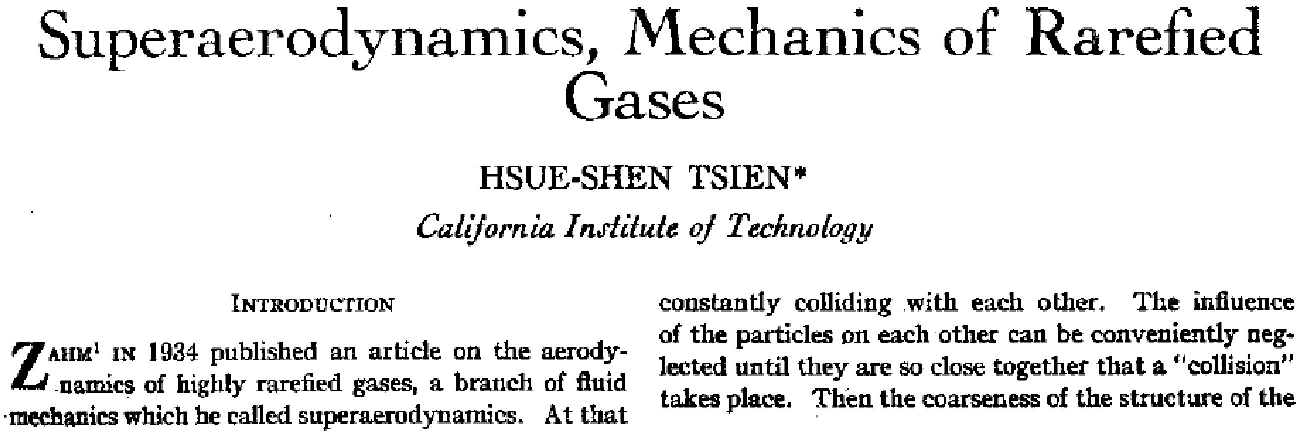
FLOW REGIMES FOR DIFFERENT MACH NUMBER AND REYNOLDS NUMBER COMBINATIONS

	R		
M	$\mathcal{O}(\epsilon)$	$\mathcal{O}(1)$	$\mathcal{O}(1/\epsilon)$
$\mathcal{O}(\epsilon)$	$K = \mathcal{O}(1)$. Creeping *micro-flow*	$K = \mathcal{O}(\epsilon)$. Moderate *micro-flow*	$K = \mathcal{O}(\epsilon^2)$. Low M Fanno Flow
$\mathcal{O}(1)$	$K = \mathcal{O}(1/\epsilon)$. Transonic Free-molecular flow	$K = \mathcal{O}(1)$. Transonic *micro-flow*	$K = \mathcal{O}(\epsilon)$. Transonic Fanno Flow
$\mathcal{O}(1/\epsilon)$	$K = \mathcal{O}(1/\epsilon^2)$. Hypersonic Free-molecular flow	$K = \mathcal{O}(1/\epsilon)$. Hypersonic Free-molecular flow	$K = \mathcal{O}(1)$. Hypersonic "Fanno" (Transitional) Flow

I. Degree of non-equilibrium: history

Hsue-Shen Tsien
(1st Director of Institute of Mechanics of Chinese Academy of Science in 1956)

Journal of the Aeronautical Sciences 13:653-664, 1946



Superaerodynamics, Mechanics of Rarefied Gases

HSUE-SHEN TSIEN*

California Institute of Technology

INTRODUCTION

ZAHM[1] IN 1934 published an article on the aerodynamics of highly rarefied gases, a branch of fluid mechanics which he called superaerodynamics. At that constantly colliding with each other. The influence of the particles on each other can be conveniently neglected until they are so close together that a "collision" takes place. Then the coarseness of the structure of the

I. Degree of non-equilibrium: Tsien's parameter

Tsien (1946) proposed a Knudsen number based on the boundary thickness *δ* (not *L*)

$$Kn_\delta = \frac{M}{\mathrm{Re}_\delta} = \frac{M}{\sqrt{\mathrm{Re}_L}} \left(= \sqrt{\frac{M^2}{\mathrm{Re}_L}} \right)$$

