Problem 1. Second order moments of the first two terms in the Boltzmann equation:

$$\begin{matrix} \frac{\partial f}{\partial t} & +\mathbf{v}\cdot\nabla f & +\frac{\mathbf{F}}{m}\cdot\nabla_{\mathbf{v}} f & = \\ (1) & (2) & (3) & \end{matrix}$$

Definitions with $\rho = mn(\mathbf{r},t)$:

$$n(\mathbf{r},t) = \int d^3v f(\mathbf{r},\mathbf{v},t) \quad (1)$$

$$\mathbf{u}(\mathbf{r},t) = \frac{1}{n(\mathbf{r},t)}\int d^3v \mathbf{v} f(\mathbf{r},\mathbf{v},t) \quad (2)$$

$$\underline{\underline{\Pi}}(\mathbf{r},t) = m\int d^3v (\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u}) f(\mathbf{r},\mathbf{v},t) \quad (3)$$

All integrals are from $-\infty$ to $+\infty$ over the three velocity components.

i) Term (1) : With $\widetilde{\mathbf{v}} = (\mathbf{v}-\mathbf{u})$or $\mathbf{v} = \widetilde{\mathbf{v}}+\mathbf{u}$

$$\begin{aligned} I_1 &= \frac{m}{2}\int d^3v v^2 \frac{\partial f(\mathbf{r},\mathbf{v},t)}{\partial t} = \frac{m}{2}\frac{\partial}{\partial t}\int d^3\widetilde{v}(\widetilde{\mathbf{v}}+\mathbf{u})\cdot(\widetilde{\mathbf{v}}+\mathbf{u}) f \\ &= \frac{m}{2}\frac{\partial}{\partial t}\int d^3\widetilde{v}\left(\widetilde{\mathbf{v}}^2+2\widetilde{\mathbf{v}}\cdot\mathbf{u}+\mathbf{u}^2\right) f \\ &= \frac{m}{2}\frac{\partial}{\partial t}\int d^3\widetilde{v}\widetilde{\mathbf{v}}^2 f + m\frac{\partial}{\partial t}\left(\mathbf{u}\cdot\int d^3v\widetilde{\mathbf{v}} f\right) + \frac{m}{2}\frac{\partial}{\partial t}\left(\mathbf{u}^2\int d^3v f\right) \end{aligned}$$

The first term with the definition of $\widetilde{\mathbf{v}}$ yields the diagonal terms of the pressure tensor

$$\frac{m}{2}\frac{\partial}{\partial t}\int d^3\widetilde{v}\widetilde{\mathbf{v}}^2 f = \frac{1}{2}\frac{\partial}{\partial t}\left(\Pi_{xx}+\Pi_{yy}+\Pi_{zz}\right) = \frac{1}{2}\frac{\partial}{\partial t}\mathrm{Tr}\underline{\underline{\Pi}} = \frac{3}{2}\frac{\partial p}{\partial t}$$

The second term is 0 because of the definition of $\mathbf{u}$. The last term yields

$$\frac{m}{2}\frac{\partial}{\partial t}\left(\mathbf{u}^2\int d^3v f\right) = \frac{m}{2}\frac{\partial}{\partial t}\left(n\mathbf{u}^2\right) = \frac{1}{2}\frac{\partial \rho\mathbf{u}^2}{\partial t}$$

such that

$$I_1 = \frac{3}{2}\frac{\partial p}{\partial t} + \frac{1}{2}\frac{\partial \rho\mathbf{u}^2}{\partial t}$$

ii) Term (2):

$$\begin{aligned} I_2 &= \frac{m}{2}\int d^3v \mathbf{v}^2\mathbf{v}\cdot\nabla f(\mathbf{r},\mathbf{v},t) = \frac{m}{2}\nabla\cdot\int d^3v\mathbf{v}^2\mathbf{v} f(\mathbf{r},\mathbf{v},t) \\ &= \frac{m}{2}\nabla\cdot\int d^3\widetilde{v}\left(\widetilde{\mathbf{v}}+\mathbf{u}\right)^2\left(\widetilde{\mathbf{v}}+\mathbf{u}\right) f \end{aligned}$$

