Finding Zeros of Analytic Functions and Local Eigenvalue Analysis Using Contour Integral Method in Examples

Erika STRAKOVÁ[1], *Dalibor LUKÁŠ*[1,2], *Petr VODSTRČIL*[1]

[1]Department of Applied Mathematics, Faculty of Electrical Engineering and Computer Science, VŠB-Technical University of Ostrava
[2] IT4Innovations, VŠB-Technical University of Ostrava, 17. listopadu 15, 708 33 Ostrava-Poruba, Czech Republic

erika.strakova@vsb.cz, dalibor.lukas@vsb.cz, petr.vodstrcil@vsb.cz

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Abstract. *A numerical method for computing zeros of analytic complex functions is presented. It relies on Cauchy's residue theorem and the method of Newton's identities, which translates the problem to finding zeros of a polynomial. In order to stabilize the numerical algorithm, formal orthogonal polynomials are employed. At the end the method is adapted to finding eigenvalues of a matrix pencil in a bounded domain in the complex plane. This work is based on a series of papers of Professor Sakurai and collaborators. Our aim is to make their work available by means of a systematic study of properly chosen examples.*

Keywords

contour integral method, zeros of analytic functions, formal orthogonal polynomials, generalized eigenvalue problem

1. Introduction

We present a numerical method for computing zeros of an analytic complex function. The method is further extended to finding eigenvalues of a matrix pencil. This is an essential problem in many areas of engineering such as analysis of mechanical vibrations, electrical networks, optical waveguides, or in quantum chemistry to name a few. Apart from traditional algorithms, cf. [11], which often compute all eigenvalues and rely on costly diagonalization of the system matrix, the presented contour integral method

- computes the roots/eigenvalues only in the region of interest
- and requires solutions to forward perturbed (possibly nonlinear) systems, which can often be achieved at a cost proportional to the problem size.

The problem to find a root of a complex function f is usually solved by fixed-point iterations, where the related mapping is contractive in a neighbourhood of the root/fixed-point. If f is smooth the Newton method is in a sense the best choice. Up to some extent the root can be eliminated from the function and the process repeats. Perhaps the main bottleneck is that the convergence of the Newton method requires to start close enough to the root.

In this paper we follow a conceptually different approach. We assume f to be analytical and we calculate moments of $F(z) := f'(z)/f(z)$ along a given curve in the complex plane. By Cauchy's residue theorem the moments give us a complete information about the poles of F, i.e., the roots of f inside the curve. This method dates back to the pioneering work of Delves and Lyness [2]. In the method, which is also referred to as the method of Newton's identities, one searches for roots of a polynomial the coefficients of which are unstable. A remedy is proposed by Kravanja, Sakurai, and van Barel [5]. They stabilize the method by formal orthogonal polynomials.

The contour integral method was further extended by Sakurai and Sugiura [12] towards computing local eigenvalues of matrix pencil (A, B) by finding poles of matrix-valued function $F(z) := V^T(zB - A)^{-1}V$. Later it was reformulated by Ikegami, Sakurai, and Nagashima [4] using the resolvent theory, see [7, 8], and a more accurate algorithm was proposed. One of the algorithmic parameters is the number of distinct eigenvalues, for which a good estimate is given in [13]. The method was also generalized to nonlinear eigenvalue problems [1].

This paper relies on Master thesis of the first author [14]. Essentialy, it is a compilation of a series of papers on contour integral method towards the local eigenvalue analysis. Our aim is to make the method available by documenting its functionality and the necessity of particular ingrediences on properly chosen examples.

The paper is organized as follows: In Section 2 we describe the method of Newton's identities and give examples when it succeeds and when it fails. In Section 3 we present the concept of formal orthogonal polynomials by which the problem is decomposed into a separate search for the distinct zeros and a subsequent search for their multiplicities. Again, we give both kinds of examples. In Section 4 we add final ingrediences by which the method of formal orthogonal polynomials becomes accurate. In Section 5 we sketch an extension of the method towards generalized local eigenvalue analysis of a matrix pencil and give an example of eigenvalue analysis of the eddy current case of Maxwell's equations. We give conclusions in Section 5.