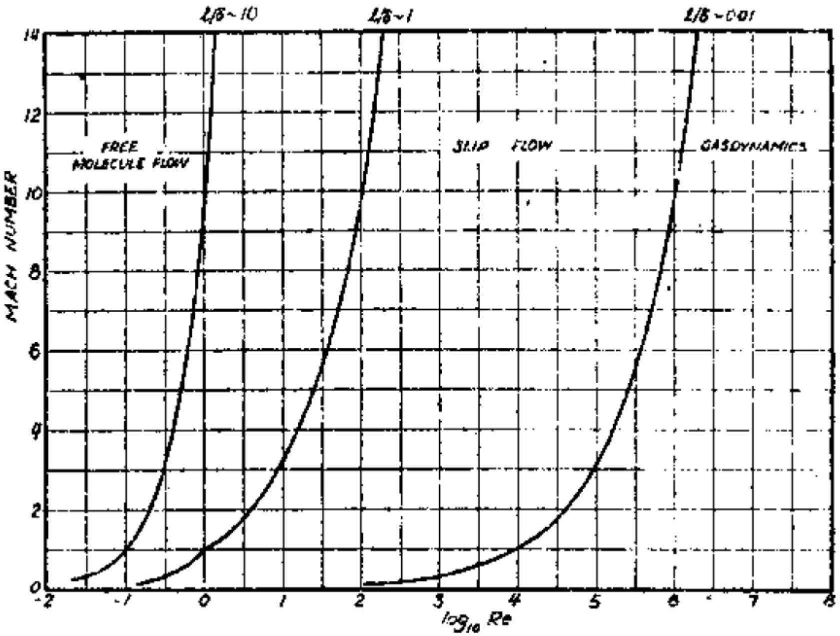
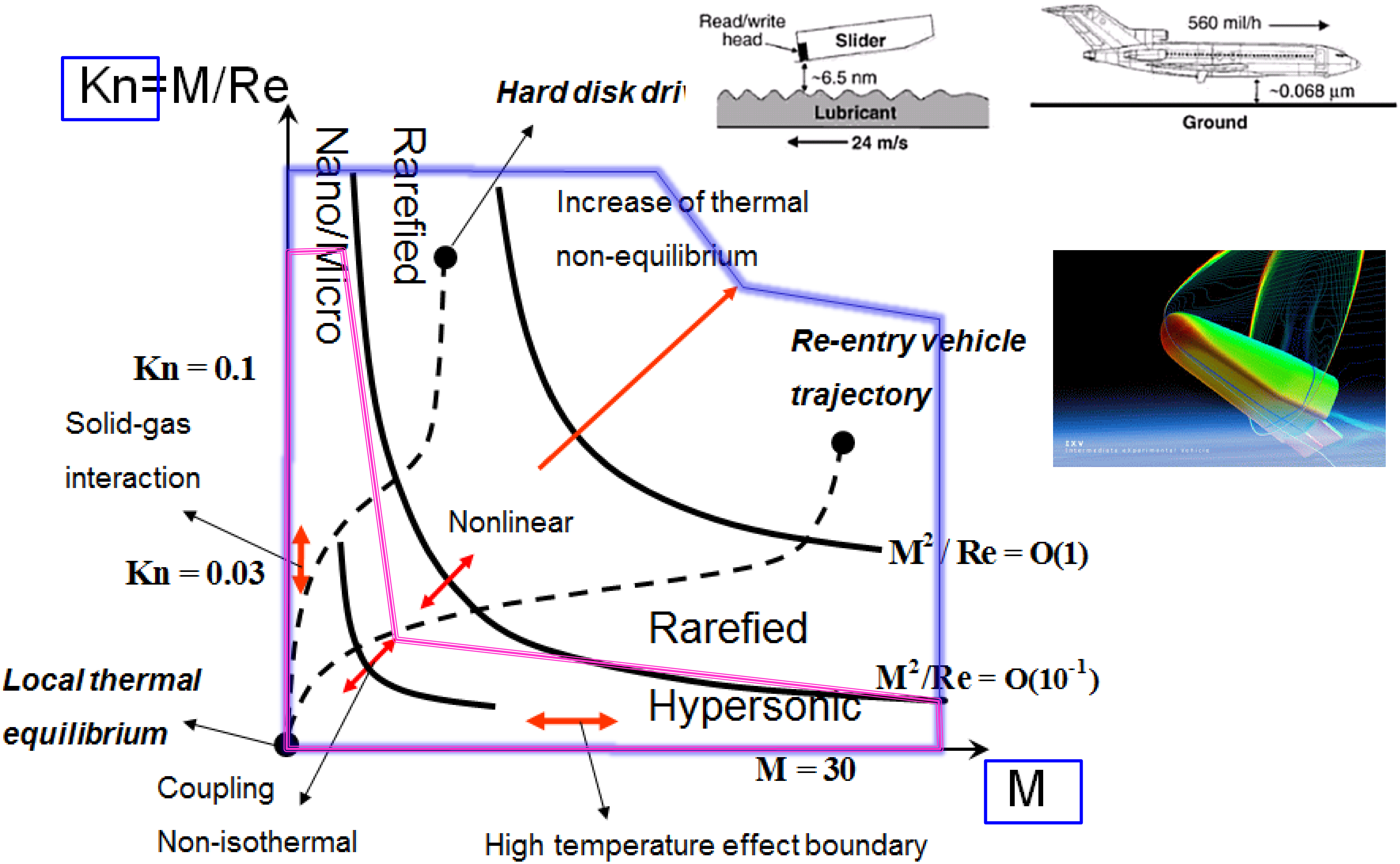