$$
\begin{aligned}
&= \frac{m}{2}\sum_i \left(\frac{\partial}{\partial x_i}\int d^3\widetilde{v}\,(\widetilde{\mathbf{v}}+\mathbf{u})^2\,(\widetilde{v}_i+u_i)\,f\right)\\
&= \frac{m}{2}\left(\sum_i \frac{\partial}{\partial x_i}\int d^3\widetilde{v}\left(\widetilde{v}_i\widetilde{\mathbf{v}}^2+2\widetilde{v}_i\widetilde{\mathbf{v}}\cdot\mathbf{u}+\widetilde{v}_i\mathbf{u}^2+u_i\widetilde{\mathbf{v}}^2+2u_i\widetilde{\mathbf{v}}\cdot\mathbf{u}+u_i\mathbf{u}^2\right)f\right)\\
&= \frac{m}{2}\left(\sum_{i,j}\frac{\partial}{\partial x_i}\int d^3\widetilde{v}\left(\widetilde{v}_i\widetilde{v}_j^2+2\widetilde{v}_i\widetilde{v}_j u_j+\widetilde{v}_i u_j^2-u_i\widetilde{v}_j{}^2-2u_i\widetilde{v}_j u_j-u_i u_j^2\right)f\right)
\end{aligned}
$$

With the heat flux $\mathbf{L}=\frac{m}{2}\int d^3v\,(\mathbf{v}-\mathbf{u})^2\,(\mathbf{v}-\mathbf{u})\,f(\mathbf{r},\mathbf{v},t)$ the first term becomes

$$
\begin{aligned}
I_2 &= \frac{m}{2}\left(\sum_{i,j}\frac{\partial}{\partial x_i}\int d^3\widetilde{v}\left(\widetilde{v}_i\widetilde{v}_j^2+2\widetilde{v}_i\widetilde{v}_j u_j+\widetilde{v}_i u_j^2-u_i\widetilde{v}_j{}^2-2u_i\widetilde{v}_j u_j-u_i u_j^2\right)f\right)\\
&= \sum_i\frac{\partial}{\partial x_i}L_i+\sum_{i,j}\frac{\partial}{\partial x_i}\left(\Pi_{ij}u_j\right)+\frac{1}{2}\sum_{i,j}\frac{\partial}{\partial x_i}\left(u_i\Pi_{jj}\right)+\frac{m}{2}\sum_{i,j}\frac{\partial}{\partial x_i}\left(nu_iu_j^2\right)
\end{aligned}
$$

In vector representation using $\sum_j \Pi_{jj}=\mathrm{Tr}\underline{\underline{\Pi}}$ this becomes

$$
I_2 = \nabla\cdot\mathbf{L}+\nabla\cdot(\Pi\cdot\mathbf{u})+\frac{3}{2}\nabla\cdot(p\mathbf{u})+\frac{1}{2}\nabla\cdot\left(\rho\mathbf{u}^2\mathbf{u}\right)
$$

iii) Combining the two terms:

$$
I_1+I_2 = \frac{3}{2}\frac{\partial p}{\partial t}+\frac{1}{2}\frac{\partial\rho\mathbf{u}^2}{\partial t}+\nabla\cdot\mathbf{L}+\nabla\cdot(\Pi\cdot\mathbf{u})+\frac{3}{2}\nabla\cdot(p\mathbf{u})+\frac{1}{2}\nabla\cdot\left(\rho\mathbf{u}^2\mathbf{u}\right)
$$

Problem 2.

(a) General second order equation

$$\frac{\partial^2 u}{\partial t^2} + \lambda c \frac{\partial^2 u}{\partial t \partial x} + c^2 \frac{\partial^2 u}{\partial x^2} = G$$

Introducing $R = \partial u/\partial t$ and $S = \partial u/\partial x$ one obtains

$$\begin{array}{ccccc} u & R & S & & \\ & \partial R/\partial t + \lambda c \partial R/\partial x & +c^2 \partial S/\partial x & = & -G \\ \partial u/\partial t & & & = & R \\ & \partial R/\partial x & -\partial S/\partial t & = & 0 \end{array}$$

(b) Nontrivial solutions require

$$\det \begin{pmatrix} 0 & \lambda_t + \lambda c \lambda_x & c^2 \lambda_x \\ \lambda_t & 0 & 0 \\ 0 & \lambda_x & -\lambda_t \end{pmatrix} = 0$$

=>

$$c^2 \lambda_x^2 \lambda_t + \lambda_t^2 (\lambda_t + \lambda c \lambda_x) = 0$$

Division by λ_t^3 and defining $r = \lambda_x/\lambda_t$ (one can equivalently define $r = \lambda_t/\lambda_x$ to get dx/dt in part c) yields

$$c^2 r^2 + \lambda c r + 1 = 0$$

or

$$r^2 + \frac{\lambda}{c} r + \frac{\lambda^2}{4c^2} = \frac{\lambda^2 - 4}{4c^2}$$

with the solutions

$$r = -\frac{\lambda}{2c} \pm \frac{1}{2c}\sqrt{\lambda^2 - 4}$$

There are two real solutions for $\lambda^2 - 4 > 0$ implying a hyperbolic PDE, one solution for $\lambda^2 - 4 = 0$ => parabolic PDE, and no real solution for $\lambda^2 - 4 < 0$ implying an elliptic PDE.

