Time-Splitting Method

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

Let $\mathcal{H}$ be a 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 $(t, \mathbf{x}) \longmapsto f(t)(\mathbf{x})$):

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

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:

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

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

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

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 $\mathbf{x}_0$. But we should remember that the equations should be written as (6).

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

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

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:

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

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 it is the same as (6). Hence we proved (3).