Chapter 10

Fluid and Plasma Simulation

10.1 Supersonic flow, shocks, flux corrected transport

MacCormack's Predictor-Corrector Scheme:

Inviscid Burger's equation

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0$$

with $f = u^2/2$

Highly effcient scheme as a basis for shock capturing methods is the MacCormack predictor-corrector method:

Predictor:

$$u_j^* = u_j^n - \frac{\Delta t}{\Delta_x}\left(F_{j+1}^n - F_j^n\right)$$

Corrector:

$$u_j^{n+1} = \frac{1}{2}\left(u_j^n + u_j^*\right) - \frac{\Delta t}{2\Delta_x}\left(F_j^* - F_{j-1}^*\right),$$

i.e., the predictor and corrector steps are one sided but from opposite sides. In fact the predictor step is the same as the upwind and represents time level $n+1$. In comparison the two step Lax Wendroff is symmetric in the evaluation of the flux:

$$\begin{aligned} u_{j+1/2}^* &= \frac{1}{2}\left(u_j^n + u_{j+1}^n\right) - \frac{\Delta t}{2\Delta_x}\left(F_{j+1}^n - F_j^n\right) \\ u_j^{n+1} &= u_j^n - \frac{\Delta t}{\Delta_x}\left(F_{j+1/2}^* - F_{j-1/2}^*\right) \end{aligned}$$

Using the predictor step the MacCormack scheme can be expressed as:

$$\begin{aligned} u_j^{n+1} &= \frac{1}{2}\left(u_j^n + u_j^n - \frac{\Delta t}{\Delta_x}\left(F_{j+1}^n - F_j^n\right)\right) - \frac{\Delta t}{2\Delta_x}\left(F_j^* - F_{j-1}^*\right) \\ &= u_j^n - \frac{\Delta t}{2\Delta_x}\left(F_{j+1}^n - F_j^n\right) - \frac{\Delta t}{2\Delta_x}\left(F_j^* - F_{j-1}^*\right) \end{aligned}$$

Importantly, the MacCormack scheme is conservative, i.e., mass, momentum etc are conserved meaning that the change of mass (or any quantity that satisfies a continuity type equation) in a volume is only changed by the fluxes in and out of the volume. This is important because shock conditions in ideal fluids (hydrodynamics, Magnetohydrodynamics) are determined by mass, momentum, and energy conservation. Using the MacCormack scheme without further modification are similar to those of the Lax-Wendroff or Leapfrog schemes (MacCormack with slightly reduced oscillations).

Flux Corrected Transport Scheme (Boris and Book, 1973):

Simple 1D example for convection equation:

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} = 0$$

Let us consider a predictor step (here Lax-Wendroff) with artificial diffusion added:

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

where ν is the diffusion coeficient. To simply subtract diffusion one would introduce antidiffusion

$$f_j^{n+1} = f_j^n - \mu\left(f_{j+1}^* - 2f_j^* + f_{j-1}^*\right)$$

with $\mu > 0$. This antidiffusion would approximately compensate the diffusion initially for $\mu = \nu$. However, we need some diffusion for shocks and discontinuities because of the dispersion errors and the resulting large oscillations. Let us consider mass flux at intermediate points $j+1/2$ and $j-1/2$:

$$F_{j+1/2} = \mu\left(f_{j+1}^* - f_j^*\right) \qquad F_{j-1/2} = \mu\left(f_j^* - f_{j-1}^*\right),$$

i.e., diffusive fluxes centered between grid cells. Now these fluxes should be adjusted such that they are only applied where diffusion is not needed (because the solution is sufficiently smooth). An example for this adjustment for flux corrected transport is the following form of the corrective flux

$$
\begin{aligned}
F^c_{j+1/2} &= \text{sign}\left(\Delta f_{j+1/2}\right)\max\left\{0,\min\left[\Delta f_{j-1/2}\text{sign}\left(f_{j+1/2}\right),\mu\left|\Delta f_{j+1/2}\right|,\right.\right.\\
&\qquad\left.\left.\Delta f_{j+3/2}\text{sign}\left(f_{j+1/2}\right)\right]\right\}\\
F^c_{j-1/2} &= \text{sign}\left(\Delta f_{j-1/2}\right)\max\left\{0,\min\left[\Delta f_{j-3/2}\text{sign}\left(f_{j-1/2}\right),\mu\left|\Delta f_{j-1/2}\right|,\right.\right.\\
&\qquad\left.\left.\Delta f_{j+3/2}\text{sign}\left(f_{j+1/2}\right)\right]\right\}
\end{aligned}
$$

with $\Delta f_{j+1/2} = f^*_{j+1} - f^*_j$. The integration is then completed by

$$f^{n+1}_j = f^*_j - F^c_{j+1/2} + F^c_{j-1/2}$$

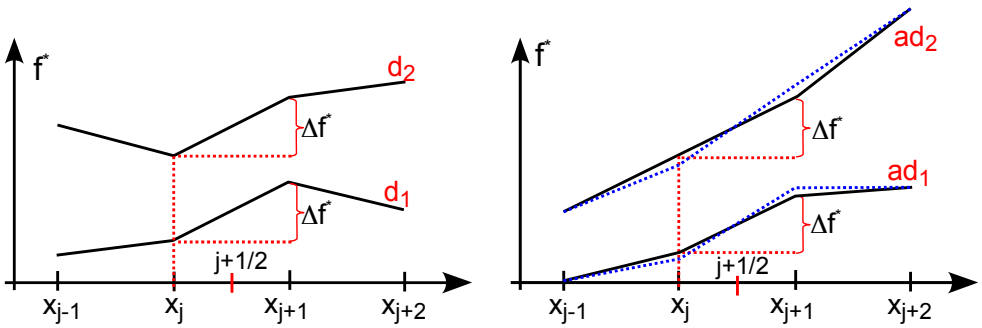


Figure 10.1: Examples (d) where the diffusive flux are not corrected vs the cases (ad) where antidiffusive fluxes are applied.

