Time-Splitting Method

Justification of the Time-Splitting Method for non-linear operators

Let $\mathcal{H}$ be a normed sub-vector space of smooth enough functions of $\mathcal{F}(\mathbb{R}^3, \mathbb{C})$, $f_0 \in \mathcal{H}$, A and B (not necessarily linear) operators $\mathcal{H} \longmapsto \mathcal{H}$.

We are looking for $f : t \in \mathbb{R} \longmapsto f(t) \in \mathcal{H}$, such that (writing f also for the function $(t, \mathbf{x}) \longmapsto f(t)(\mathbf{x})$):

$$\partial_t f = A(f) + B(f) \quad , \quad \text{and} \;\; f(0) = f_0 \tag{1}$$

We want to solve this numerically. So, for fixed t and small enough ϵ, we want an approximation of $f(t+\epsilon)$ as a function of $f(t)$. Let $f^{(1)}, f^{(2)}, f^{(3)} \in \mathcal{H}$ such that:

$$\begin{aligned} \partial_t f^{(1)} &= A(f^{(1)}) \quad , \quad f^{(1)}(0) = f(t) \\ \partial_t f^{(2)} &= B(f^{(2)}) \quad , \quad f^{(2)}(0) = f^{(1)}(\frac{\epsilon}{2}) \\ \partial_t f^{(3)} &= A(f^{(3)}) \quad , \quad f^{(3)}(0) = f^{(2)}(\epsilon) \end{aligned} \tag{2}$$

We are going to show that:

$$f(t+\epsilon) - f^{(3)}(\frac{\epsilon}{2}) \;=\; \mathcal{O}(\epsilon^3) \tag{3}$$

For $\mathbf{x} \in \mathbb{R}^3$, we define the functionals $A_{\mathbf{x}} : g \longmapsto A(g)(\mathbf{x}) \in \mathbb{C}$ and $B_{\mathbf{x}} : g \longmapsto B(g)(\mathbf{x}) \in \mathbb{C}$. We will assume that for all $\mathbf{x}$, $A_{\mathbf{x}}$ and $B_{\mathbf{x}}$ are smooth enough so that their functional derivatives exist and they can be Taylor-expanded to the 1$^{\text{st}}$ order:

$$F(g+\epsilon h) = F(g) + \int \mathrm{d}^3\mathbf{x} \frac{\delta F}{\delta f}\Big|_g (\mathbf{x}) \epsilon h(\mathbf{x}) + \mathcal{O}(\epsilon^2) \tag{4}$$

for $F = A_{\mathbf{x}}, B_{\mathbf{x}}$. It also follows that:

$$\frac{\mathrm{d}}{\mathrm{d}t} F(g(t)) = \int \mathrm{d}^3\mathbf{x} \frac{\delta F}{\delta f}\Big|_{g(t)} (\mathbf{x}) \;\partial_t g(t, \mathbf{x}) \tag{5}$$

Let $\mathbf{x}_0 \in \mathbb{R}^3$. We have:

$$f(t+\epsilon, \mathbf{x}_0) = f(t, \mathbf{x}_0) + \epsilon \partial_t f(t, \mathbf{x}_0) + \frac{\epsilon^2}{2} \partial_t^2 f(t, \mathbf{x}_0) + \mathcal{O}(\epsilon^3)$$

From (1) and using (5) we get:

$$\begin{aligned} f(t+\epsilon,\mathbf{x}_0) =& f(t,\mathbf{x}_0) \;+\; \epsilon(A_{\mathbf{x}_0}+B_{\mathbf{x}_0})(f(t)) \\ &+\frac{\epsilon^2}{2}\int \mathrm{d}^3\mathbf{x}\left[\frac{\delta A_{\mathbf{x}_0}}{\delta f}\Big|_{f(t)}(\mathbf{x})+\frac{\delta B_{\mathbf{x}_0}}{\delta f}\Big|_{f(t)}(\mathbf{x})\right]\;(A_{\mathbf{x}_0}+B_{\mathbf{x}_0})(f(t))(\mathbf{x})\;+\;\mathcal{O}(\epsilon^3) \end{aligned} \tag{6}$$

In the following we will drop the $\mathbf{x}_0$, keeping in mind that the equations have in fact the form of (6).

