Computational Astrophysics 2

The Equations of Hydrodyamics

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Outline

- The Boltzmann equation
- The Collision Integral
- The Local Thermodynamical Equilibrium
- The Euler equations
- The Equation-Of-State
- The Chapman-Enskog expansion
- Non-LTE effect in a Coulomb gas.

The Boltzmann equation

Due to collisions, particles are scattered in and out of the phase-space element.

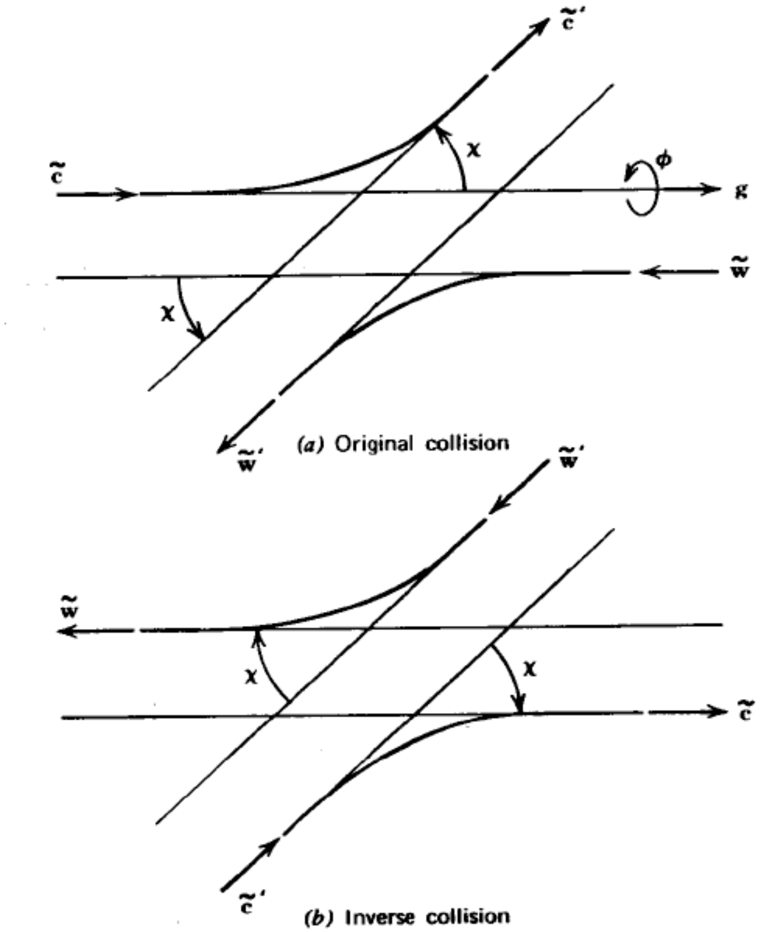
$$\frac{d}{dt} f(\mathbf{r}, \mathbf{p}, t) = \left(\frac{\partial f(\mathbf{r}, \mathbf{p}, t)}{\partial t} \right)_{collisions} \equiv \mathbf{I}[f]$$

Same structure equation as the Vlassov equation, with a source term

$$\frac{\partial f(\mathbf{r}, \mathbf{p}, t)}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{r}} f(\mathbf{r}, \mathbf{p}, t) - \nabla_{\mathbf{r}} V_{ext}(\mathbf{r}, t) \cdot \nabla_{\mathbf{p}} f(\mathbf{r}, \mathbf{p}, t) = \mathbf{I}[f].$$

$\mathbf{I}[f]$ is called the **Collision Integral**

The Collision Integral


(a) Original collision

(b) Inverse collision

Rarefied gases: only 2-body collisions.

Depleting collisions empty the phase space element from (p,q) to (p',q')

Repleneshing collisions fill up the phase space element with "inverse collisions" from (p',q') to (p,q)

The probability to get a scattering event in phase-space is given by σ, the Differential Cross-Section, and is given by Quantum Mechanics.

$$I[f] = \int_{-\infty}^{+\infty} \int_{4\pi} \left[f(q')f(p') - f(q)f(p) \right] \sigma(v,\chi) d\Omega d^3 q$$

Microscopic Conservation Laws

Particle mass, momentum and energy are *collisional invariants*

1: $$\int_{-\infty}^{+\infty} mI[f]d^3\mathbf{p} = 0$$ mass conservation

2: $$\int_{-\infty}^{+\infty} \mathbf{p}I[f]d^3\mathbf{p} = 0$$ momentum conservation

3: $$\int_{-\infty}^{+\infty} \frac{p^2}{2m}I[f]d^3\mathbf{p} = 0$$ energy conservation

$$\left.\begin{array}{l} \int m\times \\ \int \mathbf{p}\times \\ \int \frac{p^2}{2m}\times \end{array}\right| \left(\partial_t f + \mathbf{v}\cdot\partial_\mathbf{x} f + \mathbf{F}\cdot\partial_\mathbf{p} f\right) d^3\mathbf{p} = 0$$

