Multiscale Methods for Dilute Fluids and Plasmas

Russel Caflisch
IPAM
Mathematics Department, UCLA

SIAM 6 July 2009
Outline

• Particle dynamics vs. continuum dynamics
  – when does the continuum description fail?

• Rarefied gas dynamics
  – Boltzmann equation
  – short range collisions

• Plasmas
  – Landau-Fokker-Planck equation
  – Coulomb collision - long-rang collisions

• Fluid dynamic (i.e., continuum) limit

• Numerical methods
  – Direct Simulation Monte Carlo (DSMC)
  – failure in fluid dynamic limit

• Multiscale numerical methods
  – robust in fluid dynamic limit

SIAM 6 July 2009
Gas Flow: Particle vs. Fluid

Particle description
- Discrete particles
- Motion by particle velocity
- Interact through collisions

Fluid (continuum) description
- Density, velocity, temperature
- Evolution following fluid eqtns (Euler or Navier-Stokes)

When does continuum description fail?

SIAM 6 July 2009
Flow with Constant Density
(Incompressible)

• Incompressible Euler equations (\(\rho=1\))
  \[ \nabla \cdot u = 0 \]
  \[ \partial_t u + u \cdot \nabla u + \nabla p = 0 \]

• No need for particles
Compressible Flow

- Compressible Euler equations
  - shock waves
    \[ \partial_t \rho + \nabla \cdot (\rho u) = 0 \]
    \[ \rho (\partial_t u + u \cdot \nabla u) + \nabla p = 0 \]
    \[ \partial_t E + \nabla \cdot (u(E + p)) = 0 \]
  - E = total energy = \( \rho(\frac{|u|^2}{2} + e) \)

- No need for particles
  - but need thermodynamics \( p = p(\rho, e) \)
  - entropy \( S \) is needed
Compressible Flow

• Compressible Euler equations
  – shock waves
    \[ \partial_t \rho + \nabla \cdot (\rho u) = 0 \]
    \[ \rho (\partial_t u + u \cdot \nabla u) + \nabla p = 0 \]
    \[ \partial_t E + \nabla \cdot (u(E + p)) = 0 \]
  – E=total energy = \( \rho(|u|^2/2 + e) \)

• No need for particles
  – but need thermodynamics \( p = p(\rho, e) \)
  – entropy \( S \) is needed

S= k log W

Boltzmann’s grave

SIAM 6 July 2009
When Does the Continuum Description Fail?

- Rarefied gases and plasmas
- Knudsen number $Kn = \varepsilon$
  - $\varepsilon = (\text{mean free path})/(\text{characteristic distance})$
  - measures significance of collisions
  - mean free path = distance traveled by a particle between collisions
Rarefied vs. Continuum Flow: Knudsen number Kn

Collisional Effects in the Atmosphere

FIGURE 6. Mean free path as a function of geometric altitude.
Collisional Effects in MEMS and NEMS

**FIGURE 8.1** The operation range for typical MEMS and nanotechnology applications under standard conditions spans the entire Knudsen regime (continuum, slip, transition and free molecular flow regimes).

SIAM 6 July 2009
Boltzmann equation for rarefied gas dynamics (RGD)

- Statistical description replaces individual particles
  - density function $f=f(x,v,t)$ in phase space (position $x$, velocity $v$) at time $t$
  - typical number of $10^{20}$ particles would be intractable
- Boltzmann equation for $f$
  \[ f_t + v g \nabla_x f = \varepsilon^{-1} Q(f, f) \]
  - $\varepsilon$ = Knudsen number
  - $Q$ represents effect of binary collisions
- General existence theorem
  - Diperna & Lions 1989
  - “renormalized” solution
  - uniqueness, conservation of energy are not established
Collisions

- **Velocities**
  - $v, w$ before collision
  - $v', w'$ after collision

- **Conservation of momentum and energy**
  - $v + w = v' + w'$
  - $|v|^2 + |w|^2 = |v'|^2 + |w'|^2$

- **Two free parameters**
  - $\Omega = (\epsilon, \theta)$ on sphere
  - $\theta =$ scattering angle
  - $\epsilon =$ angle of plane of collision
Equilibrium and Fluid Limit of Boltzmann