It is illustrative to examine the properties of these corrective fluxes more closely. Considering the case $\Delta f_{j+1/2} > 0$ Figure (10.1) shows 4 examples, where the examples labeled (d) result in no correction for the diffusion, and the examples labeled (ad) provide antidiffusive fluxes. For $\Delta f_{j+1/2} > 0$ we can ignore the sign function.

- The corrective flux $F^c_{j+1/2}$ is subtracted from f^*_j and added to f^*_{j+1}. Thereby mass is conserved.
- The min [..] is always negative if f^* has a minimum or a maximum at x_j or x_{j+1} because the product $\Delta f_{j-1/2}\Delta f_{j+1/2}$or $\Delta f_{j+1/2}\Delta f_{j+3/2}$ is negative. The condition min [..] < 0 implies $F^c_{j+1/2} = 0$.
- For $\Delta f_{j-1/2} > 0$ and $\Delta f_{j+3/2} > 0$ the flux is $F^c_{j+1/2} = \min\left[\Delta f_{j-1/2}, \mu\left|\Delta f_{j+1/2}\right|, \Delta f_{j+3/2}\right]$. This insures that the flux correction does not cause a local minimum or maximum at j or $j+1$.

In short the FCT approach is conservative, reduces or avoids oscillations associated with numerical dispersion for large gradients, and can be 2nd order accurate in regions without large gradients. The time step limitation is slighly more restrictive with the condition $c = u\Delta t/\Delta x < 0.5$. Clearly the values chosen for μ and ν determine the specific properties. For smallvalues almost no dissipation

is introduced and the method still leads to oscillations. Large values introduce strong diffusion and a reasonable choice is $\mu = \nu = 1/8$. In order to minimize dispersion a choice of

$$\nu = \frac{1}{6} + \frac{c^2}{3} \qquad and \qquad \mu = \frac{1}{6} - \frac{c^2}{6}$$

is recommended (Boris and Book, 1976).

10.2 Shock Wave propagation using FCT:

Following we use the method described above for a system of equations given by

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0 \tag{10.1}$$

$$With\ \mathbf{q} = \begin{Bmatrix} \rho \\ \rho u \\ \frac{p}{\gamma - 1} + \frac{1}{2}\rho u^2 \end{Bmatrix} \qquad \mathbf{F} = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \left(\frac{\gamma p}{\gamma - 1} + \frac{1}{2}\rho u^2\right) u \end{Bmatrix} \tag{10.2}$$

The solution to these equations defined by the Lax-Wendroff (9.6), Leapfrog (9.5) or MacCormack's methods is 2nd order accurate, implying that they have no or very little 2nd order diffusion. This solution is denoted as $\mathbf{q}^{ND}$ and refers to time index $n+1$.

$$\begin{aligned}
Leapfrog: \qquad & \mathbf{q}_j^{ND} = \mathbf{q}_j^{n-1} - \frac{\Delta t}{2\Delta_x}\left(\mathbf{F}_{j+1}^n - \mathbf{F}_{j-1}^n\right) \\
Lax-Wendroff: \qquad & \mathbf{q}_{j+1/2}^{*} = \frac{1}{2}\left(\mathbf{q}_j^n + \mathbf{q}_{j+1}^n\right) - \frac{\Delta t}{2\Delta_x}\left(\mathbf{F}_{j+1}^n - \mathbf{F}_j^n\right) \\
& \mathbf{q}_j^{ND} = \mathbf{q}_j^n - \frac{\Delta t}{\Delta_x}\left(\mathbf{F}_{j+1/2}^{*} - \mathbf{F}_{j-1/2}^{*}\right) \\
MacCormack: \qquad & \mathbf{q}_j^{*} = \mathbf{q}_j^n - \frac{\Delta t}{\Delta_x}\left(\mathbf{F}_{j+1}^n - \mathbf{F}_j^n\right) \\
& \mathbf{q}_j^{ND} = \frac{1}{2}\left(\mathbf{q}_j^n + \mathbf{q}_j^{*}\right) - \frac{\Delta t}{2\Delta_x}\left(\mathbf{F}_j^{*} - \mathbf{F}_{j-1}^{*}\right)
\end{aligned}$$

The actual flux corrected solution will introduce diffusion in a selective manner and involves the following steps:

1) Generation of diffusive and anti-diffusive fluxes:

$$\begin{aligned}
\mathbf{F}_{j+1/2}^{D} &= \nu_{j+1/2}\left(\mathbf{q}_{j+1}^n - \mathbf{q}_j^n\right) \\
\mathbf{F}_{j+1/2}^{AD} &= \mu_{j+1/2}\left(\mathbf{q}_{j+1}^{ND} - \mathbf{q}_j^{ND}\right)
\end{aligned}$$

2) Determine the solution with 2nd order diffusion:

$$\mathbf{q}_j^D = \mathbf{q}_j^{ND} + \mathbf{F}_{j+1/2}^D - \mathbf{F}_{j-1/2}^D$$