These invariants define the 3 moments of the Boltzmann equation

Conservation of Mass

Using $\mathbf{v}\cdot\partial_{\mathbf{x}}f = \nabla\cdot(f\mathbf{v})$, we integrate over ***p***

$$\int m\left(\partial_t f + \mathbf{v}\cdot\partial_{\mathbf{x}}f + \mathbf{F}\cdot\partial_{\mathbf{p}}f\right)d^3\mathbf{p} = 0$$

which gives $\partial_t\rho + \nabla\cdot\mathbf{m} + \mathbf{F}\cdot\cancel{(f_{+\infty} - f_{-\infty})} = 0$

Mass density: $\rho(\mathbf{x},t) = \int m f(\mathbf{x},\mathbf{p},t)d^3\mathbf{p}$

Mass flux or momentum density: $\mathbf{m}(\mathbf{x},t) = \int \mathbf{p} f(\mathbf{x},\mathbf{p},t)d^3\mathbf{p}$

Average or Fluid velocity: $\mathbf{u} = \mathbf{m}/\rho$

Peculiar or Thermal velocity: $\mathbf{w} = \mathbf{v} - \mathbf{u}$

Conservation of Momentum

$$\int \mathbf{p} \times \left(\partial_t f + \mathbf{v} \cdot \partial_{\mathbf{x}} f + \mathbf{F} \cdot \partial_{\mathbf{p}} f\right) d^3\mathbf{p} = 0$$

(a) (b) (c)

(a): net change of momentum density $\partial_t \mathbf{m}$

(c): integration by parts $-\rho \mathbf{F}$

(b): $\nabla \cdot \mathcal{F}$ where the momentum flux is $\mathcal{F}_{ij} = \int m \mathrm{v_i} \mathrm{v_j} f d^3\mathbf{p}$

We further decompose the momentum flux into $\mathcal{F}_{ij} = \rho \mathrm{u_i} \mathrm{u_j} + \mathcal{P}_{ij}$

We define the Pressure Tensor $\mathcal{P}_{ij} = \int m \mathrm{w_i} \mathrm{w_j} f d^3\mathbf{p}$

We get finally $\partial_t \mathbf{m} + \nabla \cdot (\rho \mathbf{u} \times \mathbf{u} + \mathcal{P}) = \rho \mathbf{F}$

Conservation of Energy

$$\int \frac{p^2}{2m} \times \left(\partial_t f + \mathbf{v} \cdot \partial_{\mathbf{x}} f + \mathbf{F} \cdot \partial_{\mathbf{p}} f \right) d^3\mathbf{p} = 0$$

(a) (b) (c)

(a): net change of total energy density $\partial_t \mathbf{E}$

Total fluid energy is decomposed into Fluid or Bulk Kinetic Energy

$$E = \int m \frac{\mathrm{v}^2}{2} f d^3\mathbf{p} = \rho \frac{\mathbf{u}^2}{2} + \rho\epsilon$$

and Peculiar or Thermal Kinetic Energy (or Internal Energy)

$$\rho\epsilon = \int m \frac{\mathrm{w}^2}{2} f d^3\mathbf{p} = \frac{1}{2} \mathrm{Tr}\left(\mathcal{P}\right)$$

(c): integration by parts: $-\rho\mathbf{u} \cdot \mathbf{F}$

(b): $\nabla \cdot \mathcal{F}$ where the energy flux is $\mathcal{F}_i = \int m \frac{\mathrm{v}^2}{2} \mathrm{v}_i f d^3\mathbf{p}$

The Energy Flux

$$\mathcal{F}_i = \int m \frac{\mathrm{v}^2}{2} \mathrm{v}_\mathrm{i} f d^3\mathbf{p}$$

We decompose the energy flux into 3 components

$$\frac{\mathrm{v}^2}{2}\mathrm{v}_\mathrm{i} = \left[\frac{\mathrm{u}^2}{2} + \frac{\mathrm{w}^2}{2}\right]\mathrm{u}_\mathrm{i} + (\mathbf{u}\cdot\mathbf{w})\,\mathrm{w}_\mathrm{i} + \frac{\mathrm{w}^2}{2}\mathrm{w}_\mathrm{i} + \ldots$$

We get $\mathcal{F} = E\mathbf{u} + \mathcal{P} : \mathbf{u} + \mathcal{Q}$

We define the Heat Flux as: $\mathcal{Q}_i = \int m \frac{\mathrm{w}^2}{2} \mathrm{w}_\mathrm{i} f d^3\mathbf{p}$

The Energy Conservation Equation writes finally

$$\partial_t E + \nabla \cdot (E\mathbf{u} + \mathcal{P} : \mathbf{u} + \mathcal{Q}) = \rho\mathbf{u}\cdot\mathbf{F}$$

Local Thermodynamical Equilibrium

The distribution function for which the Collision Integral vanishes is given by the Maxwellian Distribution:

$$I[f_0] = 0 \qquad f_0(\mathbf{p}) = n(\mathbf{x}, t)\left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-\frac{mw^2}{2k_B T}} \qquad \mathbf{w} = \mathbf{v} - \mathbf{u}$$

The Boltzmann constant $k_B \simeq 1.38 \times 10^{-16}$ in c.g.s units.

Global Thermodynamical Equilibrium if *n*, ***u*** and *T* are uniform.