Let us now compute $f^{(3)}(\frac{\epsilon}{2})$. We will use (2), (4) and (5) and keep only 2$^{\text{nd}}$ order terms in ϵ at most.

$$\begin{aligned} f^{(3)}(\frac{\epsilon}{2}) &= f^{(3)}(0)+\epsilon\partial_t f^{(3)}(0)+\frac{\epsilon^2}{8}\partial_t^2 f^{(3)}(0)+\mathcal{O}(\epsilon^3) \\ &= f^{(3)}(0)+\frac{\epsilon}{2}A(f^{(3)}(0))+\frac{\epsilon^2}{8}\int\frac{\delta A}{\delta f}\Big|_{f^{(3)}(0)}A(f^{(3)}(0))\;+\;\mathcal{O}(\epsilon^3) \end{aligned}$$

We have $f^{(3)}(0)=f^{(2)}(\epsilon)=f^{(2)}(0)+\epsilon\partial_t f^{(2)}(0)+\frac{\epsilon^2}{2}\partial_t^2 f^{(2)}(0)+\mathcal{O}(\epsilon^3)$. So, Taylor-expanding:

$$\begin{aligned} f^{(3)}(\frac{\epsilon}{2}) &= f^{(2)}(0)+\epsilon\partial_t f^{(2)}(0)+\frac{\epsilon^2}{2}\partial_t^2 f^{(2)}(0)+\frac{\epsilon}{2}\left(A(f^{(2)}(0)+\int\frac{\delta A}{\delta f}\Big|_{f^{(2)}(0)}\epsilon\partial_t f^{(2)}(0)\right) \\ &\quad+\frac{\epsilon^2}{8}\int\frac{\delta A}{\delta f}\Big|_{f^{(2)}(0)}A(f^{(2)}(0))\;+\;\mathcal{O}(\epsilon^3) \\ &= f^{(2)}(0)+\epsilon\left[B(f^{(2)}(0)+\frac{1}{2}A(f^{(2)}(0)\right] \\ &\quad+\frac{\epsilon^2}{2}\left[\int\frac{\delta B}{\delta f}\Big|_{f^{(2)}(0)}B(f^{(2)}(0))+\int\frac{\delta A}{\delta f}\Big|_{f^{(2)}(0)}B(f^{(2)}(0))+\frac{1}{4}\int\frac{\delta A}{\delta f}\Big|_{f^{(2)}(0)}A(f^{(2)}(0))\right]\;+\;\mathcal{O}(\epsilon^3) \end{aligned}$$

Again we have $f^{(2)}(0)=f^{(1)}(\frac{\epsilon}{2})=f^{(1)}(0)+\frac{\epsilon}{2}\partial_t f^{(1)}(0)+\frac{\epsilon^2}{8}\partial_t^2 f^{(1)}(0)+\mathcal{O}(\epsilon^3)$, so:

$$\begin{aligned} f^{(3)}(\frac{\epsilon}{2}) &= f^{(1)}(0)+\frac{\epsilon}{2}\partial_t f^{(1)}(0)+\frac{\epsilon^2}{8}\partial_t^2 f^{(1)}(0) \\ &\quad+\epsilon\left(B(f^{(1)}(0))+\int\frac{\delta B}{\delta f}\Big|_{f^{(1)}(0)}\frac{\epsilon}{2}\partial_t f^{(1)}(0)+\frac{1}{2}A(f^{(1)}(0))+\frac{1}{2}\int\frac{\delta A}{\delta f}\Big|_{f^{(1)}(0)}\frac{\epsilon}{2}\partial_t f^{(1)}(0)\right) \\ &\quad+\frac{\epsilon^2}{2}\left(\int\frac{\delta B}{\delta f}\Big|_{f^{(1)}(0)}B(f^{(1)}(0))+\int\frac{\delta A}{\delta f}\Big|_{f^{(1)}(0)}B(f^{(1)}(0))+\frac{1}{4}\int\frac{\delta A}{\delta f}\Big|_{f^{(1)}(0)}A(f^{(1)}(0))\right)\;+\;\mathcal{O}(\epsilon^3) \end{aligned}$$

Gathering terms, we get:

$$\begin{aligned} f^{(3)}(\frac{\epsilon}{2}) =& f^{(1)}(0)\;+\;\epsilon(A+B)(f^{(1)}(0)) \\ &+\frac{\epsilon^2}{2}\int\left[\frac{\delta A}{\delta f}\Big|_{f^{(1)}(0)}+\frac{\delta B}{\delta f}\Big|_{f^{(1)}(0)}\right]\;(A+B)(f^{(1)}(0))\;+\;\mathcal{O}(\epsilon^3) \end{aligned} \tag{7}$$

Since $f^{(1)}(0)=f(t)$, we see that the expression is the same as (6). Hence we proved (3).