3) Compute the variation (differences) of this diffusive solution

$$\Delta\mathbf{q}_{j+1/2}^D = \mathbf{q}_{j+1}^D - \mathbf{q}_j^D$$

4) Modify the anti-diffusive flux depending on the variation of the diffusive solution $\Delta\mathbf{q}^D$ in comparison with the anti-diffusive flux $\mathbf{F}_{j+1/2}^{AD}$ of the non-diffusive solution.

$$\begin{aligned} \mathbf{F}_{j+1/2}^{FCT} &= \sigma_{j+1/2}\max\left\{0, \min\left[\sigma_{j+1/2}\Delta\mathbf{q}_{j-1/2}^D, \left|\mathbf{F}_{j+1/2}^{AD}\right|, \sigma_{j+1/2}\Delta\mathbf{q}_{j+3/2}^D\right]\right\} \\ with \quad & \sigma_{j+1/2} = \operatorname{sgn}\mathbf{F}_{j+1/2}^{AD} \end{aligned}$$

This is slightly different from the simple prior example of the advection equation.

5) The final step is the application of the corrected anti-diffusive flux to the solution with diffusion to compensate diffusion where it is not required.:

$$\mathbf{q}_j^{n+1} = \mathbf{q}_j^D + \mathbf{F}_{j+1/2}^{FCT} - \mathbf{F}_{j-1/2}^{FCT}$$

The diffusion and anti-diffusion coefficients are chosen as

$$\nu_{j+1/2} = \alpha_0 + \alpha_1\left(u_{j+1/2}\frac{\Delta t}{\Delta x}\right)^2 \qquad and \qquad \mu = \alpha_0 + \alpha_2\left(u_{j+1/2}\frac{\Delta t}{\Delta x}\right)^2$$

with $\alpha_0 = 1/6$, $\alpha_1 = 1/3$, and $\alpha_2 = -1/6$. The overall approach is rather similar to the simple fixed convection example in the previous section.

Notes on the program on web page uses the example of shock propagation:

It is convenient to normalize equations to typical quantities, i.e., $\rho = \rho_0\widehat{\rho} \quad p = p_0\widehat{p} \quad u = u_0\widehat{u}$, but these are not independent. Specifically a measure of the flow velocity in units of the sound speed implies $u_0 = \sqrt{\gamma p_0/\rho_0}$ (we also obtain the relation $x_0/t_0 = u_0$). Substituting these quantities into (10.1) generates

$$\begin{aligned} \frac{\partial\hat{\mathbf{q}}}{\partial\hat{t}} + \frac{\partial\hat{\mathbf{F}}}{\partial\hat{x}} &= 0 \\ With\ \hat{\mathbf{q}} = \begin{Bmatrix} \hat{\rho} \\ \hat{\rho}\hat{u} \\ \frac{\hat{p}/\gamma}{\gamma-1} + \frac{1}{2}\hat{\rho}\hat{u}^2 \end{Bmatrix} \qquad & \mathbf{F} = \begin{Bmatrix} \hat{\rho}\hat{u} \\ \hat{p}/\gamma + \hat{\rho}\hat{u}^2 \\ \left(\frac{\hat{p}}{\gamma-1} + \frac{1}{2}\hat{\rho}\hat{u}^2\right)\hat{u} \end{Bmatrix} \end{aligned}$$

These equations are almost identical to those in physical units except that p is replaced by p/γ. For the case of shock propagation it is convenient to use the down stream values for the normalization. In normalized units the pressure, density, and soundspeed in the downstream region are all unity (and the sound speed in normalized units is now $\hat{c}_s = \sqrt{\hat{p}/\hat{\rho}}$ (also measured in units of $u_0 = \sqrt{\gamma p_0/\rho_0}$). In the following expressions we ommit the $\hat{}$ for normalized quantities.

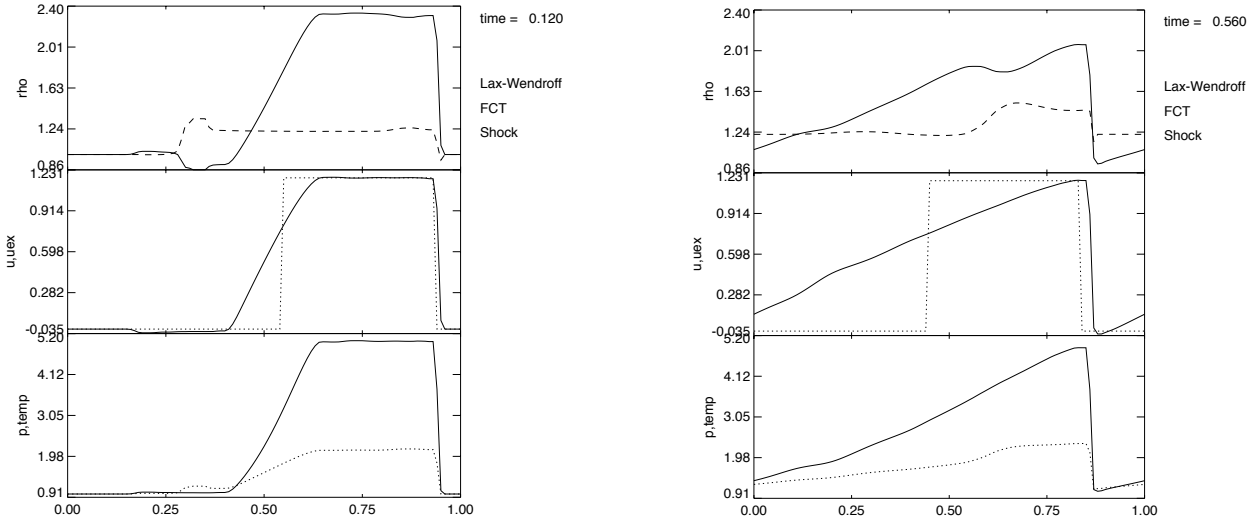
The jump conditions can be derived from the Rankine-Hugoniot conditions and are oft expressed in terms of the upstream Machnumber $M = u/c_s$ with $c_s^2 = \gamma p/\rho$ by the relations