(c) The vector (λ_x, λ_t) represents the normal to a curve given by (x,t) and is therefore equivalent to $(dt, -dx)$ or $r = -dt/dx$ such that ** back to equation for r^2

$$
\begin{aligned}
c^2 - \lambda c \frac{dx}{dt} + \left(\frac{dx}{dt}\right)^2 &= 0 \\
\left(\frac{dx}{dt} - \frac{\lambda c}{2}\right)^2 &= \frac{\lambda^2 c^2}{4} - c^2 \\
\frac{dx}{dt} &= \frac{\lambda c}{2} \pm \sqrt{\frac{\lambda^2 c^2}{4} - c^2} = \frac{\lambda c}{2}\left[1 \pm \sqrt{1 - \frac{4}{\lambda^2}}\right]
\end{aligned}
$$

for the characteristics.

Problem 3.

Consistency requires that the discretized algebraic equation converges to the actual partial differential equation $\partial f/\partial t + v\partial f/\partial x = 0$ in the limit of Δt, $\Delta x \to 0$.

Inserting the definition $c = v\Delta t/\Delta x$ the discretized equation is

$$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} = -\frac{4v}{3}\frac{1}{2\Delta x}\left(f_{j+1}^n - f_{j-1}^n\right) + \frac{v}{3}\frac{1}{4\Delta x}\left(f_{j+2}^n - f_{j-2}^n\right)$$

Taylor expansion of the left side of the equation

$$\begin{aligned}\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} &= \frac{1}{2\Delta t}\left\{(1-1)f_j^n + (1+1)\Delta t f_{t,j}^n + \frac{1}{2}(1-1)\Delta t^2 f_{tt,j}^n + \frac{1}{6}(1+1)\Delta t^3 f_{ttt,j}^n\right.\\ &\qquad \left. + \frac{1}{24}(1-1)\Delta t^4 f_{tttt,j}^n + \frac{1}{120}(1+1)\Delta t^5 f_{ttttt,j}^n\right\}\\ &= f_{t,j}^n + \frac{1}{6}\Delta t^2 f_{ttt,j}^n + \frac{1}{120}\Delta t^4 f_{ttttt,j}^n\end{aligned}$$

The Taylor expansion for the first term on the right is the same replacing t with x

$$\frac{1}{2\Delta x}\left(f_{j+1}^n - f_{j-1}^n\right) = f_{x,j}^n + \frac{1}{6}\Delta x^2 f_{xxx,j}^n + \frac{1}{120}\Delta x^4 f_{xxxxx,j}^n$$

For the second term on the right we need to replace Δx with $2\Delta x$

$$\frac{1}{4\Delta x}\left(f_{j+2}^n - f_{j-2}^n\right) = f_{x,j}^n + \frac{4}{6}\Delta x^2 f_{xxx,j}^n + \frac{16}{120}\Delta x^4 f_{xxxxx,j}^n$$

multiplication of these equations with $-4v/3$ and with $v/3$ and adding the results yields

$$RHS = -v f_{x,j}^n - v\frac{1}{30}\Delta x^4 f_{xxxxx,j}^n$$

Finally using $f_t = -v f_x$ and $f_{tt} = -v f_{xt} = v^2 f_{xx}$ and $f_{ttt} = v^2 f_{xxt} = -v^3 f_{xxx}$ and the definition $v\Delta t = c\Delta x$

$$\begin{aligned}\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} &= f_{t,j}^n - \frac{1}{6}\Delta t^2 v^3 f_{xxx,j}^n - \frac{1}{120}\Delta t^4 v^5 f_{xxxxx,j}^n + ..\\ &= f_{t,j}^n - \frac{v}{6}c^2\Delta x^2 f_{xxx,j}^n - \frac{v}{120}c^4\Delta x^4 f_{xxxxx,j}^n + ..\end{aligned}$$

and combining the different Taylor expansions

$$\begin{aligned}f_{t,j}^n + v f_{x,j}^n &= \frac{v}{6}c^2\Delta x^2 f_{xxx,j}^n + \frac{v}{120}c^4\Delta x^4 f_{xxxxx,j}^n - v\frac{1}{30}\Delta x^4 f_{xxxxx,j}^n + O\left(\Delta x^6\right)\\ &= \frac{v}{6}\Delta x^2\left[c^2 f_{xxx,j}^n + \left(\frac{c^4-4}{20}\right)\Delta x^2 f_{xxxxx,j}^n\right]\end{aligned}$$

such that despite the higher accuracy of the spatial derivative the leading error term $\frac{v}{6}\Delta x^2 c^2 f_{xxx,j}^n$ is determined by the temporal derivative. Therefore the scheme satisfies consistency but is accurate only up to 2nd order in Δx.