Local Thermodynamical Equilibrium if they vary both in time and space.

$$\int_{-\infty}^{+\infty} m f_0(\mathbf{p}) d^3\mathbf{p} = n(\mathbf{x}, t) m = \rho(\mathbf{x}, t) \qquad \text{mass density}$$

$$\int_{-\infty}^{+\infty} \mathbf{p} f_0(\mathbf{p}) d^3\mathbf{p} = \rho(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t) \qquad \text{momentum}$$

$$\int_{-\infty}^{+\infty} \frac{1}{2} m w^2 f_0(\mathbf{p}) d^3\mathbf{p} = \frac{3}{2} n(\mathbf{x}, t) k_B T(\mathbf{x}, t) \qquad \text{internal energy density}$$

Local Thermodynamical Equilibrium

Property of Maxwell fluids :

1- Zero Heat Flux

2- Isotropic Pressure tensor $\mathcal{P} = P\mathcal{I}$

Perfect gas Equation-Of-State (EOS) $P = nk_BT$

The Euler equations under the LTE approxmation:

$$\partial_t \rho + \nabla \cdot \mathbf{m} = 0$$

$$\partial_t \mathbf{m} + \nabla \cdot (\rho \mathbf{u} \times \mathbf{u}) + \partial_x P = \rho \mathbf{F}$$

$$\partial_t E + \nabla \cdot \mathbf{u}(E + P) = \rho \mathbf{u} \cdot \mathbf{F}$$

The Equation-Of-State

In real life (except may be in astrophysics), fluids are not rarefied.

- 3-body collisions
- degenerate matter (Maxwell becomes Fermi-Dirac distribution)
- ionization and molecular states (internal degrees of freedom)
- crystal structure (solid state)

Fluid description may beak down, but in most cases, one can capture all these microscopic processes into the Equation-Of-State.

$$\epsilon(\rho, T)$$ specific internal energy

$$P(\rho, T)$$ pressure

The Equation-Of-State

Total energy conservation equation inherits from the First Law of Thermodynamics

$$\rho \frac{\mathrm{D}\epsilon}{\mathrm{D}t} = -P \nabla \cdot \mathbf{u}$$

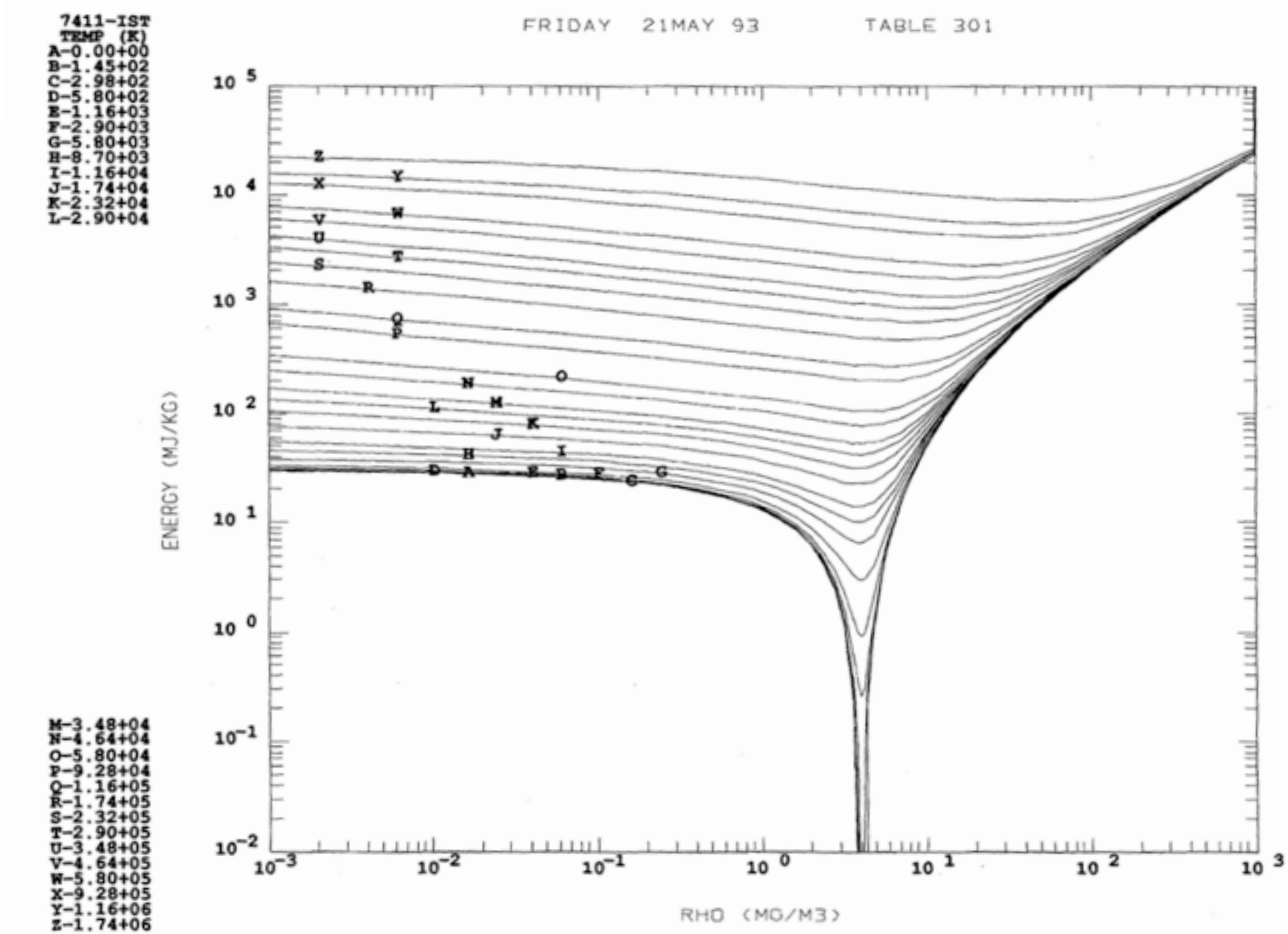
Usually, given the mass and total energy of the fluid element, one computes the specific internal energy.