- **Maxwellian equilibrium**
  - $Q(f,f) = 0$ implies $f = M(v; \rho, u, T)$
  
  $$M(v) = \rho (2\pi T)^{-3/2} \exp(-(v-u)^2 / 2T)$$

- **Equilibration**
  - $f=f(v,t)$ spatially homogeneous
  - $H=-\text{Entropy}$
  - Boltzmann’s H-theorem
  - $dH / dt \leq 0$
  - H-theorem implies $f \to M$ as $t \to \infty$

- **Fluid Limit (Hilbert, Grad, Nishida, REC)**
  - $\varepsilon \to 0$
  - $f(v,x,t) \to M(v; \rho, u, T)$, with $\rho = \rho(x,t)$, etc.
  - $\rho, u, T$ satisfy Euler (or Navier-Stokes)

SIAM 6 July 2009
Plasmas

• **Plasma**
  – gas of ionized particles
  – 99% of visible matter

• **Examples**
  – fluorescent lights
  – sun
  – fusion energy plasmas
New experimental facilities are driving plasma physics

• ITER
  – tokamak (magnetic confinement fusion)
  – reactor chamber 840 m³
  – originally the International Thermonuclear Experimental Reactor
  – international (China, EU, India, Japan, Korea, Russia, US)
  – located in southern France
Where are collisions significant in plasmas?
Example: Tokamak edge boundary layer

From G. W. Hammett, review talk 2007
APS Div Plasmas Physics
Annual Meeting, Orlando, Nov. 12-16.
New experimental facilities are driving plasma physics

- **NIF**
  - National Ignition Facility
  - 192 lasers
  - laser-based inertial confinement fusion (ICF) device
  - Lawrence Livermore National Laboratory
Interactions of Charged Particles in a Plasma

- **Boltzmann equation for plasma with collisions**

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + m^{-1} F_{EM} \cdot \nabla_v f = \left( \frac{\partial f}{\partial t} \right)_{col} \]

\[ F_{EM} = q \left( E + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \]

- **Long range interactions**
  - \( r > \lambda_D \) (\( \lambda_D = \text{Debye length} \))
  - Electric and magnetic fields \( E, B \)

- **Short range interactions**
  - \( r < \lambda_D \)
  - Coulomb “collisions”

m=mass, q=charge
Landau-Fokker-Planck equation for collisions

- **Coulomb interactions**
  - collision rate $\approx u^{-3}$ for two particles with relative velocity $u$

- **Fokker-Planck equation**

\[
\left( \frac{\partial f}{\partial t} \right)_{col} = - \frac{\partial}{\partial \mathbf{v}} \mathbf{F}_d(\mathbf{v}) f(\mathbf{v}) + \frac{1}{2} \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}'} : \mathbf{D}(\mathbf{v}) f(\mathbf{v})
\]

\[
\begin{align*}
\mathbf{F}_d(\mathbf{v}) &= c_1 \frac{\partial H}{\partial \mathbf{v}} = c_1 \frac{\partial}{\partial \mathbf{v}} 2 \int \frac{f(\mathbf{v}')}{|\mathbf{v} - \mathbf{v}'|} d\mathbf{v}' \\
\mathbf{D}(\mathbf{v}) &= c_2 \frac{\partial^2 G}{\partial \mathbf{v} \partial \mathbf{v}'} = c_2 \frac{\partial^2}{\partial \mathbf{v} \partial \mathbf{v}'} \int f(\mathbf{v}') |\mathbf{v} - \mathbf{v}'| d\mathbf{v}'
\end{align*}
\]
Derivation of Landau Equation

• Linear Boltzmann equation (idealized)
  – collision integral
    \[ Lf(v) = \int k(v, v') f(v') dv' - \alpha(v) f(v) \]
  – conservation of mass
    \[ \int k(v, v') d\omega = \alpha(v) \]