$$\frac{\rho_d}{\rho_u} = \frac{(\gamma+1)M_u^2}{2+(\gamma-1)M_u^2} \qquad \frac{u_d}{u_u} = \frac{\rho_u}{\rho_d} \qquad \frac{p_d}{p_u} = \frac{2\gamma M_u^2-(\gamma-1)}{\gamma+1}$$

where up- and downstream velocities are measured in the rest frame of the shock. However, here we express these conditions through the pressure ratio assuming the downstrean density and sound speed are unity (i.e., normalization is with respect to downstream fluid properties) and the downstream velocity is 0:

$$\begin{aligned} u_u &= \sqrt{2}\left(\frac{p_u}{p_d}-1\right)\left[\gamma(\gamma-1)\frac{p_d}{p_u}+\gamma(\gamma+1)\right]^{-1/2} \\ \rho_u &= \left(1+\frac{\gamma+1}{\gamma-1}\frac{p_d}{p_u}\right)\left(\frac{p_d}{p_u}+\frac{\gamma+1}{\gamma-1}\right)^{-1} \\ u_s &= \left(\frac{\gamma-1}{2\gamma}+\frac{\gamma+1}{2\gamma}\frac{p_d}{p_u}\right)^{1/2} \end{aligned}$$

where u_s is the shock speed relative to the rest frame in the downstream region. The following figure shows two snapshot of a square shock propagating using the above initial conditions and a Lax-Wendroff method for the initial solution in the FCT scheme.



The program for shock propagation can be found on the class web page and is named `shock1.f`. It uses an input file `shock.dat` and an include file `shin`. The program solves the fluid equations

as specified at the beginning of this chapter and uses the normalization discussed above. The program also allows to choose between the Lax-Wendroff, Leapfrog, and MacCormack's methods. These methods can be used with or without FCT and there is a choice between 3 different initial configurations. All cases use periodic boundary conditions.

10.3 MHD Simulation

MHD Equations:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\nabla \cdot \rho \mathbf{u} \\
\frac{\partial \rho \mathbf{u}}{\partial t} &= -\nabla \cdot \left[\rho \mathbf{u}\mathbf{u} + \left(p + \frac{1}{2\mu_0} B^2 \right) \mathbf{1} - \frac{1}{\mu_0} \mathbf{B}\mathbf{B} \right] \\
\frac{\partial \mathbf{B}}{\partial t} &= \nabla \times [\mathbf{u} \times \mathbf{B} - \eta \mathbf{j}] \\
\frac{\partial w}{\partial t} &= -\nabla \cdot \left[\mathbf{u} \cdot \left(w + \left(p + \frac{1}{2\mu_0} B^2 \right) \right) - \frac{1}{\mu_0} (\mathbf{u} \cdot \mathbf{B}) \mathbf{B} + \eta \mathbf{j} \times \mathbf{B} \right]
\end{aligned}$$

with the electric field $\mathbf{E} = -\mathbf{u} \times \mathbf{B} + \eta \mathbf{j}$, the current density $\mu_0 \mathbf{j} = \nabla \times \mathbf{B}$ and with total energy density

$$w = \frac{1}{2} \rho u^2 + \frac{1}{2\mu_0} B^2 + \frac{p}{\gamma - 1}$$

and $\gamma = 5/3$. Intrinsic phase/group velocities: Speed of sound $c_s = \sqrt{\gamma p / \rho}$, Alfven speed $v_A = B/\sqrt{\mu_0 \rho}$, and fast mode speed $c_f = \sqrt{c_s^2 + v_A^2}$. Helpfull dimensionless parameter: plasma β

$$\beta = \frac{p_{th}}{p_B} = \frac{2\mu_0 p}{B^2} = \frac{2}{\gamma} \frac{c_s^2}{v_A^2}$$

Normalization

The MHD equations are normalized to typical values for a system, i.e.:

$$\begin{array}{ccc}
B = B_0 \widehat{B} & \rho = \rho_0 \widehat{\rho} & \mathbf{u} = u_0 \widehat{\mathbf{u}} \\
\mathbf{r} = l_0 \widehat{\mathbf{r}} & \nabla = \frac{1}{l_0} \widehat{\nabla} & t = \tau_0 \widehat{t} \\
p = p_0 \widehat{p} & \mathbf{j} = j_0 \widehat{\mathbf{j}} & \mathbf{E} = E_0 \mathbf{E}
\end{array}$$

Substitution into the MHD equations specifies the normalization values to yield a new set of equations for the normalized quantities. With

$$\begin{array}{ccc}
u_0 = v_A = B_0/\sqrt{\mu_0 \rho_0} & p_0 = B_0^2/(2\mu_0) & E_0 = v_A B_0 \\
\tau_0 = \tau_A = l_0/v_A & j_0 = B_0/(\mu_0 l_0) & \\
\widehat{\eta} = \eta/(\mu_0 l_0 v_A) & \widehat{\nu} = \nu \tau_A / l_0^2 &
\end{array}$$

In the following we omit the hat such that all quantities are assumed normalized!