$$\rho\epsilon = E - \frac{1}{2}\mathbf{u}^2$$

Using the EOS, one then computes the temperature and the pressure

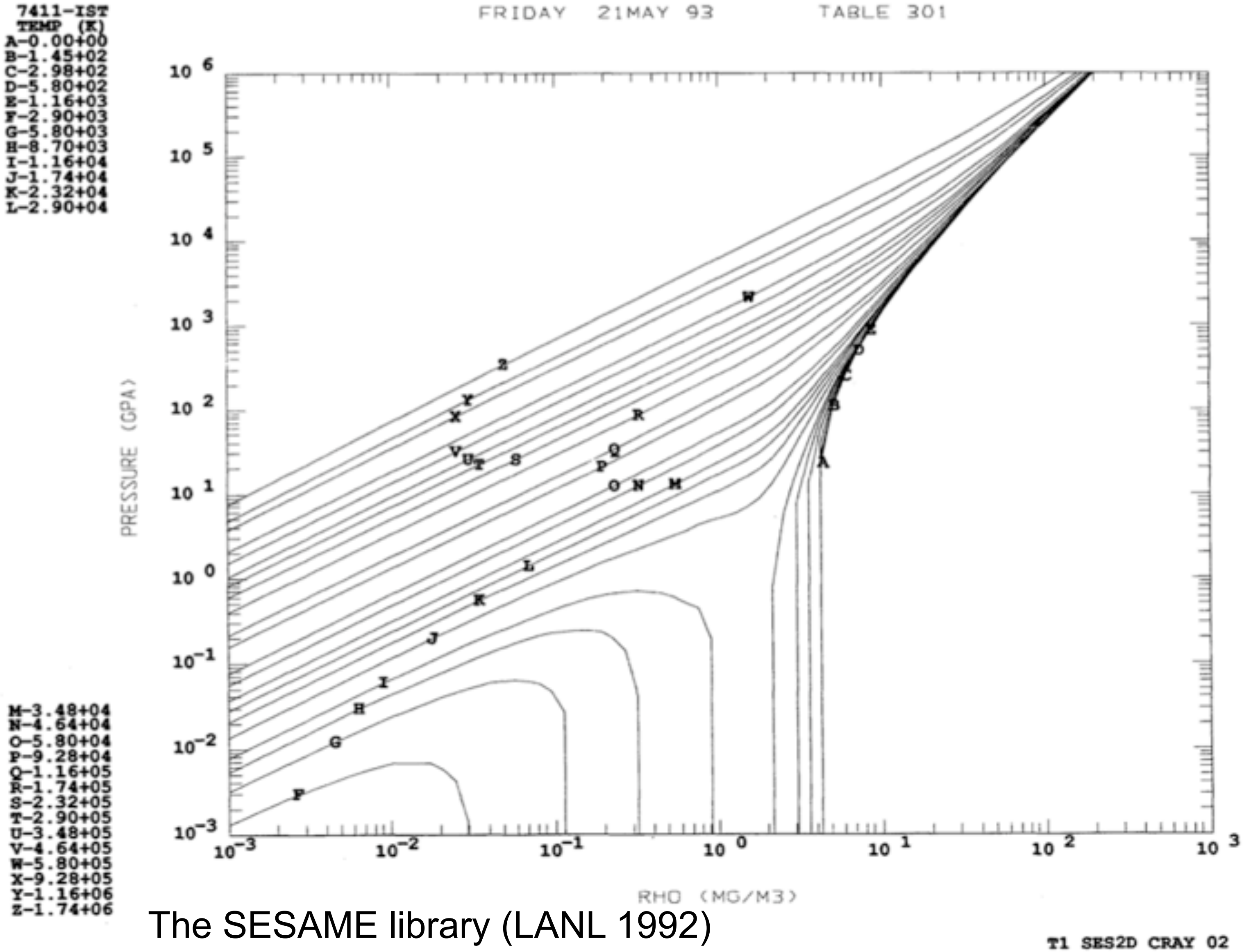
$P(\rho, \epsilon)$ and $T(\rho, \epsilon)$

Equation-Of-State for Aluminium



The SESAME library (LANL 1992)

Equation-Of-State for Aluminium



The SESAME library (LANL 1992)

Mie-Gruneisen EOS

A fairly general EOS formulation: $P - P_c(\rho) = \Gamma\rho\left(\epsilon - \epsilon_c(\rho)\right)$

