Algorithmic Solution of High Order Partial Differential Equations in Julia via the Fokas Transform Method

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$*$ Equations of the form

$$f\left(x_1, \ldots, x_n, u, u_{x_1}, \ldots, u_{x_n}, u_{x_1 x_1}, \ldots, u_{x_1 x_n}, \ldots\right) = 0,$$

which relate an unknown function $u(x_1, \ldots, x_n)$ to its partial derivatives $u_{x_i \cdots x_j} := \frac{\partial}{\partial x_i} \cdots \frac{\partial}{\partial x_j} u$.

Algorithmic Solution of High Order Partial Differential Equations in Julia via the Fokas Transform Method*

* A method to solve a certain class of PDE problems algorithmically[1].

[1] Athanassios S. Fokas. *A Unified Approach to Boundary Value Problems*. Society for Industrial and Applied Mathematics, 2008. ISBN: 978-0-89871-651-1. DOI: 10.1137/1.9780898717068. URL: http://epubs.siam.org/doi/book/10.1137/1.9780898717068.

Algorithmic Solution of High Order Partial Differential Equations in Julia* via the Fokas Transform Method

* A free, open-source, high-performance language for numerical computing[2].

[2] *The Julia Language*. https://julialang.org/. URL: `https://julialang.org/` (visited on 03/19/2019).

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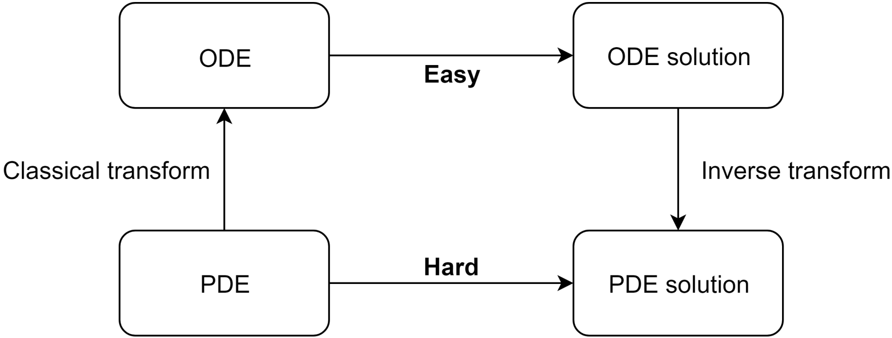
Motivation

- PDEs can model various physical phenomena. E.g.,
  - heat equation $u_t = K u_{xx}$
  - wave equation $u_{tt} = c^2(u_{xx} + u_{yy})$
  - (linear) Schrödinger equation $ihw_t + \frac{h}{2m} w_{xx} = 0$
- Problems involving PDEs are usually formulated as initial-boundary value problems (IBVPs), consisting of
  - a PDE in temporal and spatial variables defined over a domain,
  - boundary conditions, and
  - initial condition.

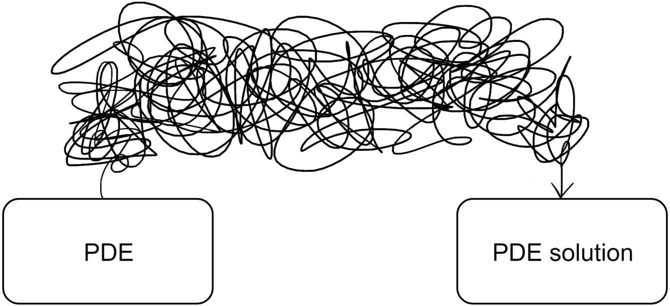
Motivation

- Some IBVPs can be solved using classical transform pairs, e.g., the Fourier transform.



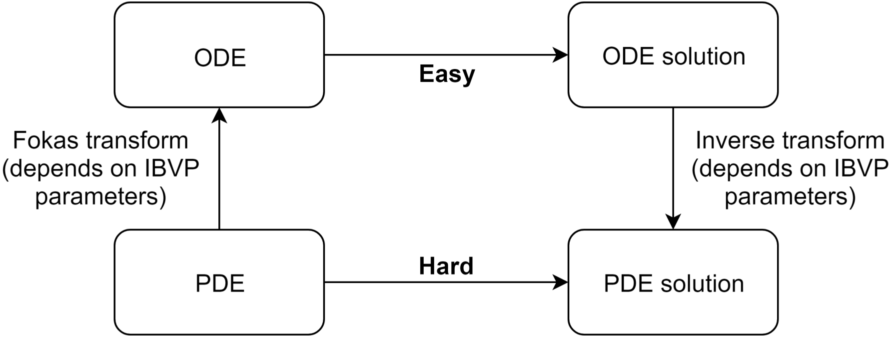
Motivation

- For more complicated IBVPs, no such classical transform pairs exist.
  - Resort to ad-hoc methods that are specific to the given IBVP.



