Implicit Filon Methods for Highly Oscillating Problems and Controlled Qubits

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Abstract

We present a numerical methods tailored for Schrödinger equations with time dependent Hamiltonians and rapidly oscillating solutions, such as those arising in the modeling of controlled qudits. Our method discretizes the Picard form of the ordinary differential equation (ODE) by Filon quadrature. The method is implicit but the size of the linear system is always the dimension of the ODE independent of order. We illustrate that the new method is superior to the classic RK4 method.

Keywords: Filon quadrature, highly oscillatory, quantum computing, qubit

1 Introduction

The Picard form of the ODE

$$\frac{\mathrm{d}v(t)}{\mathrm{d}t} = F(t, v(t)), \quad v(0) = u_0, \quad 0 \le t \le \Delta t,$$

is

$$v(t) = u_0 + \int_0^{\Delta t} F(t, v(t))\mathrm{d}t. \tag{1}$$

We assume that f is smooth, and that the components in the right hand side will be highly oscillatory and best approximated by methods for integrals of the type

$$I_\omega[f] = \int_{-1}^{1} f(x)e^{i\omega x}\mathrm{d}x. \tag{2}$$

In particular our implicit Filon method approximates the solution $v(t_n)$ by replacing the integral in (1) by Filon quadrature , [1]. This results in schemes in the form

$$u_{n+1} = u_n + \Delta t \sum_{k=0}^{1}\sum_{l=0}^{m} b_{k,l} f^{(l)}(t_{n+k}, u_{n+k}).$$

The ω dependent weights of the Filon quadrature for (2) are found by insisting that the quadrature is exact for

$$\mathcal{F}_\omega^m = \int_{-1}^{1} p(x)e^{i\omega x}\mathrm{d}x,$$

where $p(x)$ is the unique degree $2m+1$ Hermite interpolation polynomial such that $p^{(l)}(\pm 1) = f^{(l)}(\pm 1)$, $l = 0, \ldots, m$.

Assuming $\omega \gg 1$, integration by parts

$$\begin{aligned}\mathcal{F}_\omega^m[f] - I_\omega[f] &= \int_{-1}^{1} (p(x) - f(x))e^{i\omega x}\mathrm{d}x \\ &= -\sum_{k=0}^{\infty} \frac{\left[(p^{(k)}(x) - f^{(k)}(x))e^{i\omega x}\right]_{-1}^{1}}{(-i\omega)^{k+1}} \\ &= \frac{1}{(-i\omega)^{m+1}} I_\omega[(p-f)^{(m+1)}]\end{aligned}$$

reveals that the error of this method is $O(\omega^{-m-2})$. As for all high frequency methods the error *decrease* as $\omega \to \infty$. But in the limit of $\omega \to 0$, spectacularly the approximation becomes $\mathcal{F}_\omega^m = \int_{-1}^{1} p(x)\mathrm{d}x \approx \int_{-1}^{1} f(x)\mathrm{d}x$, so that $\mathcal{F}_\omega^m$ becomes the Birkhoff-Hermite quadrature [2] and our implicit Filon methods resemble Hagstrom's Hermite-in-time methods [3].

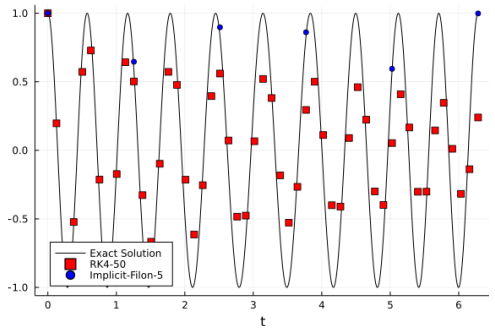

Figure 1: Comparison of implicit Filon method and the 4th order accurate RK method.

2 Examples of the Implicit Filon Method

Consider the ODE

$$\frac{\mathrm{d}v}{\mathrm{d}t} = (\lambda + ig(t))v, \; v(0) = u_0, \; 0 \le t \le \Delta t, \tag{3}$$

where $\lambda \in \mathbb{C}$ and $g(t)$ is smooth. Generally dv/dt is not in the form $f(t)e^{i\omega t}$, so we rewrite

$$\frac{\mathrm{d}v(t)}{\mathrm{d}t} = f(t)e^{i\omega t}, \; f(t, v(t)) \equiv (\lambda + ig(t))v(t)e^{-i\omega t}.$$

Here, the assumption is that f oscillates over a larger timescale than v, and that it is easier to discretize f than v.

As $f(t, v(t))$ depends on $v(t)$, the quantities $f^{(l)}(t_{n+1}, u_{n+1})$, $l = 0, \ldots, m$ in the approximation are defined implicitly. If we set $q(t) \equiv (\lambda + ig(t))$, and $r(t) \equiv e^{-i\omega t}$, so that $f(t) = q(t)r(t)v(t)$, then the chain rule gives $f'(t) = (q(t)r(t))'v(t) + (q(t)r(t))v'(t)$. Thus, this relation together with the ODE (3) recursively defines the derivatives of f in terms of u_{n+1} alone.