$\epsilon_c(\rho)$ and $P_c(\rho)$ are the cold energy and cold pressure (Cold Curves) defined at T=0 K

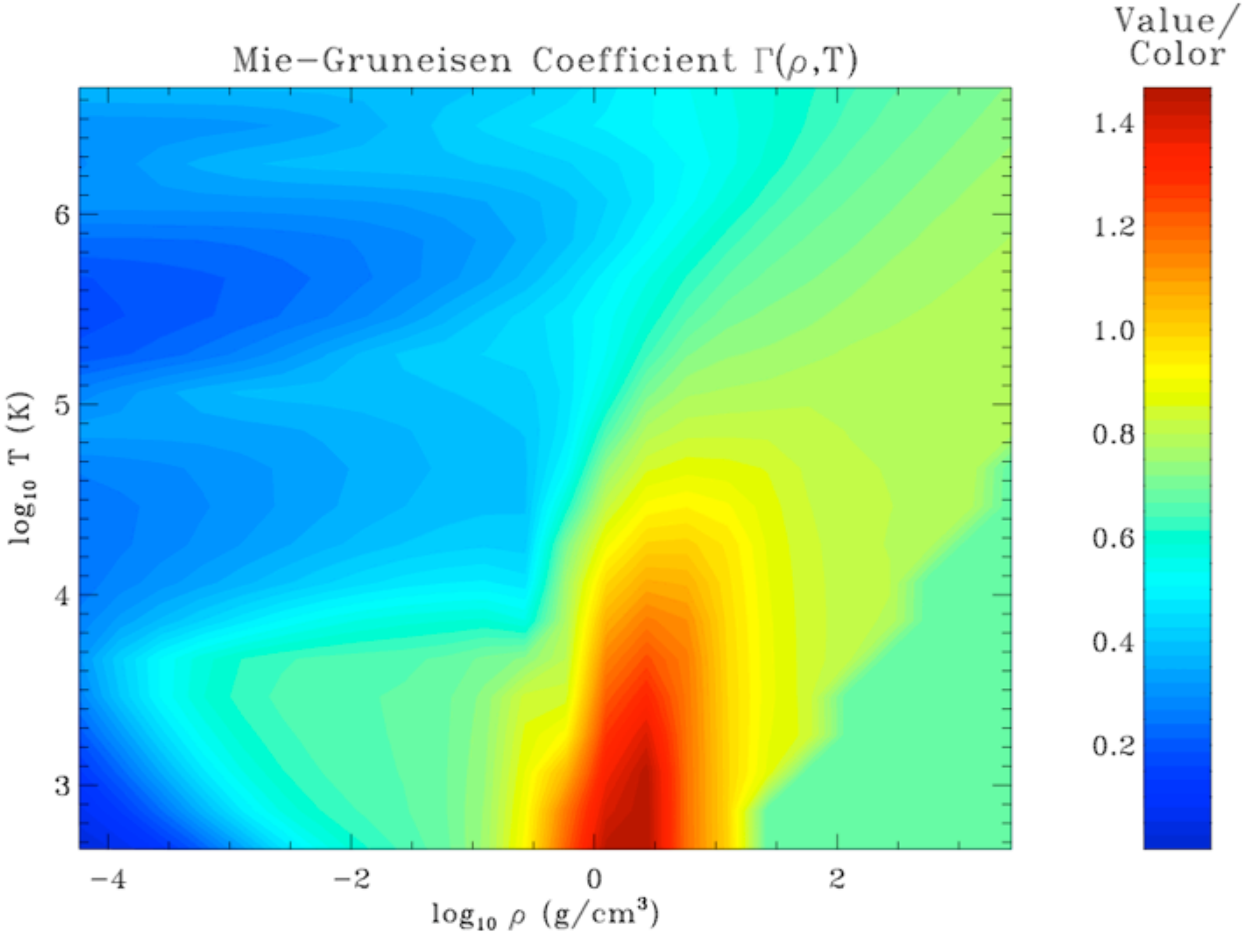
Thermnodynamical consistency : $\rho^2\epsilon_c'(\rho) = P_c$