Motivation

- The Fokas method extends the idea of classical transform pair to a class of complicated IBVPs by constructing transform pairs depending on the problems' parameters.
  - Even better, this class of IBVPs can have arbitrary spatial order.



Motivation

- The Fokas method advances the understanding of high order PDEs by providing an algorithmic procedure to solve an entire class of IBVPs of arbitrary spatial order.

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- However, it is still laborious to use the Fokas method by hand.

Thus, capstone:

> Implement the Fokas method[1] as a software library[2] that supplies various computer aid[3] in the process of solving IBVPs[4].

[1] This is the first time that the Fokas method is implemented computationally in any generality.

[2] In Julia: Open-source allows for checking correctness.

[3] Numeric and symbolic features.

[4] For this class of IBVPs, no other solver algorithm yet exists.

IBVPs solvable by the Fokas method

The Fokas method allows solving any well-posed IBVP of the form

$$
\begin{aligned}
(\partial_t + a(-i)^n \partial_x^n)\, q(x,t) &= 0 && \forall (x,t) \in (0,1)\times(0,T) && \text{(2.1a)}\\
q(x,0) &= f(x) \in \Phi && \forall x \in [0,1] && \text{(2.1b)}\\
q(\cdot,t) &\in \Phi && \forall t \in [0,T], && \text{(2.1c)}
\end{aligned}
$$

where

- $a \in \mathbb{C}$ (for the IBVP to be well-posed, we require at least that $a = \pm i$ if n is odd and $\mathrm{Re}(a) \geq 0$ if n is even),
- Φ is a set of functions that satisfy a set of homogeneous boundary conditions

  $$\Phi := \{\phi \in C^\infty[0,1] : \, B_j\phi = 0 \, \forall j \in \{1,2,\dots,n\}\},$$

  where B_j-s are boundary forms with boundary coefficients b_{jk}, $\beta_{jk} \in \mathbb{R}$,

  $$B_j\phi := \sum_{k=0}^{n-1} \left(b_{jk}\phi^{(k)}(0) + \beta_{jk}\phi^{(k)}(1) \right), \; j \in \{1,2,\dots,n\}.$$

IBVPs solvable by the Fokas method

E.g., the linearized Korteweg-de Vries (KdV) equations:

Problem 1

$$\begin{aligned} q_t(x,t) + q_{xxx}(x,t) &= 0, && (x,t) \in (0,1) \times (0,T) \\ q(x,0) &= f(x), && x \in [0,1] \\ q(0,t) = q(1,t) &= 0, && t \in [0,T] \\ 2q_x(1,t) &= q_x(0,t) && t \in [0,T]. \end{aligned}$$

Problem 2

$$\begin{aligned} q_t(x,t) + q_{xxx}(x,t) &= 0, && (x,t) \in (0,1) \times (0,T) \\ q(x,0) &= f(x), && x \in [0,1] \\ q(0,t) = q(1,t) = q_x(1,t) &= 0, && t \in [0,T]. \end{aligned}$$

Algorithm: Overview

Consider an IBVP of the form

$$
\begin{aligned}
(\partial_t + a(-i)^n \partial_x^n)\, q(x,t) &= 0 && \forall (x,t) \in (0,1) \times (0,T) \\
q(x,0) &= f(x) \in \Phi && \forall x \in [0,1] \\
q(\cdot,t) &\in \Phi && \forall t \in [0,T].
\end{aligned}
$$

$$
\begin{tikzcd}
\boxed{\begin{array}{c}(\partial_t + a\lambda^n)\hat{q}(\lambda,t) = 0 \\ \hat{q}(\lambda,0) \text{ known}\end{array}} \arrow[r, "\text{Solve}"] & \boxed{\hat{q}(\lambda,t) = e^{-a\lambda^n t} F_\lambda(f)} \arrow[d, "\text{Inverse transform } f_x"] \\
\boxed{\begin{array}{c}(\partial_t + a(-i)^n \partial_x^n) q(x,t) = 0 \\ q(x,0) = f(x) \in \Phi \\ q(\cdot,t) \in \Phi\end{array}} \arrow[u, "\text{Transform } F_\lambda"] \arrow[r, dashed] & \boxed{q(x,t) = f_x(e^{-a\lambda^n t} F_\lambda(f))}
\end{tikzcd}
$$