FIG. 3. Realms of fluid mechanics.

"… *The order of magnitude of the additional (second-order) heat flux or stresses is then M*Kn). That is, the additional terms are only of importance if the product of Mach number and Knudsen number is large. Therefore, for the gas dynamical flow with small mean free path, the ordinary terms suffice. This is also true for the slip flows if the Mach number is small.* …" (page 656 in H. S. Tsien's 1946 paper)

Tsien clearly recognized the difference between high *M* rarefied flow and low *M* microscale flow, which was rediscovered a half century later in study of microscale gases.

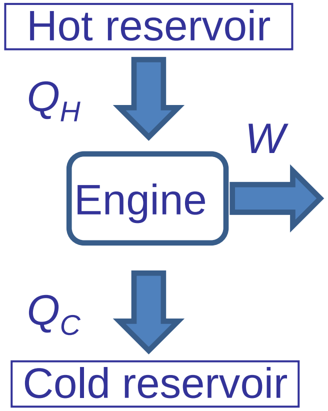
I. New flow classification



Memo

II. Irreversible processes and thermodynamics

- The second law of thermodynamics
  - **Clausius principle**: It is impossible to transfer heat from a colder to a hotter body **without converting at the same time a certain amount of work into heat at the end of a cycle of changes**.
  - **Kelvin principle**: In a cycle of processes it is impossible to transfer heat from a heat reservoir and convert it all into work, **without transferring at the same time a certain amount of heat** from a hotter to a colder body.