Full set of normalized MHD Equations:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\nabla \cdot \rho \mathbf{u} \\
\frac{\partial \rho \mathbf{u}}{\partial t} &= -\nabla \cdot \left[\rho \mathbf{u}\mathbf{u} + \frac{1}{2}\left(p + B^2\right)\mathbf{1} - \mathbf{B}\mathbf{B} \right] \\
\frac{\partial \mathbf{B}}{\partial t} &= \nabla \times \left[\mathbf{u} \times \mathbf{B} - \eta \mathbf{j} \right] \\
\frac{\partial w}{\partial t} &= -\nabla \cdot \left[\mathbf{u} \cdot \left(w + \frac{1}{2}\left(p + B^2\right) \right) - \left(\mathbf{u} \cdot \mathbf{B}\right)\mathbf{B} + \eta \mathbf{j} \times \mathbf{B} \right]
\end{aligned}$$

with total energy density

$$w = \frac{1}{2}\rho u^2 + \frac{1}{2}B^2 + \frac{p}{2\left(\gamma - 1\right)}$$

Alternative versions of the energy equation using temperature $T = p/\rho$ and (i) thermal pressure$p$ (ii) $h = (p/2)^{1/\gamma}$, (iii) $R = T^{1/(\gamma-1)}$, (iv) local entropy $S = p/\rho^{\gamma}$:

$$\begin{aligned}
\frac{\partial p}{\partial t} &= -\nabla \cdot p\mathbf{u} - \left(\gamma - 1\right) p \nabla \cdot \mathbf{u} + 2\left(\gamma - 1\right)\eta \mathbf{j}^2 \\
\frac{\partial h}{\partial t} &= -\nabla \cdot h\mathbf{u} + \frac{\gamma - 1}{\gamma} h^{1-\gamma} \eta \mathbf{j}^2 \\
\frac{\partial R}{\partial t} &= -\nabla \cdot R\mathbf{u} + 2\frac{R}{p}\eta \mathbf{j}^2 \\
\frac{\partial S}{\partial t} + \mathbf{u} \cdot \nabla S &= \left(\gamma - 1\right)\frac{2\eta \mathbf{j}^2}{\rho^{\gamma}}
\end{aligned}$$

Example: Continuity Equation

$$\frac{\partial n}{\partial t} = -\frac{\partial nu}{\partial x} + \nu \frac{\partial^2 n}{\partial x^2}$$

Here the diffusion term can either represent physical density diffusion or as in the code is used to a diffusion term to balance numerical dispersion and the resulting grid oscillations.

Discretization: with $d_x = 1/\left(2\Delta x\right)$, $D_t = 2\Delta t$, $d_x^2 = 1/\Delta x^2$

$$\frac{n_i^+ - n_i^-}{2\Delta t} = -d_x\left((nu)_{i+1}^0 - (nu)_{i-1}^0 \right) + \nu d_x^2 \left(n_{i+1}^0 + n_{i-1}^0 - n_i^+ - n_i^- \right)$$

$$\left(1+\nu D_t d_x^2\right) n_i^+ = n_i^- \left(1+\nu D_t d_x^2\right) - D_t d_x \left((nu)_{i+1}^0 - (nu)_{i-1}^0\right) + \nu D_t d_x^2 \left(n_{i+1}^0 + n_{i-1}^0 - 2n_i^-\right)$$

$$\begin{aligned}
n_i^+ &= n_i^- - \frac{D_t d_x}{(1+\nu D_t d_x^2)} \left((nu)_{i+1}^0 - (nu)_{i-1}^0\right) + \frac{\nu D_t d_x^2}{(1+\nu D_t d_x^2)} \left(n_{i+1}^0 + n_{i-1}^0 - 2n_i^-\right) \\
&= n_i^- - \frac{D_t d_x \left(1+\nu D_t d_x^2\right) - D_t d_x \nu D_t d_x^2}{(1+\nu D_t d_x^2)} \left((nu)_{i+1}^0 - (nu)_{i-1}^0\right) \\
&\qquad + \frac{\nu D_t d_x^2}{(1+\nu D_t d_x^2)} \left(n_{i+1}^0 + n_{i-1}^0 - 2n_i^-\right) \\
&= n_i^- - D_t d_x \left((nu)_{i+1}^0 - (nu)_{i-1}^0\right) + \frac{\nu D_t d_x^2}{(1+\nu D_t d_x^2)} D_t d_x \left((nu)_{i+1}^0 - (nu)_{i-1}^0\right) \\
&\qquad + \frac{\nu D_t d_x^2}{(1+\nu D_t d_x^2)} \left(n_{i+1}^0 + n_{i-1}^0 - 2n_i^-\right)
\end{aligned}$$

In terms of fluxes:

$$\begin{aligned}
n_i^+ &= n_i^- - (1-\lambda) F_i^0 + \lambda H_i \\
&\text{with} \\
F_i^0 &= D_t d_x \left((nu)_{i+1}^0 - (nu)_{i-1}^0\right) \\
H_i &= \left(n_{i+1}^0 + n_{i-1}^0 - 2n_i^-\right) \\
\lambda &= \frac{\nu D_t d_x^2}{(1+\nu D_t d_x^2)}
\end{aligned}$$

Here we can again define a parameter $s = \nu D_t d_x^2 = 2\nu\Delta t/\Delta x^2$ (similar to the simple diffusion equation). We can interpret $\nu_{grid} = \nu D_t d_x^2$ as a grid diffusivity/viscosity, used for the damping of grid oscillations. An efficient diffusion on the gridscale requires $s \approx 1$ such that a good choice to avoid strong grid oscillations is $\nu \approx 1/D_t d_x^2 = \Delta x^2/2\Delta t$. Note, in general the grid is nonuniform, and in the provided MHD program this type of diffusion is only applied to locations where grid oscillations occur.