Algorithm: Overview

- Input: An IBVP of the form

$$
\begin{aligned}
(\partial_t + a(-i)^n \partial_x^n)\, q(x,t) &= 0 && \forall (x,t) \in (0,1)\times(0,T) \\
q(x,0) &= f(x) \in \Phi && \forall x \in [0,1] \\
q(\cdot,t) &\in \Phi && \forall t \in [0,T].
\end{aligned}
$$

- Construct adjoint boundary conditions of the spatial ordinary BVP.
- Using the spatial adjoint boundary conditions and other information about the IBVP, construct the Fokas transform pair F_λ and f_x.
- Output: Solution of the IBVP $q(x,t) = f_x(e^{-a\lambda^n t} F_\lambda(f))$.

Algorithm: Constructing adjoint boundary conditions

An algorithm to find adjoint boundary conditions is developed based on literature[3], which includes (among definitions of various relevant objects)

- a constructive existence theorem on the adjoint, and
- a theorem to check whether a candidate adjoint is indeed valid.

These results are expanded and adapted to an algorithm to construct valid adjoint boundary conditions.

[3] E. A. Coddington and N. Levinson. *Theory of Ordinary Differential Equations*. New York: McGraw-Hill Publishing, 1977, p. 429. ISBN: 9780070992566.

Algorithm: Constructing Fokas transform pair

Integrand construction

Let $b^\star, \beta^\star$ be the matrices associated with the adjoint boundary conditions. Let $\alpha := e^{2\pi i/n}$. For complex variable λ, define $n \times n$ matrices $W^+(\lambda)$, $W^-(\lambda)$ entry-wise by

$$W^+_{kj}(\lambda) := \sum_{r=0}^{n-1} (-i\alpha^{k-1}\lambda)^r b^\star_{jr}$$

$$W^-_{kj}(\lambda) := \sum_{r=0}^{n-1} (-i\alpha^{k-1}\lambda)^r \beta^\star_{jr}.$$

Define $n \times n$ matrix W entry-wise by

$$W_{kj}(\lambda) := W^+_{kj}(\lambda) + W^-_{kj}(\lambda) e^{-\alpha^{k-1}\lambda}.$$

Define

$$\Delta(\lambda) := \det W(\lambda).$$

Algorithm: Constructing Fokas transform pair

Integrand construction

Let X^{lj} be the $(n-1)\times(n-1)$ submatrix of the block matrix $\mathbb{W} := \begin{bmatrix} W & W \\ W & W \end{bmatrix}$, where X^{lj}_{11} is $\mathbb{W}_{l+1,j+1}$.

For $\lambda \in \mathbb{C}$ such that $\Delta(\lambda) \neq 0$, define the integrands

$$F^+_\lambda(f) := \frac{1}{2\pi\Delta(\lambda)} \sum_{j=1}^{n} \sum_{l=1}^{n} (-1)^{(n-1)(l+j)} \det X^{lj}(\lambda) W^+_{1j}(\lambda) \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\,dx$$

$$F^-_\lambda(f) := \frac{-e^{-i\lambda}}{2\pi\Delta(\lambda)} \sum_{j=1}^{n} \sum_{l=1}^{n} (-1)^{(n-1)(l+j)} \det X^{lj}(\lambda) W^-_{1j}(\lambda) \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\,dx.$$