Hot reservoir

Q_H

W

Engine

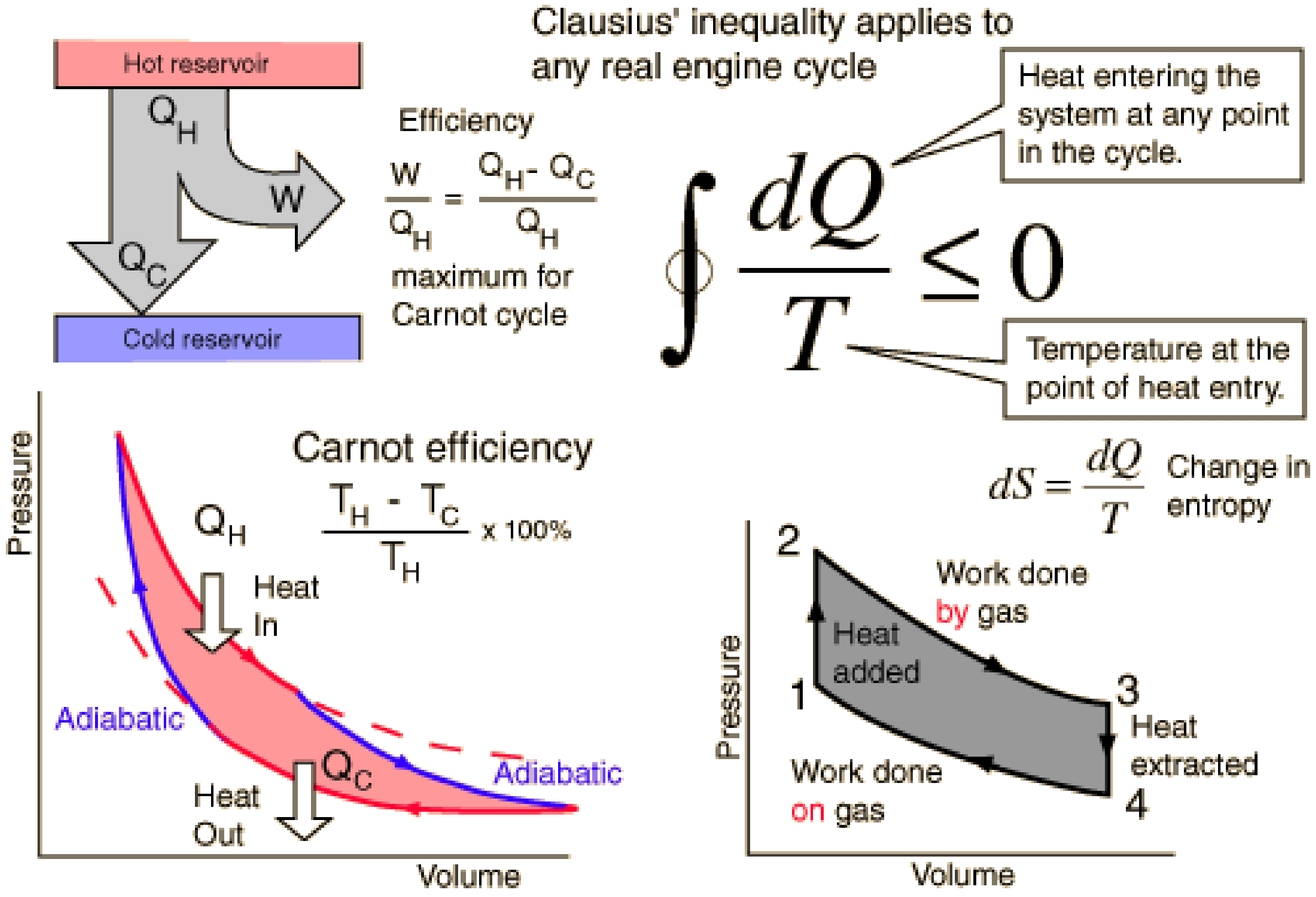
Q_C

Cold reservoir

Q_C cannot be zero!

II. Irreversible processes and thermodynamics

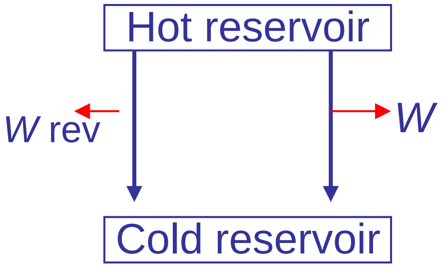
- Popular explanation



II. Irreversible processes and thermodynamics

- Original form by Clausius (1865)

$$\eta_{\mathrm{rev}} = \frac{-W_{\mathrm{rev}}}{Q_{\mathrm{H}}} = \frac{Q_{\mathrm{H}} - Q_{\mathrm{C}}}{Q_{\mathrm{H}}} \underset{\text{ideal gas}}{=} 1 - \frac{T_{\mathrm{C}}}{T_{\mathrm{H}}}, \qquad \eta_{\mathrm{irr}} = \frac{-W}{Q_{\mathrm{H}}} = \frac{Q_{\mathrm{H}} - Q_{\mathrm{C}}}{Q_{\mathrm{H}}} = 1 - \frac{Q_{\mathrm{C}}}{Q_{\mathrm{H}}}$$



By the Carnot theorem $\eta_{\mathrm{rev}} \geq \eta_{\mathrm{irr}}$

$$1 - \frac{T_{\mathrm{C}}}{T_{\mathrm{H}}} \geq 1 - \frac{Q_{\mathrm{C}}}{Q_{\mathrm{H}}}, \quad -\frac{Q_{\mathrm{C}}}{T_{\mathrm{C}}} + \frac{Q_{\mathrm{H}}}{T_{\mathrm{H}}} \geq 0$$

Or $-\oint \frac{dQ}{T} \geq 0$ for a series of infinitesimal cycles

Clausius recognized another quantity, the ‘uncompensated heat’ N

$$N = \underline{-\oint \frac{dQ}{T} \geq 0} \quad \Rightarrow$$

For reversible process

$$\boxed{\oint \frac{dQ}{T} = 0 = \oint dS_{\mathrm{e}}}$$

$$\boxed{dS_{\mathrm{e}} = T^{-1}(dE + dW)}: \ \textbf{equilibrium} \text{ Gibbs relation}$$

II. Irreversible processes and thermodynamics

- Refined theory by Eu (2002)