Sound speed: $$c^2 = P_c'(\rho) + (\Gamma + 1)\,\frac{P - P_c}{\rho}$$

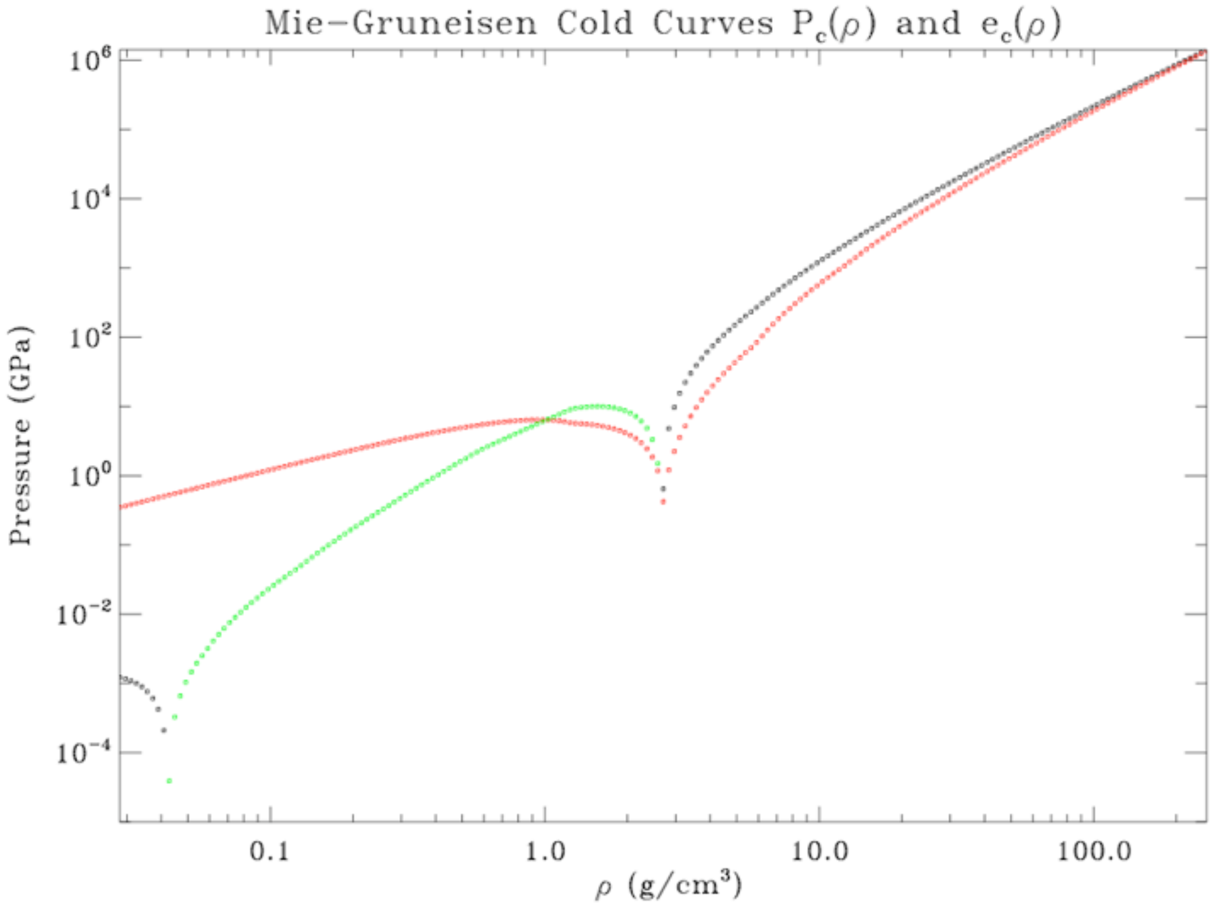
General case: $\Gamma(\rho, \epsilon)$

Numerical trick: assume Γ is a constant over the time step.

