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

$$\underset{(1)}{\frac{\partial f}{\partial t}} \quad \underset{(2)}{+\mathbf{v}\cdot\nabla f} \quad \underset{(3)}{+\frac{\mathbf{F}}{m}\cdot\nabla_{\mathbf{v}} f} \quad =$$

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

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

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

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

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

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

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

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

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

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

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

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):

$$\begin{aligned}
I_2 &= \frac{m}{2}\int d^3v\mathbf{v}^2\mathbf{v}\cdot\nabla f(\mathbf{r},\mathbf{v},t) = \frac{m}{2}\nabla\cdot\int d^3v\mathbf{v}^2\mathbf{v}f(\mathbf{r},\mathbf{v},t) \\
&= \frac{m}{2}\nabla\cdot\int d^3\widetilde{v}\left(\widetilde{\mathbf{v}}+\mathbf{u}\right)^2\left(\widetilde{\mathbf{v}}+\mathbf{u}\right)f \\
&= \frac{m}{2}\sum_i\left(\frac{\partial}{\partial x_i}\int d^3\widetilde{v}\left(\widetilde{\mathbf{v}}+\mathbf{u}\right)^2\left(\widetilde{v}_i+u_i\right)f\right) \\
&= \frac{m}{2}\left(\sum_i\frac{\partial}{\partial x_i}\int d^3\widetilde{v}\left(\widetilde{v}_i\widetilde{\mathbf{v}}^2+2\widetilde{v}_i\widetilde{\mathbf{v}}\cdot\mathbf{u}+\widetilde{v}_i\mathbf{u}^2+u_i\widetilde{\mathbf{v}}^2+2u_i\widetilde{\mathbf{v}}\cdot\mathbf{u}+u_i\mathbf{u}^2\right)f\right) \\
&= \frac{m}{2}\left(\sum_{i,j}\frac{\partial}{\partial x_i}\int d^3\widetilde{v}\left(\widetilde{v}_i\widetilde{v}_j^2+2\widetilde{v}_i\widetilde{v}_ju_j+\widetilde{v}_iu_j^2-u_i\widetilde{v_j}^2-2u_i\widetilde{v}_ju_j-u_iu_j^2\right)f\right)
\end{aligned}$$

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

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

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

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

iii) Combining the two terms:

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

Problem 2.

General second order equation

$$A\frac{\partial^2 u}{\partial t^2} + B\frac{\partial^2 u}{\partial t \partial x} + C\frac{\partial^2 u}{\partial x^2} + D\frac{\partial u}{\partial t} + E\frac{\partial u}{\partial x} + Fu = G$$

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

$$\begin{array}{ccccc} u & R & S & & \\ & A\partial R/\partial t + B\partial R/\partial x & +C\partial S/\partial x & = & -DR - ES - Fu - G \\ \partial u/\partial t & & & = & R \\ & \partial R/\partial x & -\partial S/\partial t & = & 0 \end{array}$$

Which yields

$$\det \begin{pmatrix} 0 & A\lambda_t + B\lambda_x & C\lambda_x \\ \lambda_t & 0 & 0 \\ 0 & \lambda_x & -\lambda_t \end{pmatrix} = 0$$

=>

$$C\lambda_x^2\lambda_t + \lambda_t^2\left(A\lambda_t + B\lambda_x\right) = 0$$

Division by λ_t^3 and defining $r = \lambda_x/\lambda_t$ yields

$$Cr^2 + Br + A = 0$$

or

$$r^2 + \frac{B}{C}r + \frac{B^2}{4C^2} = \frac{B^2 - 4CA}{4C^2}$$

with the solutions

$$r = -\frac{B}{2C} \pm \frac{1}{2C}\sqrt{B^2 - 4CA}$$

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

Problem 3.

(a) Taylor expansion of

$$
\begin{aligned}
\frac{d^2 f}{dx^2} \approx a f_{i-1} + b f_i + c f_{i+1} + d f_{i+2} &= (a+b+c+d)\, f_i + (-a+c+2d)\,\Delta x \frac{df}{dx} \\
&+ (a+c+4d)\,\frac{\Delta x^2}{2}\frac{d^2 f}{dx^2} + (-a+c+8d)\,\frac{\Delta x^3}{6}\frac{d^3 f}{dx^3} \\
&+ (a+c+16d)\,\frac{\Delta x^4}{24}\frac{d^4 f}{dx^4} + (-a+c+32d)\,\frac{\Delta x^5}{120}\frac{d^5 f}{dx^5}
\end{aligned}
$$

Conditions for a, b, c, and d

$$
\begin{aligned}
a+b+c+d &= 0 \\
-a+c+2d &= 0 \\
a+c+4d &= 2/\Delta x^2 \\
-a+c+8d &= 0
\end{aligned}
$$