By realizing dQ: compensated heat exchange to perform the task (work)

N: energy (work) unavailable to the given task

$$N = -\left(\frac{Q_1}{T_1} - \frac{Q_n}{T_n}\right) = -\left(\frac{Q_1}{T_1} - \frac{Q_2}{T_2} + \frac{Q_2}{T_2} - \cdots - \frac{Q_n}{T_n}\right) = -\sum_{j=1}^{n-1}\int_j^{j+1} d\left(\frac{Q}{T}\right) = -\int_1^n \frac{dQ}{T} - \underline{\int_1^n Q\,d\left(\frac{1}{T}\right)} \geq 0$$

Uncompensated heat associated with heat transfer

Or the Carnot theorem may be written as an equation instead of an inequality

$$\frac{T_2}{T_1} = \frac{Q_2}{Q_1} - \frac{W_{\text{unavailable}}}{Q_1} \Rightarrow \frac{Q_2}{T_2} = \frac{Q_1}{T_1} + N \text{ where } N = \frac{W_{\text{unavailable}}}{T_2}$$

we can consider *N* as an independent entity

$$\oint dN = -\oint \frac{dQ}{T} \geq 0 \Rightarrow \boxed{\oint\left(\frac{dQ}{T} + dN\right) = 0} \Rightarrow \oint d\Psi = 0 \text{ where } \Psi \text{ is nonequil. entropy}$$

$\boxed{d\Psi = T^{-1}(dE + dW) + dN}$: extended **nonequilibrium** Gibbs relation

III. Theory and simulation methods

- Pure vs PDE-based
- Microscopic, mesoscopic, and macroscopic
- Limits of validity of statistical average definition and 2nd law of thermodynamics

Molecular			Continuum	Molecular				Continuum
Pure (or Semi-) Simulation				**PDE-based Approach**				
MD	DSMC	Gas-Kinetic Scheme	LBM	Liouville Equation	Boltzmann and Simplified Boltzmann	Method of Moments	Chapman-Enskog and Burnett	NSF
Microscopic	Mesoscopic		Macroscopic	Microscopic	Mesoscopic			Macroscopic

III. Theory and simulation methods

An innovative tent, requiring only 5 second for set-up!

Do you want to purchase it for next summer vacation?

III. Theory and simulation methods

A game of reducing the degree of freedom of BTE from 10^{23} to 10^{3} -10^{10}

DSMC

A representative particle to cover real particles in order of 10^{13}

Then describing the motion of the particles via deterministic movement and stochastic collision

No PDE

Gas-kinetic scheme

Solving a discretized version of conservation laws

and discretized BGK-BTE in an iterative way

Only discretized PDE

LBM

Solving BTE on discrete lattice

Introducing finite numbers of discrete velocity

Finally replace by 1st-order accurate BGK

← Molecular

Macroscopic →

III. Theory and simulation methods

A game of reducing the degree of freedom of BTE from 10^{23} to 10^{3} -10^{10}

Boltzmann

Describing the motion of the particles movement and collision

Stochastic PDE in 7-d phase space

Molecular chaos and break of time reversal

Moment method

Differentiating the statistical definition

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

with time

and combining with BTE

PDE of high order

Chapman-Enskog

Assuming

$$f(t,\mathbf{r},\mathbf{v}) \simeq f\left[\mathbf{W}(t,\mathbf{r}), \nabla\mathbf{W}(t,\mathbf{r}), \mathbf{v}, \varepsilon\right]$$

and inserting into BGK-BTE and deriving 1st, 2nd, 3rd approximations

PDE of high order

Need of extra BC due to $\nabla\mathbf{W}(t,\mathbf{r})$

← **Molecular**

Macroscopic →

III. Theory and simulation methods

DSMC

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right)f(t,\mathbf{r},\mathbf{v})=0$$

Kinematic: the collision-less movement of molecules

$$\frac{\partial f}{\partial t}=\int\left|\mathbf{v}-\mathbf{v}_2\right|(f^*f_2^*-ff_2)d\mathbf{v}_2$$

Molecular collisions

$$\rho=\iiint mf(t,\mathbf{r},\mathbf{v})dv_x dv_y dv_z$$

Sampling

Constraints:

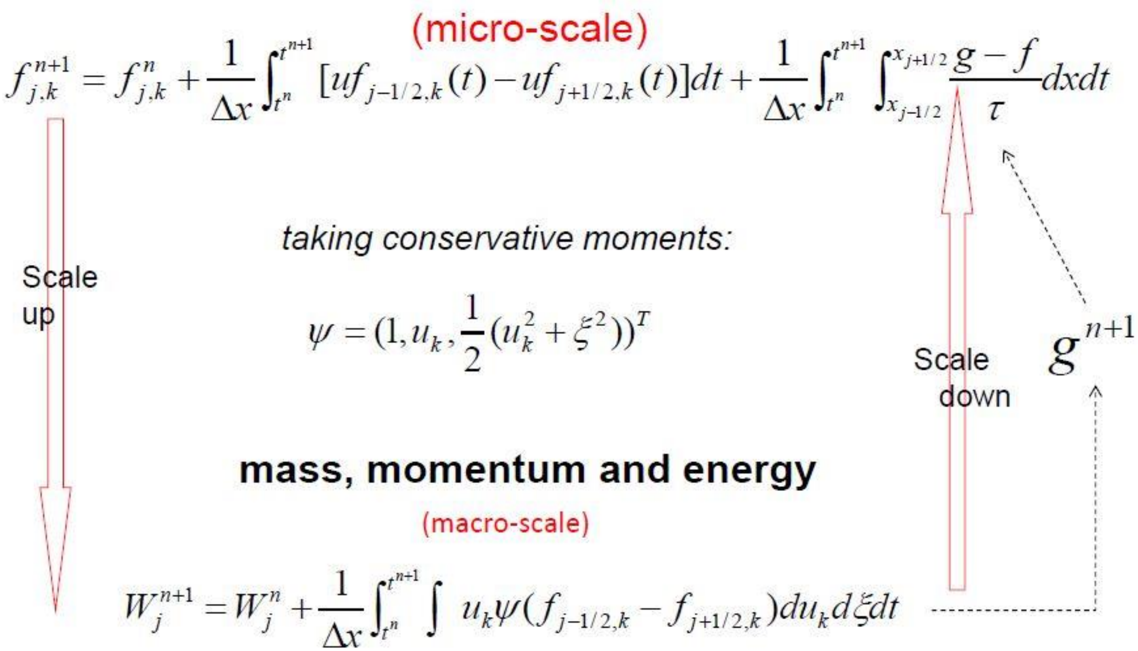
Δt < mean collision time

Δx < mean free path

Particles cross less than

1 cell/timestep

Gas-kinetic scheme



(micro-scale)

$$f_{j,k}^{n+1}=f_{j,k}^{n}+\frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}[uf_{j-1/2,k}(t)-uf_{j+1/2,k}(t)]dt+\frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int_{x_{j-1/2}}^{x_{j+1/2}}\frac{g-f}{\tau}dxdt$$

taking conservative moments:

$$\psi=(1,u_k,\frac{1}{2}(u_k^2+\xi^2))^T$$

mass, momentum and energy

(macro-scale)

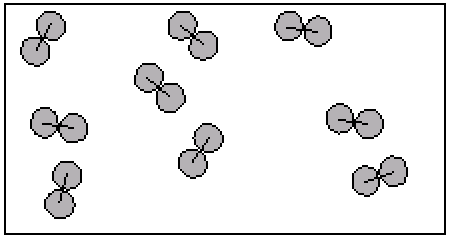
$$W_j^{n+1}=W_j^n+\frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int u_k\psi(f_{j-1/2,k}-f_{j+1/2,k})du_k d\xi dt$$

K. Xu (2014)

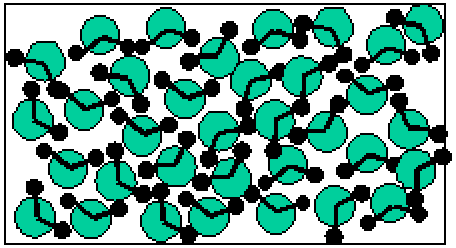
IV. Liquid?

- How we can define **‘degree of non-equilibrium’ in liquid?**
  - Something similar to Kn (or Kn*M) in gas?

Gases (STP)



Liquids



Molecular diameter	0.3 nm	Molecular diameter	0.3 nm
Number density (m^{-3})	3 E25	Number density (m^{-3})	2 E28
Intermolecular spacing	3 nm	Intermolecular spacing	0.4 nm
Displacement distance	100 nm	Displacement distance	1 pm
Molecular Velocity	500 m/s	Molecular Velocity	10^3 m/s

Q & A