• grazing collisions
  \[ k(v, v') \approx \alpha \delta(v' - (v + \Delta v)) \]
  \[ \approx \alpha \delta(v' - v) + \beta \partial_v \delta(v' - v) + \gamma \partial^2_v \delta(v' - v) \]
  – derivation of Landau collision operator
    \[ Lf(v) \approx \int \left( \alpha - \beta \partial_v + \gamma \partial^2_v \right) \delta(v' - v) f(v') dv' - \alpha f(v) \]
    \[ = \left( \alpha + \partial_v \beta + \partial^2_v \gamma \right) f(v) - \alpha f(v) \]
    \[ = \left( \partial_v \beta + \partial^2_v \gamma \right) f(v) \]
Collisions in Gases vs. Plasmas

• Collisions between velocities $v$ and $v_*$
  – $q = |v - v_*|$ relative velocity

• Gas collisions
  – hard spheres, $\sigma =$ cross section area of sphere
  – collision rate is $\sigma q$
  – any two velocities can collide $\rightarrow$ smoothing in $v$

• Plasma (Coulomb) collisions
  – very long range, potential $O(1/r)$
  – collisions are grazing, localized as in Landau eqtn
  – differential eqtn in $v$, as well as $x,t$
  – waves in phase space
  – Landau damping (interaction between waves and particles)
Boltzmann → Continuum: The original multiscale problem

- Maxwell calculated fluid transport coefficients
  - viscosity coefficient independent of density
- Hilbert performed perturbation expansion to derive Euler eqtns from Boltzmann eqtn

\[ f = f_0 + \epsilon f_1 + O(\epsilon^2) \]
Derivation of Euler equations

- Insert expansion into Boltzmann eqtn

\[ f = f_0 + \varepsilon f_1 + O(\varepsilon^2) \]

\[ f_t + \nu g \nabla_x f = \varepsilon^{-1} Q(f, f) \]

- Expansion of eqtn

\[ O(\varepsilon^{-1}) : \quad Q(f_0, f_0) = 0 \]

\[ \Rightarrow f_0 = M = \rho (2\pi T)^{-3/2} \exp\left(-|v - u|^2 / 2T\right) \]

\[ O(\varepsilon^0) : \quad (\partial_t + \nu g \nabla_x) f_0 = 2Q(f_0, f_1) \]

\[ \int (1, v, v^2) Q dv = 0 \quad \Rightarrow \int (1, v, v^2) (\partial_t + \nu g \nabla_x) M dv = 0 \]

conservation of mass, momentum, energy

SIAM 6 July 2009
- Solveability condition (conservation)
  \[ \int \left(1, v, v^2 \right) \left( \partial_t + v g \nabla_x \right) Mdv = 0 \]
- Equivalent to Euler eqtns
  \[ \partial_t \rho + \nabla \cdot (\rho u) = 0 \]
  \[ \rho (\partial_t u + u \cdot \nabla u) + \nabla p = 0 \]
  \[ \partial_t E + \nabla \cdot (u (E + p)) = 0 \]
- Using integrals
  \[ \int \left(1, v, v^2 \right) Mdv = (\rho, \rho u, 2E) \]
  \[ \int \left(1, v, v^2 \right) v Mdv = (\rho u, \rho uu + pI, 2u (E + p)) \]
  \[ E = \rho \left( |u|^2 + 3T \right) / 2 \quad p = \rho T \]
Dominant numerical method for dilute flows

- **DSMC = Direct Simulation Monte Carlo**
  - Invented by Graeme Bird, early 1970’s
  - Represents density $f$ as collection of particles
    \[ F(v) = \sum_{k=1}^{N} \delta(v - v_k(t))\delta(x - x_k(t)) \]
  - Directly simulates RGD by randomizing collisions
    - Collision $v,w \rightarrow v',w'$ conserving momentum, energy
    - Random choice of collision angles $(\varepsilon, \theta)$
  - Particle advection \[ dx_k / dt = v_k \]
  - Convergence (Wagner 1992)

- **Limitation of DSMC**
  - DSMC becomes computationally intractable near fluid regime, since collision time-scale becomes small

SIAM 6 July 2009
What can mathematics contribute to DSMC?

- Traditionally, math contributed little to DSMC
  - only difficulties are computational complexity
  - no stability, consistency issues
- Flows near fluid limit
  - DSMC becomes intractable
  - math needed to design methods that overcome this difficulty!
Current Multiscale Methods: What’s New?