Algorithm: Constructing Fokas transform pair

Contour construction

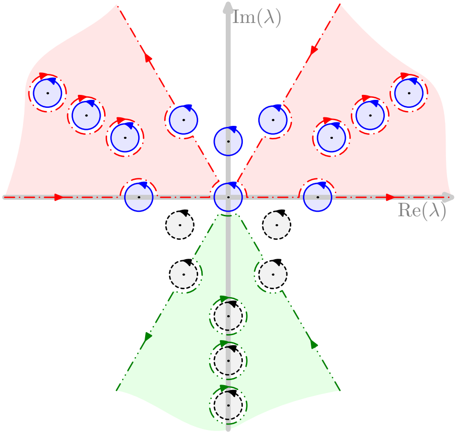
Define the contours

$$
\begin{aligned}
\Gamma_a^\pm &:= \partial\Big(\{\lambda \in \mathbb{C}^\pm : \operatorname{Re}(a\lambda^n) > 0\} \setminus \bigcup_{\substack{\sigma\in\mathbb{C};\\ \Delta(\sigma)=0}} D(\sigma, 2\epsilon)\Big) \\
\Gamma_a &:= \Gamma_a^+ \cup \Gamma_a^- \\
\Gamma_0^+ &:= \bigcup_{\substack{\sigma\in\operatorname{cl}\mathbb{C}^+;\\ \Delta(\sigma)=0}} C(\sigma, \epsilon) \\
\Gamma_0^- &:= \bigcup_{\substack{\sigma\in\mathbb{C}^-;\\ \Delta(\sigma)=0}} C(\sigma, \epsilon) \\
\Gamma_0 &:= \Gamma_0^+ \cup \Gamma_0^- \\
\Gamma &:= \Gamma_0 \cup \Gamma_a.
\end{aligned}
$$

Algorithm: Constructing Fokas transform pair

Contour construction

Sample contour drawn by hand[4]:

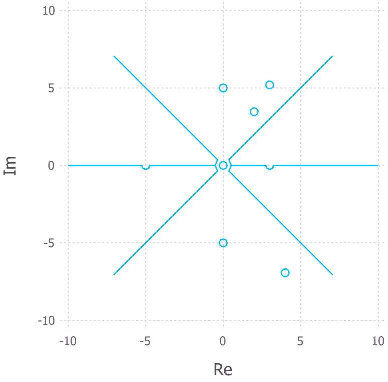


[4] David Andrew Smith and Athanassios S. Fokas. "Evolution PDEs and augmented eigenfunctions. Finite interval". In: *Journal of Spectral Theory* 6.1 (2013), pp. 185–213. ISSN: 1664-039X. DOI: 10.4171/JST/123. arXiv: 1303.2205. URL: `http://www.ems-ph.org/doi/10.4171/JST/123http://arxiv.org/abs/1303.2205`.

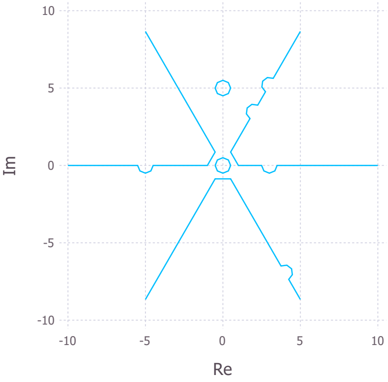
Algorithm: Constructing Fokas transform pair

Contour construction

Sample contours drawn by the implemented library[5]:



(a) $n = 2$, $a = 1$.



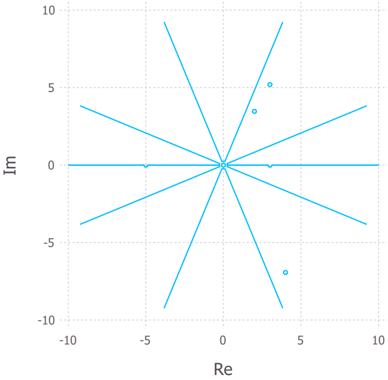
(b) $n = 3$, $a = -i$.

[5] Linfan Xiao. *Documentation of the implementation of the Fokas method*. URL: https://gitlab.com/linfanxiaolinda/capstone{_}repo/blob/master/work{_}in{_}julia/The{_}Fokas{_}method{_}documentation.ipynb.

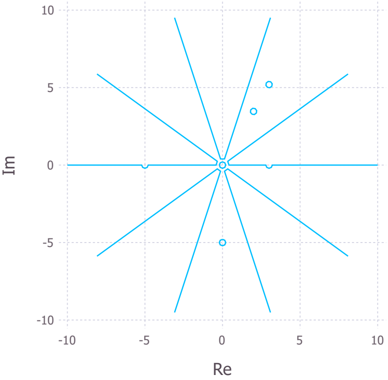
Algorithm: Constructing Fokas transform pair

Contour construction

Sample contours drawn by the implemented library[6]:



(a) $n = 4$, $a = 1$.



(b) $n = 5$, $a = -i$.

[6] Xiao, *Documentation of the implementation of the Fokas method*.