In the paper we use mathematical terminology which might be behind the scope of the journal. We recommend readers interested in a deeper understanding to consult the monographs [10] and [3].

2. Newton's identities

Let $\Omega \subset \mathbb{C}$ be a simply connected domain, $f : \mathbb{C} \to \mathbb{C}$ be holomorfic in Ω, and γ be a positively oriented curve such that f is nonvanishing along γ. We consider the problem of locating zeros of f in the interior of γ. According to Cauchy's residue theorem, we obtain

$$\frac{1}{2\pi i}\int_\gamma z^k \frac{f'(z)}{f(z)}\,dz = \sum_{i=1}^{n} \alpha_i z_i^k =: s_k, \tag{1}$$

where $z_1, \cdots, z_n$ are the mutually distinct zeros of f inside γ and $\alpha_1, \cdots, \alpha_n$ are their respective multiplicities. We denote by $N := s_0$ the total number of the zeros and construct the polynomial

$$P_N(z) := z^N + \sigma_1 z^{n-1} + \ldots + \sigma_N \tag{2}$$

having the same zeros (including their multiplicities) as function f in the interior of γ. The coefficients of $P_N(z)$ are given by following Newton's identities:

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ s_1 & 2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ s_{N-1} & \cdots & s_1 & N \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \vdots \\ \sigma_N \end{bmatrix} = - \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_N \end{bmatrix}. \tag{3}$$

We obtain s_k from (1) by numerical integration. However, the method of Newton's identities is usually ill-conditioned due to bad conditioning of the polynomial, i.e., small changes of σ_k generate larger changes in the zeros of (2). Therefore, the contour integrals have to be approximated with high accuracy.

Adaptive numerical integration

For the sake of simplicity we assume the circular curve γ with the parametrization $z(t) := c + \rho e^{2\pi i t}$, $t \in \langle 0, 1\rangle$. We employ the composite trapezoidal rule

$$\frac{1}{2\pi i}\int_\gamma z^k \frac{f'(z)}{f(z)}\,dz = \int_0^1 g_k(t)\,dt$$
$$\approx \frac{1}{n}\left[\frac{g_k(0)+g_k(1)}{2} + \sum_{j=1}^{n-1} g_k(j/n)\right] =: I_n(g_k; 0, 1), \tag{4}$$

where $g_k(t) := \rho z^k(t) f'(z(t))/f(z(t))$. As g_k is periodic with period 1, then

$$I_n(g_k; 0, 1) = \frac{1}{n}\sum_{j=0}^{n-1} g_k(j/n)$$

and

$$I_{2n}(g_k; 0, 1) = \frac{I_n(g_k; 0, 1)}{2} + \frac{1}{2n}\sum_{j=0}^{n-1} g_k\left(\frac{2j+1}{2n}\right).$$

This allows us to double n successively until $|I_{2n}(g_k; 0, 1) - I_n(g_k; 0, 1)| < \varepsilon_{\text{int}}$.

In all examples throuhout the paper we underline the accurate digits.

Example 1. *Let*

$$f(z) := \sin z - z^3 - i, \quad z(t) := 4e^{2\pi i t}.$$

The choice $\varepsilon_{\text{int}} := 0.01$ *suffices to obtain the following highly precise results:*

$$\begin{aligned} z_1 &= \underline{1.09201015578401}4 - \underline{0.33368801461735}86i, \\ z_2 &= -1.933642457 \cdot 10^{-16} + \underline{0.66139340353310}01i, \\ z_3 &= -\underline{1.09201015578401}5 - \underline{0.33368801461735}85i. \end{aligned}$$