For example, if we consider the Dahlquist equation (when $g(t) = 0$) the 4th order Filon method can be expressed as

$$S_+(\omega, \Delta t, \lambda)u_{n+1} = S_-(\omega, \Delta t, \lambda)u_n,$$

$$S_+ = 1 - \frac{\Delta t}{2} e^{-i\frac{\omega \Delta t}{2}} \left(\lambda b_{2,0} + \frac{\Delta t}{2}(\lambda^2 - i\omega\lambda) b_{2,1} \right),$$
$$S_- = 1 + \frac{\Delta t}{2} e^{i\frac{\omega \Delta t}{2}} \left(\lambda b_{1,0} + \frac{\Delta t}{2}(\lambda^2 - i\omega\lambda) b_{1,1} \right).$$

Note that here all the quadrature weights are evaluated at $\omega\frac{\Delta t}{2}$.

The stability of the method is governed by the absolute value of $Q = S_-/S_+$. At the time of writing we have not been able to prove that this quantity is always less than unity in the left half of the complex plane but in Figure 2 we display contours of $|Q|$ for $\omega\Delta t/2 = 0$ and 35. In both cases it appears that the method is A-stable. In addition, from [3] we know that

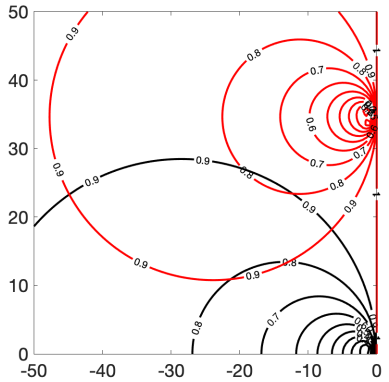

Figure 2: Contours for the stability function Q for $\omega = 0$ (black contours) and $\omega\Delta t/2 = 35$ (red countours). The x and y axis correspond to the real and imaginary parts of $\lambda\Delta t/2$.

the methods are A-stable in the limit $\omega \to 0$.

A comparison between solutions obtained with the 4-th order implicit Filon and the classic fourth order Runge-Kutta method (RK4) for the case $\lambda = i\omega = i10$ and $g(t) = \cos(t)$ is provided in Figure 1. The implicit Filon method achieves a relative error 6.1×10^{-2} using **five time steps**, while RK4 does not achieve a single digit of precision using 50 time steps.

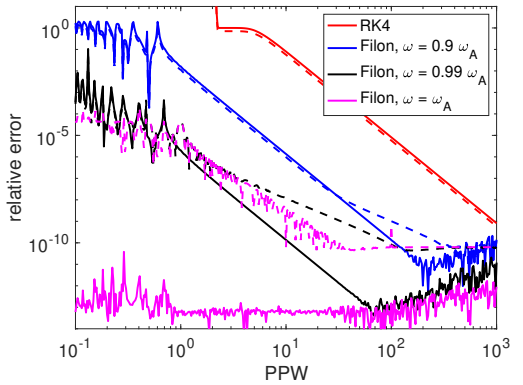

Figure 3: Errors for the qubit example and (3) as a function of points-per-wavelength.

3 Application to Controlled Qubit

A controlled qubit can be modeled by the Schrödinger equation

$$\frac{d\mathbf{u}(t)}{dt} = -i \left(\begin{bmatrix} 0 & 0 \\ 0 & \omega_{\mathrm{A}} \end{bmatrix} + g_{\mathrm{c}}(t) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right) \mathbf{u}(t),$$

where $\mathbf{u}$ is the state vector and $g_{\mathrm{c}}(t)$ is the control. Here we can apply the Filon quadrature component-wise, using $\omega = 0$ in the first component and $\omega = \omega_{\mathrm{A}}$ in the second component. With these choices and with $\omega_{\mathrm{A}} = 10^6$ and $g_c(t) = \cos(t)$, we evolve the qubit until time $10 \times 2\pi/\omega_{\mathrm{A}}$. In Figure 3 we display (in dashed lines) the errors at the final time as a function of the points per wavelength. We display results using $\omega = \omega_{\mathrm{A}}, 0.99\omega_{\mathrm{A}}$, and $0.9\omega_{\mathrm{A}}$ in the second component and, as a reference, we also display the errors using RK4. In the same figure in solid lines we display the errors for the scalar problem (3) with $g(t) = g_{\mathrm{c}}(t)$ and $\lambda = i\omega_{\mathrm{A}}$ and with the same choices of ω. The reference result for RK4 is also displayed. Clearly our method drastically outperforms RK4 in all cases.

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