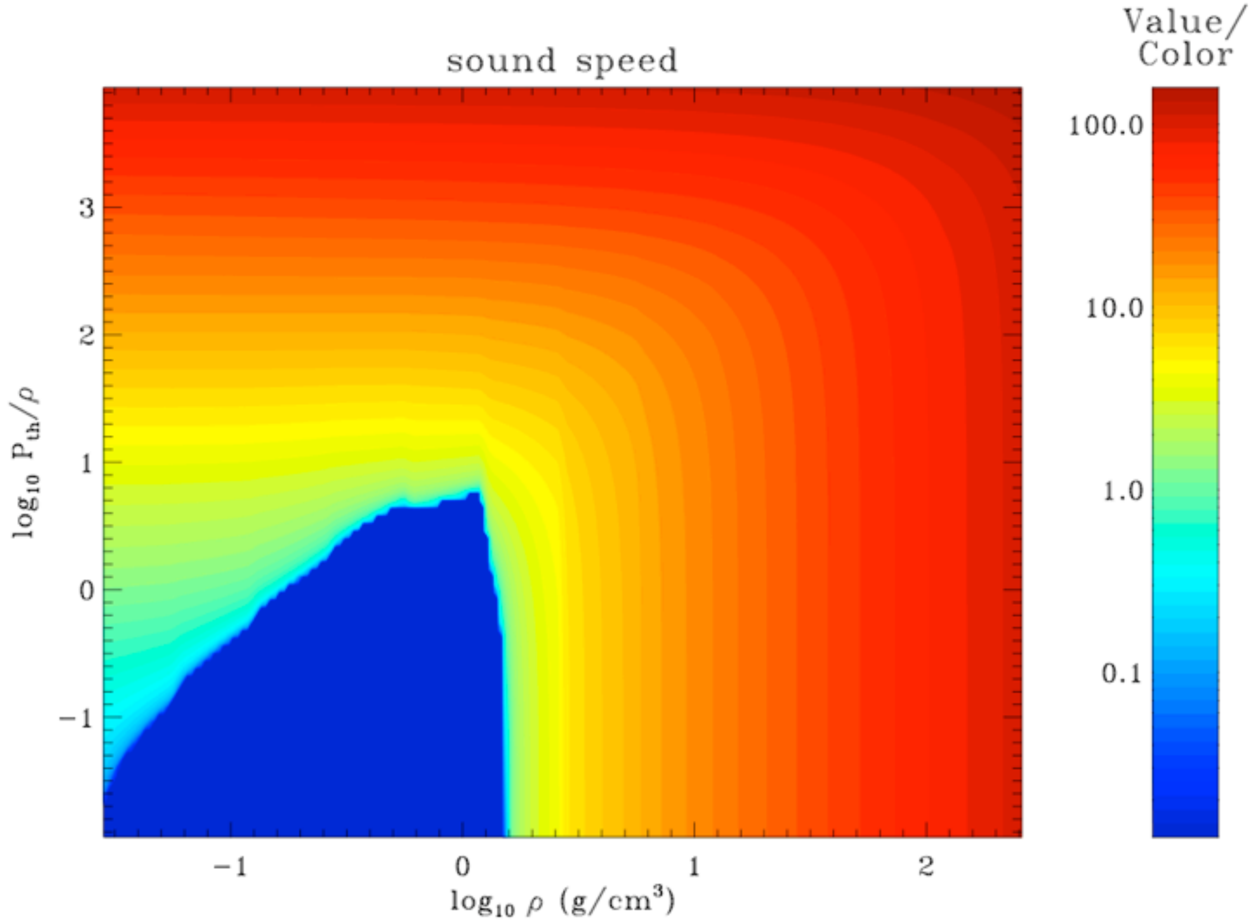
Mie-Gruneisen coefficient for Aluminium



Cold Curves for Aluminium



Sound Speed for Aluminium



Beyond LTE: Chapman-Enskog expansion

Not too far from LTE, the Boltzmann equation can be written using the Relaxation Time Approximation

$$\partial_t f + \mathbf{v} \cdot \partial_\mathbf{x} f + \mathbf{F} \cdot \partial_\mathbf{p} f = I[f] \simeq -\frac{f - f_0}{\tau}$$

$\tau(p)$,the relaxation time is defined by:

$$\frac{1}{\tau(p)} = \int_{-\infty}^{+\infty} \int_{4\pi} \sigma(p-q,\chi) f_0(q) d\Omega d^3 q$$

We assume no body force, and we perform a *Chapman-Enskog expansion*.

$$f = f_0 + \Delta f$$

Assuming stationnarity, we get to leading order (perturbative solution).

$$\Delta f = -\tau \mathbf{v} \cdot \partial_\mathbf{x} f_0$$

Recall:

$$f_0(\mathbf{p}) = n(\mathbf{x},t) \left(\frac{m}{2\pi k_B T(\mathbf{x},t)} \right)^{3/2} e^{-\frac{m(\mathbf{u}(\mathbf{x},t)-\mathbf{v}(\mathbf{x},t))^2}{2k_B T(\mathbf{x},t)}}$$

Modification to the pressure tensor

Only terms that are quadratic in velocity contribute to the pressure tensor

$$\Delta \mathcal{P}_{ij} = \int m \mathrm{w_i} \mathrm{w_j} \Delta f d^3\mathbf{p} \qquad \Delta f = -\tau \mathbf{v} \cdot \partial_{\mathbf{x}} f_0$$

$$\partial_{\mathrm{x_i}} f_0 = -\frac{m}{k_B T} \mathrm{w_j} \frac{\partial u_j}{\partial x_i} f_0$$ plus zero-th and second order terms.

$$\Delta \mathcal{P}_{ij} = \tau \frac{\partial u_j}{\partial x_i} \frac{m}{k_B T} \int m \mathrm{w_i} \mathrm{w_j} f_0 d^3\mathbf{p}$$

We define the correction to the pressure tensor as the ***dynamical viscosity*** of the fluid,

$$\Delta \mathcal{P}_{ij} = \mu \frac{\partial u_j}{\partial x_i}$$

and the viscosity coefficient

$$\mu = \tau \frac{\rho k_B T}{m}$$

Modification to the heat flux

Only terms that are quadratic in velocity contribute to the heat flux

$$\Delta Q_i = \int m \frac{\mathrm{w}^2}{2} \mathrm{w}_\mathrm{i} \Delta f d^3\mathbf{p} \qquad \Delta f = -\tau \mathbf{v} \cdot \partial_\mathbf{x} f_0$$

$$\partial_{\mathrm{x}_\mathrm{i}} f_0 = \frac{1}{T}\left(\frac{m\mathrm{w}^2}{2k_B T} - \frac{3}{2}\right)\frac{\partial T}{\partial x_i} f_0$$

and first order terms

We define the heat flux or thermal flux as $$\Delta Q_i = -\kappa \frac{\partial T}{\partial x_i}$$

Exercise: show that $\kappa \propto \rho k_B \tau \frac{k_B T}{m}$

Non-LTE effects in a Coulomb plasma

Electrons and ions interact through the Coulomb potential.

It features a long-range force, with a cut-off scale at the Debye length.

Spitzer-Harm used the Chapman-Enskog expansion to derive non-LTE coefficients,

$$\mu \simeq \frac{m^{1/2}(k_B T)^{5/2}}{e^4 \ln \Lambda} \qquad \kappa \simeq \frac{k_B (k_B T)^{5/2}}{m^{1/2} e^4 \ln \Lambda}$$

The mass of each particle is the key parameter.

Electron and ions temperature generally differ.