Problem 4. Is the scheme

$$f_j^{n+1} - f_j^{n-1} = -\frac{4c}{3}\left(f_{j+1}^n - f_{j-1}^n\right) + \frac{c}{6}\left(f_{j+2}^n - f_{j-2}^n\right)$$

with $c = v\Delta t/\Delta x$ stable?

(a) Amplification factor: Substituting the amplification factor $g = f_j^{n+1}/f_j^n$ and $f_{j+1}^n = f_j^n \exp\left[ik\Delta_x\right]$ yields

$$\begin{aligned} g - \frac{1}{g} &= -\frac{4c}{3}\left[\exp\left(ik\Delta_x\right) - \exp\left(-ik\Delta_x\right)\right] + \frac{c}{6}\left[\exp\left(i2k\Delta_x\right) - \exp\left(-i2k\Delta_x\right)\right] \\ &= -\frac{8c}{3} ic\sin\left(k\Delta_x\right) + \frac{c}{3} ic\sin\left(2k\Delta_x\right) \\ &= \frac{c}{3} i\left[8\sin\left(k\Delta_x\right) + 2\sin\left(k\Delta_x\right)\cos\left(k\Delta_x\right)\right] = 2ih\left(k\Delta_x\right) \end{aligned}$$

with $h\left(k\Delta_x\right) = \frac{c}{3}\sin\left(k\Delta_x\right)\left[4 + \cos\left(k\Delta_x\right)\right]$ which yields for g:

$$\begin{aligned} g^2 - 2gih - 1 = 0 \quad or \quad (g - ih)^2 = 1 - h^2 \\ \Longrightarrow \qquad g \;=\; ih \pm \sqrt{1 - h^2} \end{aligned}$$

(b) Stability: Since g is complex we consider the absolute value of g

(1) Assuming $h^2 \le 1$, i.e., $-1 \le h \le 1$ the magnitude of the amplification factor is given by

$$|g|^2 = gg^* = h^2 + \left(1 - h^2\right) = 1,$$

i.e., the scheme is stable in the range $-1 \le h \le 1$.

(2) Assuming $h^2 > 1$, i.e., $h > 1$ or $h < -1$:

$$\begin{aligned} g^2 &= i^2\left(h \pm \sqrt{h^2 - 1}\right)^2 \\ &= -\left[2h^2 \pm 2h\sqrt{h^2 - 1} - 1\right] \end{aligned}$$

Choosing the '$+$' sign and $h > 1$:

$$g^2 = -\left[2h^2 + 2h\sqrt{h^2 - 1} - 1\right] < -\left[h^2 + 2h\sqrt{h^2 - 1}\right] < -1.$$

For $h < -1$ and the '$-$' sign:

$$g^2 = -\left[2h^2 - 2h\sqrt{h^2 - 1} - 1\right] < -\left[h^2 - 2h\sqrt{h^2 - 1}\right] < -1,$$

i.e., the scheme is unstable for $h > 1$and $h < -1$. Therefore overall stability requires $-1 \le h \le 1$. To identify the stable range of c is given by

$$\left|\frac{c}{3}\sin\left(k\Delta_x\right)\left[4 + \cos\left(k\Delta_x\right)\right]\right| \le 1$$

or with $x = k\Delta_x$ and $f = \sin x\,(4+\cos x)$ the stable range is $|c| \le 3/\max\left(f\left(x\right)\right)$. The maxima and minima of $f\left(x\right)$ are given by $df/dx = \cos x\,(4+\cos x) - \sin x\,(\sin x) = 2\cos^2 x + 4\cos x - 1 = 0$ or

$$\begin{aligned} \cos x &= -1+\sqrt{3/2} \qquad \sin x = \pm\sqrt{-\frac{3}{2}+\sqrt{6}} \\ \Longrightarrow \quad \max\left(f\left(x\right)\right) &= \sqrt{\sqrt{6}-\frac{3}{2}}\left(3+\sqrt{3/2}\right) \approx \pm 4.12 \quad \text{and} \\ |c| &\le \min\left(\frac{3}{|\sin x\,(4+\cos x)|}\right) = \frac{3}{\max f} \approx 0.73 \end{aligned}$$

A cruder estimate using $\sin x \le 1$ and $4+\cos x \le 5$ yields $|c| \le 3/5 = 0.6$.