The implementation of the other MHD equations is similar albeit a bit more tedious because the respective expressions for the fluxes involve more terms. Similar the to prior discussion of diffusion and convection any physical diffusion is implemented in the same manner as outlined for the continuity eqation. This also requires that the numerical diffusivity must be smaller than the physical diffusion. This particularly applies to the resisitivity in the magnetic field equation.

10.4 Particle simulation

Particle simulations are applied frequently in plasma or astrophysics but are also employed to investigate Brownian motion, diffusion and similar random walk problems to investigate diffusive

transport. In astrophysics particle motion is used to examine selfgravitating systems such that the force which governs stellar or interstellar dynamics is the gravitational force. In plasma physics the dominant forces are electromagnetic forces but there are some applications where electromagnetic and gravitational forces are important such as the dynamics of dusty material in planetary ring systems or charge particle motion in the magnetosphere of neutran stars or pulsars.

Most of these applications consider physical systems where the direct collisional interaction is either small or competes with the collective interaction through the forces. Typical are collisionless plasmas or astrophysical systems. A particle model is called selfconsistent if the collective interaction is important (see also sections 2.1 and 2.2) and considered in combination with the particle motion. However important insight can also be gained from the particle dynamics in the cases of prescribed forces (electric and magnetic field or gravity ususally addressed as test particle simulations. For instance, currents which are generated by typical particle drifts can be estimated by test particle simulation. Also the energization or acceleration of particles can be investigated by test particle simulations.

In terms of selfconsistent models in plasma physics two methods dominate these applications. A full electromagnetic particle simulation solves the full dynamics of electrons and ions in combination to evaluating the forces which arise from the charge and current distributions of all particles. The major constraint of the full particle simulations are the very small spatial scales (debye length, electron gyroradius, plasma skin depth) and the extremely short time scales (plasma period, electron gyro-frequency). These spatial and temporal scales imply very large numbers of spatial grid cells and time steps to solve fully kinetic problems. This implies particularly small integration domains and temporal scale in three spatial dimensions. It also limits applications of full elctrodynamic particle simulations.

The second method is the so-called hybrid simulation. This model solves only the ion dynamics of the particle motion while electrons are treated as a neutralizing fluid. Electron continuity (number density) is determined by charge neutrality and the electron equation of motion is equivalent to Ohm's law where terms such as the Hall term and or electron pressure can be considered. The strength of hybrid simulation is the resolution of ion kinetics which provides insight into various non-MHD effects such as ion-cylclotron waves, gyro-viscosity, or the ion physics of shocks. Questions such as stability and accuracy are somewhat difficult in full particle or hybrid simulations. For instance, a sufficient resolution of the Debye scale through the particle distribution is important because an insufficient resolution does not provide the basic plasma oscillations.

This section will focus on the solution of the Lorentz equation of motion in the presence of electric amd magnetic fields. Therefore also concepts regarding stability or accuracy are exclusively applied to the method to solve the particle motion. This is sufficient in the case of test particle simulations and a necessary requirement for all particle simulations. The basic equations for particle motion in a plasma are:

Lorentz equations of motion

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i \tag{10.3}$$

$$\frac{d\mathbf{v}_i}{dt} = \frac{q_i}{m_i}\left(\mathbf{E}+\mathbf{v}\times\mathbf{B}\right)_{\mathbf{r_i},t}. \tag{10.4}$$

where i is the particle index. Similar to other models it is convenient to normalize the equations,

$$\begin{aligned}\frac{d\tilde{\mathbf{r}}}{d\tilde{t}} &= \frac{t_0}{L_0} v_0 \tilde{\mathbf{v}} \\ \frac{d\tilde{\mathbf{v}}}{d\tilde{t}} &= t_0 \frac{q}{m} B_0 \left(\frac{E_0}{v_0 B_0} \tilde{\mathbf{E}} + \tilde{\mathbf{v}} \times \tilde{\mathbf{B}} \right).\end{aligned}$$

where the normalization depends on the application. Here the typical gyrofrequency is $\omega_{c0} = |q| B_0/m$, such that the natural choice for the timescale is $t_0 = t_{c0} = 1/\omega_{c0}$ (note that the lorentz force can be positive or negative depending on the particle charge). This also implies the natural electric field normalization $E_0 = v_0 B_0$ and $L_0 = v_0/\omega_{c0}$ which represents the gyro-radius of a particle with velocity v_0. The normalization of velocity can be to any typical velocity such as a thermal speed or the Alfven speed of a plasma. Note that in this normalization the value of $\tilde{B}$The normalized equation thus become

$$\begin{aligned}\frac{d\tilde{\mathbf{r}}}{d\tilde{t}} &= \tilde{\mathbf{v}} \\ \frac{d\tilde{\mathbf{v}}}{d\tilde{t}} &= s_q \left(\tilde{\mathbf{E}}(\tilde{\mathbf{r}}, t) + \tilde{\mathbf{v}} \times \tilde{\mathbf{B}}(\tilde{\mathbf{r}}, t) \right) \qquad \text{with} \qquad s_q = \operatorname{sign}(q).\end{aligned}$$

In the following we omit the tilde to indicate normalized quatities. The equation are just a set of ordinary differential equations and typical solution methods are the same as for many other sets of first order ordinary differential equations of the form

$$\frac{dx}{dt} = f(x,t)$$

where x is representative of the velocity. We will further assume that the the explit time dependence of the force term is negligible. The following examples are found in the book by Hockney and Eastwood (1988):