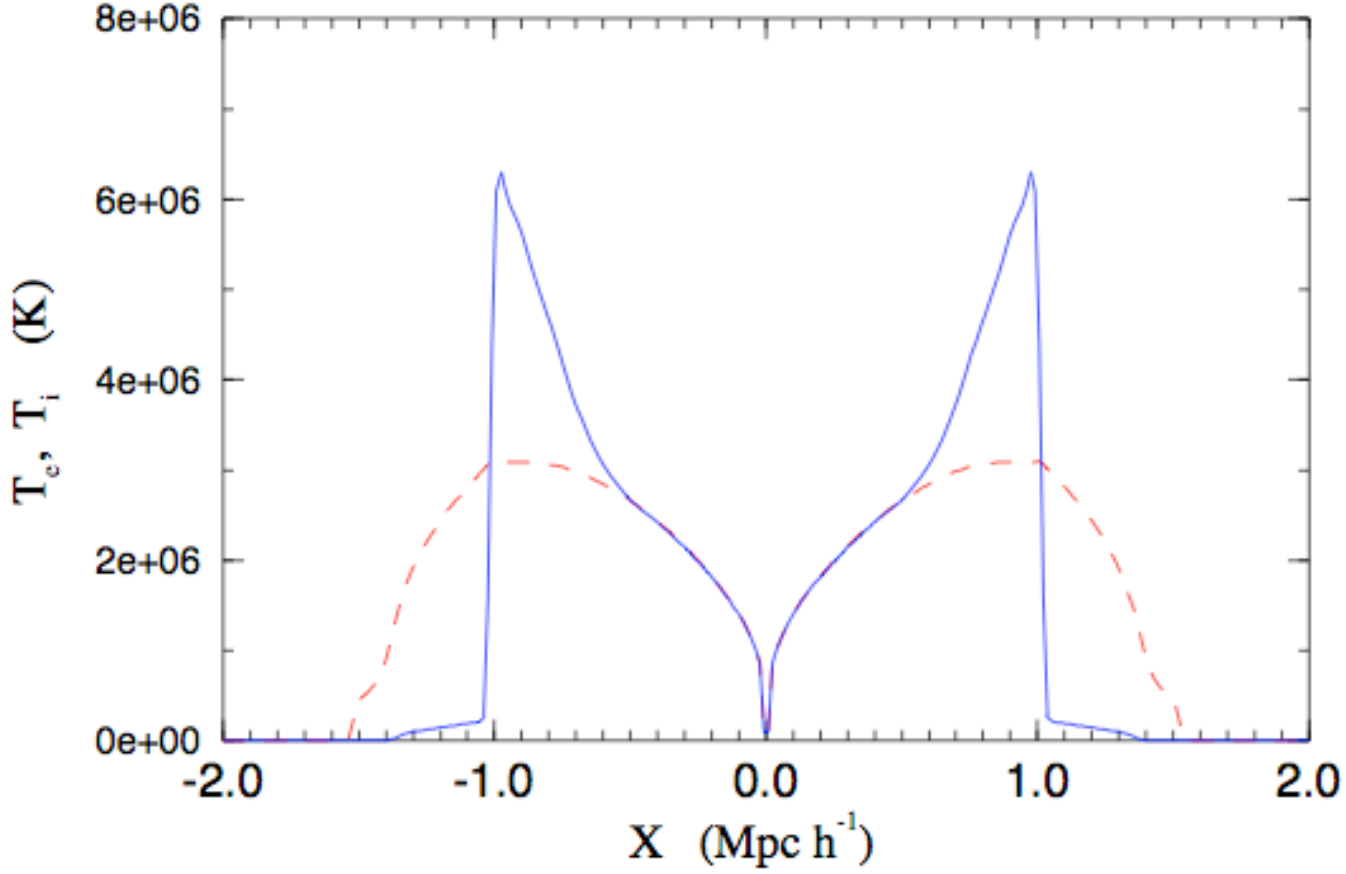
$$\frac{\mathrm{D}T_e}{\mathrm{D}t} = -\frac{\mathrm{D}T_e}{\mathrm{D}t} = -\omega_{ep}(T_e - T_i)$$

Equipartition rate:

Timescale to return to LTE.

$$\omega_{ep} \simeq \frac{m_e^{1/2} e^4 \ln \Lambda}{m_p (k_B T)^{3/2}} n$$

Non-LTE shock-waves in cosmic pancakes



Conclusion

- Kinetic theory as the origin of the Euler equation
- Microscopic conservation laws result in fluid conservation laws.
- Relaxation time approximation to the Collision Integral
- Chapman-Enskog expansion to get *first order* non-LTE effects
- Application to astrophysical plasmas using Spitzer coefficients.

Next lecture: Hydrodynamics 2

Kinetic theory is also used to derive numerical scheme.

The BGK solver is based on the relaxation time approximation.

Prendergast, K.H., Xu, K., "A gas-kinetic BGK scheme for the compressible Navier-Stokes equations",1993, JCP, **109**, 53

Spitzer, L.Jr., Harm, R., "Transport Phenomena in a Completely Ionized Gas", 1953, Phys. Rev., **87**, 977

Mihalas, D., Weibel-Mihalas, B., "Foundations of Radiation Hydrodynamics", on Amazon

The SESAME EOS Library: http://t1web.lanl.gov/newweb_dir/t1sesame.html