• Current multiscale methods
  – e.g. quasi-continuum, HMM, equations-free method
  – combine multiple scales and multiple physics into a single numerical method

• Multiscale methods for dilute fluids and plasmas (my title!)
  – applicable in near fluid regime
  – combine fluid and particle descriptions
  – provide considerable acceleration over traditional methods
Accelerated Methods for RGD

• **Domain decomposition**
  – DSMC in one region, CFD in another region

• **Asymptotic-preserving methods**
  – Fluid limit for numerical method consistent with limit for Boltzmann
  – Larsen (neutron transport), Levermore, Jin, Degond, …

• **Hybrid methods**
  – Combine fluids and Monte Carlo throughout space

• **Complex particle methods**
  – add additional degrees of freedom to particles, representing fluid state
  – not closely related to the other types of methods
Domain decomposition

- Method required for finding domain interfaces
- Fluid/particle BCs needed across interfaces
- On Boltzmann side of interface, computation is still stiff

SIAM 6 July 2009
Asymptotic Preserving Methods

Boltzmann solver $(\varepsilon,N,dx)$ \(\xrightarrow{\varepsilon\to 0}\) limit of Boltzmann solver $(N,dx)$

\[ N \to \infty \quad dx \to 0 \]

Boltzmann eqtn $(\varepsilon)$ \(\xrightarrow{\varepsilon\to 0}\) Fluid eqtns

\[ N \to \infty \quad dx \to 0 \]
Hybrid method

• Combine fluid and particle methods
• Pareschi & REC
  – Representation of density function as combination of Maxwellian and particles
    \[ F(v) = \alpha M(v) + m \sum_{k=1}^{(1-\alpha)N} \delta(v - v_k(t)) \]
    \[ M(v) = \rho (2\pi T)^{-3/2} \exp(-(v-u)^2 / 2T) \]
  – \( \rho, u, T \) solved from fluid eqtns, using Boltzmann scheme for CFD
  – DSMC used for particles
• Thermalization coefficient \( \alpha \)
  – independent of \( v \) (cf. plasma)
  – \( \alpha = 0 \) \( \leftrightarrow \) DSMC
  – \( \alpha = 1 \) \( \leftrightarrow \) CFD
  – Remains robust near fluid limit
Comparison of DSMC (blue) and IFMC (red) for a shock with Mach=1.4 and Kn=0.019
Direct convection of Maxwellians

ρ comparison of shock plots using IFMC and DSMC, (Mach,Kn) = (1.4,0.01901) 07/27/05 11:31

ρ prescribed DSMC IFMC

u comparison of shock plots using IFMC and DSMC, (Mach,Kn) = (1.4,0.01901) 07/27/05 11:31

u prescribed DSMC IFMC

T comparison of shock plots using IFMC and DSMC, (Mach,Kn) = (1.4,0.01901) 07/27/05 11:31

T prescribed DSMC IFMC

SIAM 6 July 2009
Comparison of DSMC (contours with num values) and IFMC (contours w/o num values) for the leading edge problem.
Hybrid method for plasmas
Thermalization/Dethermalization Method

• Hybrid representation (as in RGD)
  \[ F(v) = m + g \]

• Thermalization and dethermalization (T/D)
  – Thermalize particle (velocity \( v \)) with probability \( p_t \)
    • Move from g to m
  – Dethermalize particle (velocity \( v \)) with probability \( p_d \)
    • Move from m to g
Hybrid Method for Bump-on-Tail

Electron Distribution from Hybrid and Nanbu Methods $t=0$

Electron Distribution from Hybrid and Nanbu Methods $t=6.4179$

Electron Distribution from Hybrid and Nanbu Methods $t=19.2538$

Electron Distribution from Hybrid and Nanbu Methods $t=38.5076$
Ion Acoustic Waves

- kinetic description needed for ion Landau damping and ion-ion collisions
- wave oscillation and decay shown at right
- agreement with “exact” solution from Nanbu

Nanbu (–), hybrid (–), older hybrid method (–)
Conclusions and Prospects

• Lots of opportunities for mathematics in plasma physics
• Current simulation methods for kinetics have trouble in the fluid and near-fluid regime
• Math leading to new methods that are robust in fluid limit