Algorithm: Constructing Fokas transform pair

Define the Fokas transform pair

$$F_\lambda : f(x) \mapsto F(\lambda) \quad F_\lambda(f) = \begin{cases} F_\lambda^+(f) & \text{if } \lambda \in \Gamma_0^+ \cup \Gamma_a^+, \\ F_\lambda^-(f) & \text{if } \lambda \in \Gamma_0^- \cup \Gamma_a^-, \end{cases}$$

$$f_x : F(\lambda) \mapsto f(x) \quad f_x(F) = \int_\Gamma e^{i\lambda x} F(\lambda)\, d\lambda,\ x \in [0,1].$$

Algorithm: IBVP solution

The solution to the IBVP is given by

$$
\begin{aligned}
q(x,t) &= f_x\left(e^{-a\lambda^n t} F_\lambda(f)\right) \\
&= \int_{\Gamma_0^+} e^{i\lambda x} e^{-a\lambda^n t} F_\lambda^+(f)\, d\lambda + \int_{\Gamma_a^+} e^{i\lambda x} e^{-a\lambda^n t} F_\lambda^+(f)\, d\lambda \\
&\quad + \int_{\Gamma_0^-} e^{i\lambda x} e^{-a\lambda^n t} F_\lambda^-(f)\, d\lambda + \int_{\Gamma_a^-} e^{i\lambda x} e^{-a\lambda^n t} F_\lambda^-(f)\, d\lambda.
\end{aligned}
$$

Sample usage: Solving IBVPs

IBVP formulation
Consider the IBVP

$$\begin{aligned} q_t - q_{xx} &= 0 && \forall (x,t) \in (0,1) \times (0,T) && \text{(4.1a)} \\ q(x,0) &= \sin(2\pi x) && \forall x \in [0,1] && \text{(4.1b)} \\ q(0,t) - q(1,t) &= 0 && \forall t \in [0,T] && \text{(4.1c)} \\ q_x(0,t) - q_x(1,t) &= 0 && \forall t \in [0,T]. && \text{(4.1d)} \end{aligned}$$

Rewriting the IBVP in the standard form, we have $n = 2$, $a = 1$,

$$\begin{aligned} B_1\phi &= 1 \cdot \varphi(0) + (-1) \cdot \varphi(1) + 0 \cdot \varphi^{(1)}(0) + 0 \cdot \varphi^{(1)}(1) \\ B_2\phi &= 0 \cdot \varphi(0) + 0 \cdot \varphi(1) + 1 \cdot \varphi^{(1)}(0) + (-1) \cdot \varphi^{(1)}(1), \end{aligned}$$

and

$$\Phi = \{\phi \in C^\infty[0,1] : \, B_j\phi = 0 \, \forall j \in \{1,2\}\}.$$

Sample usage: Solving IBVPs

Adjoint boundary conditions construction

The matrices associated with the spatial adjoint boundary conditions are

$$b^\star = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \beta^\star = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

Fokas transform pair construction

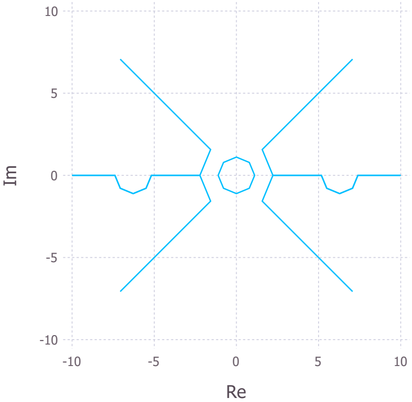
We compute the integrands $F_\lambda^+(f)$, $F_\lambda^-(f)$ to be

$$F_\lambda^+(f) = \frac{\left(\int_0^1 e^{i\lambda x} f(x)\,dx\right) e^{i\lambda}}{2\pi(e^{i\lambda}-1)}, \quad F_\lambda^-(f) = \frac{\int_0^1 e^{i\lambda x} f(x)\,dx}{2\pi(e^{i\lambda}-1)}.$$

Sample usage: Solving IBVPs

Fokas transform pair construction

We compute the contours to be:



IBVP solution

$q(x,t)$ can be evaluated at given (x_0, t_0) within 20s.

Sample usage: Symbolic features

- Applying the Fokas method requires two technical lemmas concerning the positions of the poles of the integrands F_λ^+, F_λ^- and their asymptotic behaviour[7].
- Thus, it is necessary to obtain symbolic formulas for the integrands.
- In the case of complicated integrands, it is of interest to derive their symbolic formulas using a computer.
- We verified that the library computes the correct symbolic formulas for F_λ^+, F_λ^- using the following two problems.

[7] Peter D. Miller and David A. Smith. "The diffusion equation with nonlocal data". In: *Journal of Mathematical Analysis and Applications* 466.2 (2017), pp. 1119–1143. DOI: 10.1016/j.jmaa.2018.05.064. arXiv: 1708.00972. URL: http://arxiv.org/abs/1708.00972.