General force - 'Leapfrog method' (note although there is some similarity this is different from Leapfrog in the PDE case):

$$\begin{aligned}\mathbf{x}^{n+1} - \mathbf{x}^n &= \Delta t \mathbf{v}^{n+1/2} \\ \mathbf{v}^{n+1/2} - \mathbf{v}^{n-1/2} &= \Delta t \mathbf{F}^n\end{aligned}$$

Lorentz force integrator for the equations:

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \qquad \frac{d\mathbf{v}}{dt} = \mathbf{v} \times \Omega$$

Second order implicit for constant magnetic field:

$$\begin{aligned}\mathbf{x}^{n+1}-\mathbf{x}^{n} &= \Delta t\,\mathbf{v}^{n+1/2}\\ \mathbf{v}^{n+1/2}-\mathbf{v}^{n-1/2} &= \frac{\Delta t}{2}\left(\mathbf{v}^{n+1/2}+\mathbf{v}^{n-1/2}\right)\times\Omega^{n}\end{aligned}$$

unconditionally stable and energy conservation! Relation between gyro-frequency Ω and numerical gyro-frequency ω

$$\tan\frac{\Delta t\,\omega}{2}=\pm\frac{\Delta t\,\Omega}{2}$$

and similarly for the gyro-radius

$$R'=\frac{|\mathbf{v}|}{\Omega}\sec\frac{\Delta t\,\omega}{2}$$

generalization to a spatially varying electric and magnetic field:

$$\begin{aligned}\mathbf{x}^{n+1}-\mathbf{x}^{n} &= \Delta t\,\mathbf{v}^{n+1/2}\\ \mathbf{v}^{n+1/2}-\mathbf{v}^{n-1/2} &= \Delta t\mathbf{E}^{n}+\frac{\Delta t}{2}\left(\mathbf{v}^{n+1/2}+\mathbf{v}^{n-1/2}\right)\times\Omega^{n}\end{aligned}$$

where the component parallel to $\mathbf{B}$ is the simple Leapfrog integration and the components perpendicular are the Lorentz force integrator scheme and unconditionally stable. For large time steps the above integration just approximate the $\mathbf{E}\times\mathbf{B}$ drift which can easily be shown by taking the cross product of the equation with Ω^{n}.

The discretization can be split into a three step process (goal to solve the implicit $\mathbf{v}^{n+1/2}$ term) by

$$\begin{aligned}\mathbf{v}_1^{*} &= \mathbf{v}^{n-1/2}+\frac{\Delta t}{2}\mathbf{E}^{n}\\ \mathbf{v}_2^{*} &= \mathbf{v}_1^{*}+\frac{\Delta t}{2}\left(\mathbf{v}_2^{*}+\mathbf{v}_1^{*}\right)\times\Omega^{n}\\ \mathbf{v}^{n+1/2} &= \mathbf{v}_2^{*}+\frac{\Delta t}{2}\mathbf{E}^{n}\end{aligned}$$

Where the second equation can be solved for $\mathbf{v}_2^{*}$ by taking the cross product with Ω^{n}

$$\begin{aligned}\mathbf{v}_2^{*} &= \mathbf{v}_1^{*}+\frac{2}{1+\left(\frac{\Omega\Delta t}{2}\right)^{2}}\mathbf{v}_3^{*}\times\Omega^{n}\\ \text{with}\qquad \mathbf{v}_3^{*} &= \mathbf{v}_1^{*}+\frac{\Delta t}{2}\mathbf{v}_1^{*}\times\Omega^{n}\end{aligned}$$

Actual implementation with $\delta = q\Delta_t/(2m)$

1st. step:

$$\mathbf{u} = \mathbf{v}^k + \delta\mathbf{E}$$

2nd step:

$$\mathbf{w} = \mathbf{u}\left(1-\delta^2B^2\right) + 2\delta\mathbf{u}\times\mathbf{B} + 2\delta^2\left(\mathbf{u}\cdot\mathbf{B}\right)\mathbf{B}$$

3rd step:

$$\mathbf{v}^{k+1} = \mathbf{w}/\left(1+\delta^2B^2\right) + \delta\mathbf{E}$$

Evaluating parallel and perpendicular energy (combining theses steps):

$$\begin{aligned}
\mathbf{v}_{k+1,\parallel} &= \mathbf{v}_{k,\parallel} + 2\delta\mathbf{E}_\parallel \\
\mathbf{v}^2_{k+1,\perp} &= \mathbf{v}^2_{k,\perp} + \left[4\delta\mathbf{E}_\perp\cdot\mathbf{v}_{k,\perp} + 4\delta^2\mathbf{E}_\perp\cdot\left(\mathbf{E}_\perp + \mathbf{v}_{k,\perp}\times\mathbf{B}\right)\right]/\left(1+\delta^2B^2\right) \\
&= \mathbf{v}^2_{k,\perp} + 4\delta\mathbf{E}_\perp\cdot\mathbf{v}_{k,\perp}/\left(1+\delta^2B^2\right)
\end{aligned}$$

which is exactly what is expected if there is an average drift (caused by gradients or curvature of the magnetic field). Other tests are the conservation of the magnetic moment and the socalled drift kinetcs (i.e., test the gradient and curvature drifts of charged particles).