Subtracting (2) from (4) yields $d = 0$ and $a = c$ such that

$$
\begin{aligned}
a = c &= 1/\Delta x^2 \\
b = -2a &= -2/\Delta x^2
\end{aligned}
$$

which yields

$$
\begin{aligned}
\frac{1}{\Delta x^2}\left(f_{i-1} - 2 f_i + f_{i+1}\right) &= \frac{d^2 f}{dx^2} + (a+c)\,\frac{\Delta x^4}{24}\frac{d^4 f}{dx^4} + \ldots \\
&= \frac{d^2 f}{dx^2} + \frac{\Delta x^2}{12}\frac{d^4 f}{dx^4} + \ldots
\end{aligned}
$$

Lowest order error:

$$
E = \frac{\Delta x^2}{12}\frac{d^4 f}{dx^4}
$$

(b) For the second approximation the Taylor expansion is

$$
\begin{aligned}
\frac{d^2 f}{dx^2} \approx a f_i + b f_{i+1} + c f_{i+2} + d f_{i+3} &= (a+b+c+d)\, f_i + (b+2c+3d)\,\Delta x \frac{df}{dx} \\
&+ (b+4c+9d)\,\frac{\Delta x^2}{2}\frac{d^2 f}{dx^2} + (b+8c+27d)\,\frac{\Delta x^3}{6}\frac{d^3 f}{dx^3} \\
&+ (b+16c+81d)\,\frac{\Delta x^4}{24}\frac{d^4 f}{dx^4} + \ldots
\end{aligned}
$$

Conditions for a, b, c, and d

$$\begin{aligned} a+b+c+d &= 0 \\ b+2c+3d &= 0 \\ b+4c+9d &= 2/\Delta x^2 \\ b+8c+27d &= 0 \end{aligned}$$

Subtracting (2) from (3) and from (4) yields

$$\begin{aligned} c+3d &= 1/\Delta x^2 \\ c+4d &= 0 \end{aligned}$$

yielding

$$\begin{aligned} d &= -1/\Delta x^2 \\ c &= 4/\Delta x^2 \end{aligned}$$

Backsubstitution:

$$\begin{aligned} b=-2c-3d &= -5/\Delta x^2 \\ a=-b-c-d &= 2/\Delta x^2 \end{aligned}$$

which yields

$$\frac{1}{\Delta x^2}\left(2f_i - 5f_{i+1} + 4f_{i+2} - f_{i+3}\right) = \frac{d^2 f}{dx^2} + (b+16c+81d)\,\frac{\Delta x^4}{24}\frac{d^4 f}{dx^4} + ...$$

Lowest order error:

$$b+16c+81d = -\frac{22}{\Delta x^2}$$

or

$$\frac{1}{\Delta x^2}\left(2f_i - 5f_{i+1} + 4f_{i+2} - f_{i+3}\right) = \frac{d^2 f}{dx^2} + \frac{11}{12}\Delta x^2 \frac{d^4 f}{dx^4} + ...$$

Comparison with (a) shows that the error has the same order but is larger by a factor of 3.

Problem 4. Is the scheme

$$f_j^{n+1} - f_j^{n-1} = c\left(f_{j+1}^n - f_{j-1}^n\right)$$

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

Stability: 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

$$\begin{aligned} g - \frac{1}{g} &= c\left[\exp\left(ik\Delta_x\right) - \exp\left(-ik\Delta_x\right)\right] \\ &= 2ic\sin\left(k\Delta_x\right) \end{aligned}$$

which yields for g:

$$\begin{aligned} g^2 - g2ic\sin\left(k\Delta_x\right) - 1 &= 0 \\ \left(g - ic\sin\left(k\Delta_x\right)\right)^2 &= 1 - c^2\sin^2\left(k\Delta_x\right) \end{aligned}$$

or

$$g = ic\sin\left(k\Delta_x\right) \pm \sqrt{1 - c^2\sin^2\left(k\Delta_x\right)}$$

Since g is complex we need the absolute value of g which is

$$\begin{aligned} |g|^2 = gg^* &= c^2\sin^2\left(k\Delta_x\right) + \left(1 - c^2\sin^2\left(k\Delta_x\right)\right) \\ &= 1 \end{aligned}$$

Since the magnitude of g is equal to 1 the scheme is always stable for $c \leq 1$.

For $c > 1$:

Assume $h = c\sin\left(k\Delta_x\right) > 1$. Then

$$g = i\left(h \pm \sqrt{h^2 - 1}\right)$$

Obviously the case with $h > 1$ and choosing the "+" sign yields $|g| > 1$. Similarly it is easy to show $|g| > 1$ if $h < -1$.

In conclusion, the Leapfrog scheme is stable for $c \leq 1$.