Sample usage: Symbolic features

Problem 1

$$\begin{aligned} q_t(x,t) + q_{xxx}(x,t) &= 0, && (x,t) \in (0,1) \times (0,T) \\ q(x,0) &= f(x), && x \in [0,1] \\ q(0,t) &= 0 = q(1,t), && t \in [0,T] \\ 2q_x(1,t) &= q_x(0,t) && t \in [0,T], \end{aligned}$$

with

$$\begin{aligned} F_\lambda^+(f) &= \frac{1}{2\pi\Delta(\lambda)} \Big[\hat{f}(\lambda)(e^{i\lambda} + 2\alpha e^{-i\alpha\lambda} + 2\alpha^2 e^{-i\alpha^2\lambda}) + \hat{f}(\alpha\lambda)(\alpha e^{i\alpha\lambda} - 2\alpha e^{-i\lambda}) \\ &\quad + \hat{f}(\alpha^2\lambda)(\alpha^2 e^{i\alpha\lambda} - 2\alpha^2 e^{-i\lambda})\Big] \\ F_\lambda^-(f) &= \frac{e^{-i\lambda}}{2\pi\Delta(\lambda)} \Big[-\hat{f}(\lambda)(2 + \alpha^2 e^{-\alpha\lambda} + \alpha e^{-\alpha^2\lambda}) - \alpha\hat{f}(\alpha\lambda)(2 - e^{-i\alpha^2\lambda}) \\ &\quad - \alpha^2\hat{f}(\alpha^2\lambda)(2 - e^{-i\alpha\lambda})\Big], \end{aligned}$$

where $\Delta(\lambda) = e^{i\lambda} + \alpha e^{i\alpha\lambda} + \alpha^2 e^{i\alpha^2\lambda} + 2(e^{-i\lambda} + \alpha e^{-i\alpha\lambda} + \alpha^2 e^{-i\alpha^2\lambda})$ and $\hat{f}(\alpha^{l-1}\lambda) = \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\,dx$.

Sample usage: Symbolic features

Problem 2

$$
\begin{aligned}
q_t(x,t) + q_{xxx}(x,t) &= 0, && (x,t) \in (0,1)\times(0,T) \\
q(x,0) &= f(x), && x \in [0,1] \\
q(0,t) &= 0, && t \in [0,T] \\
q(1,t) &= 0 && t \in [0,T] \\
q_x(1,t) &= 0 && t \in [0,T],
\end{aligned}
$$

with

$$
\begin{aligned}
F_\lambda^+(f) &= \frac{1}{2\pi\Delta(\lambda)}\left[\hat{f}(\lambda)(\alpha e^{-\alpha\lambda} + \alpha^2 e^{-i\alpha^2\lambda}) - (\alpha\hat{f}(\alpha\lambda) + \alpha^2\hat{f}(\alpha^2\lambda))e^{-i\lambda}\right] \\
F_\lambda^-(f) &= \frac{e^{-i\lambda}}{2\pi\Delta(\lambda)}\left[-\hat{f}(\lambda) - \alpha\hat{f}(\alpha\lambda) - \alpha^2\hat{f}(\alpha^2\lambda)\right],
\end{aligned}
$$

where $\Delta(\lambda) = e^{-i\lambda} + \alpha e^{-i\alpha\lambda} + \alpha^2 e^{-i\alpha^2\lambda}$ and $\hat{f}(\alpha^{l-1}\lambda) = \int_0^1 e^{-i\alpha^{l-1}\lambda x} f(x)\,dx$.

Discussion

- Next step: Speed up
  - Measures have been taken to bring down computation time to a reasonable range (e.g., by replacing double integral with explicit formulas).
  - Yet to analyze the IBVP solution in-depth, evaluating it at a given (x_0, t_0) should take less than milliseconds to allow graphing.

- Idea: Develop a custom integrator tailored to the efficient evaluation of these contour integrals by exploiting the mathematical properties of the integrand and the contour.

Summary

- The Fokas method allows solving an entire class of IBVPs of arbitrary spatial order.
- A library has been developed in Julia to provide computer aid in the process of applying the Fokas method to solve IBVPs.
  - Functionalities of the library include symbolic formulas of important mathematical objects, their numeric representations, and contour visualization.
  - The library's code, unit tests, and documentations are available on a public GitLab repository[8].
- Looking ahead, in order to analyze the solution graphically, it is of interest to develop a custom integrator to bring the time it takes to evaluate the solution at a given point down to the order of milliseconds.

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[8] Xiao, *Documentation of the implementation of the Fokas method*.