Note that one can correct for the gyrofrequency by separating parallel and perpendicular velocities. The perpendicular velocity equation can be manipulated to read

$$\mathbf{v}_\perp^{n+1/2} - \mathbf{v}_\perp^{n-1/2} = \alpha\left[\Delta t\mathbf{E}_\perp^n + \frac{\Delta t}{2}\left(\mathbf{v}_\perp^{n+1/2} + \mathbf{v}_\perp^{n-1/2}\right)\times\Omega^n\right]$$

with

$$\alpha = \left(\tan\frac{\Delta t\,\omega}{2}\right)/\left(\frac{\Delta t\,\Omega}{2}\right)$$

Expansion methods

$$\frac{dx}{dt} = f(x,t)$$

Easiset approximation is through a Taylor expansion of $x(t)$ with

$$\begin{aligned}
x(t_{i+1}) &= x(t_i+s) = x(t_i) + s\left[\frac{dx}{dt}(t_i) + .. + \frac{d^n}{dt^n}x(t_i)\frac{s^{n-1}}{n!}\right] + O\left(s^{n+1}\right) \\
&= x(t_i) + s\left[f(x_i,t_i) + .. + \frac{d^{n-1}}{dt^{n-1}}f(x_i,t_i)\frac{s^{n-1}}{n!}\right] + O\left(s^{n+1}\right)
\end{aligned}$$

requires the higher derivatives of f.

Runge-Kutta similar but do not require the explicit evaluation of derivatives of $f(x,t)$, but rather use linear combinations of $f(x,t)$to evaluate $x(t)$. The linear combination is than compared to the Taylor series expansion to determine the coefficients of the linear combination. Example: Match

$$\begin{array}{lll} x_{i+1} & = & x_i + s\left[a_1 f(x_i,t_i) + a_2 f(\tilde{x}_i,\tilde{t}_i)\right] \\ and & & \tilde{t}_i = t_i + sb_1 \qquad \tilde{x}_i = x_i + b_2 s f(x_i,t_i) \end{array} \tag{10.5}$$

with the expansion

$$x(t_{i+1}) = x(t_i) + s\left[f(x_i,t_i) + \frac{d}{dt}f(x_i,t_i)\frac{s}{2} + \frac{d^2}{dt^2}f(x_i,t_i)\frac{s^2}{6} + ..\right]. \tag{10.6}$$

Expansion of (10.5):

$$\begin{array}{rcl} T_{rk} & = & a_1 f(x_i,t_i) + a_2 f(x_i + b_2 s f, t_i + sb_1) \\ & = & (a_1+a_2) f + a_2 s\left(b_2 f f_x + b_1 f_t\right) + \frac{a_2 s^2}{2}\left(b_2^2 f^2 f_x^2 + 2b_1 b_2 f f_{tx} + b_1^2 f_{tt}\right) \end{array}$$

and (10.6):

$$\begin{array}{rcl} T_t & = & f(x_i,t_i) + \frac{s}{2}\frac{d}{dt}f(x_i,t_i) + \frac{s^2}{6}\frac{d^2}{dt^2}f(x_i,t_i) + O\left(s^3\right) \\ & = & f + \frac{s}{2}\left(f f_x + f_t\right) + \frac{s^2}{6}\left(f^2 f_{xx} + 2 f f_{tx} + f_{tt} + f_t f_x + f f_x^2\right) + O\left(s^3\right) \end{array}$$

Comparing coefficients:

$$\begin{array}{ll} s^0: & a_1 + a_2 = 1 \\ s^1: & a_2 b_2 = a_2 b_1 = \frac{1}{2} \end{array}$$

Defining $a_2 = c$ implies $a_1 = 1-c$ and $b_1 = b_2 = 1/2c$. Choosing for instance $c = 1$ (Euler-Cauchy method):

$$x_{i+1} = x_i + s f\left(x_i + \frac{s}{2} f(x_i,t_i), t_i + \frac{s}{2}\right)$$

or $c = 1/2$ (improved)

$$x_{i+1} = x_i + s\left[\frac{1}{2}f(x_i,t_i) + \frac{1}{2}f(x_i + sf(x_i,t_i), t_i + s)\right]$$

Higher order Runge-Kutta example (classic 4th order)

$$\begin{aligned} x_{i+1} &= x_i + \frac{s}{6}[K_1 + K_2 + K_3 + K_4] \\ K_1 &= f(x_i,t_i) \\ K_2 &= f\left(x_i + \frac{s}{2}K_1, t_i + \frac{s}{2}\right) \\ K_3 &= f\left(x_i + \frac{s}{2}K_2, t_i + \frac{s}{2}\right) \\ K_3 &= f(x_i + sK_3, t_i + s) \end{aligned}$$

Application to particle simulation with $d\mathbf{x}/dt = \mathbf{F}(\mathbf{x})$. There is no explicit time dependence in the force.

$$\begin{aligned} \mathbf{k}_1 &= \Delta t\mathbf{F}(\mathbf{x}^n) \\ \mathbf{k}_2 &= \Delta t\mathbf{F}\left(\mathbf{x}^n + \frac{1}{2}\mathbf{k}_1\right) \\ \mathbf{k}_3 &= \Delta t\mathbf{F}\left(\mathbf{x}^n + \frac{1}{2}\mathbf{k}_2\right) \\ \mathbf{k}_4 &= \Delta t\mathbf{F}(\mathbf{x}^n + \mathbf{k}_3) \\ \mathbf{x}^{n+1} &= \mathbf{x}^n + \frac{1}{6}(\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4) \end{aligned}$$

Properties:

- High accuracy,
- velocity and position at the same value in time,
- time step can be easily changed,
- smaller truncation error than the finite difference methods.

General question address conservation of particle properties ()energy, magnetic moment etc. Often reported that higher order Runge Kutta necessary. Main disadvantage is the higher need for storage and some sofisticated approach needed to save memory requirements.