Example 2. *Let*

$$f(z) := (z-1)^{10}(z-5)^5, \quad z(t) := 6e^{2\pi i t}.$$

Clearly, $z_1 = 1$, $\alpha_1 = 10$, $z_2 = 5$, $\alpha_2 = 5$. *However, the method of Newton's identities and* $\varepsilon_{\text{int}} := 0.01$ *now give very poor results:*

$$
\begin{aligned}
z_1 &= 0.638482651241363 + 0.1123392797585549i,\\
z_2 &= 0.638587425742418 - 0.1126503196732164i,\\
z_3 &= 0.763900657783945 + 0.3022377533042421i,\\
z_4 &= 0.764166341345210 - 0.3024211941351311i,\\
z_5 &= 0.981330371128332 + 0.3925444707253891i,\\
z_6 &= 0.981647031382095 - 0.3925384311440422i,\\
z_7 &= 1.223616331736505 + 0.3378606328576522i,\\
z_8 &= 1.223870848730167 - 0.3376746496432903i,\\
z_9 &= 1.392149341950558 + 0.1355311955012755i,\\
z_{10} &= 1.392248774201433 - 0.1352287380346158i,\\
z_{11} &= 4.969215063333387 + 0.0229039229183072i,\\
z_{12} &= 4.969232020549779 - 0.0229259755221052i,\\
z_{13} &= 5.012225738075729 + 0.0354938759143295i,\\
z_{14} &= 5.012250530712597 - 0.0354846773469500i,\\
z_{15} &= 5.037076872119689 + 0.0000128545195791i.
\end{aligned}
$$

The poor results of the last example are caused by the instability of the mapping of the polynomial coefficients to the roots. In the next section we introduce the concept of formal orthogonal polynomials that will allow to separate the problem into two subtasks:

- first determine all mutually distinct zeros of f
- and then determine their multiplicities.

By this approach the last example gets well-posed.

3. Formal orthogonal polynomials

Let $\mathcal{P}$ be the linear space of polynomials with complex coefficients and $\langle\cdot,\cdot\rangle : \mathcal{P}\times\mathcal{P}\to\mathbb{C}$ be the following symmetric bilinear form

$$
\langle \phi,\psi\rangle := \frac{1}{2\pi i}\int_\gamma \phi(z)\psi(z)\frac{f'(z)}{f(z)}\,\mathrm{d}z = \sum_{i=1}^{n}\alpha_i\phi(z_i)\psi(z_i). \tag{5}
$$

Note that (1) and (5) are related, $s_p = \langle 1, z^p\rangle$.

Definition 1. *A monic polynomial $\varphi_t(z) = u_0 + \cdots + u_{t-1}z^{t-1} + z^t$ of degree t is called a formal orthogonal polynomial (FOP) if and only if (iff)*

$$
\left\langle z^k, \varphi_t(z)\right\rangle = 0 \quad \text{for all } k \in \{0,1,\cdots,t-1\}. \tag{6}
$$

By definition the coefficients of an FOP solve the following linear system with a Hankel matrix:

$$
\underbrace{\begin{bmatrix} s_0 & \cdots & s_{t-1}\\ \vdots & \ddots & \vdots\\ s_{t-1} & \cdots & s_{2t-2}\end{bmatrix}}_{=:H_t}\begin{bmatrix} u_0\\ \vdots\\ u_{t-1}\end{bmatrix} = -\begin{bmatrix} s_t\\ \vdots\\ s_{2t-1}\end{bmatrix}. \tag{7}
$$

Thus, FOP φ_t is unique iff H_t is nonsingular. In such a case φ_t is called a *regular FOP* and the index t is a *regular index*.

We further introduce Hankel matrix

$$
H_t^{(1)} := \begin{bmatrix} s_1 & \cdots & s_t\\ \vdots & & \ddots\\ s_t & \cdots & s_{2t-1}\end{bmatrix}.
$$

Theorem 1. *[5]*

1. rank $H_{n+p} = n$ *for all* $p \in \mathbb{N}\cup\{0\}$.
2. *For a regular index $t \geq 1$ the zeros of FOP φ_t are the eigenvalues of matrix pencil $H_t^{(1)} - \lambda H_t$.*
3. *For each $t \geq n$ zeros $z_1,\cdots,z_n$ are eigenvalues of matrix pencil $H_t^{(1)} - \lambda H_t$. We have no information about the remaining $t-n$ eigenvalues.*

Theorem 1 suggests to replace the computation of the zeros of φ_n by determining the eigenvalues of matrix pencil $H_n^{(1)} - \lambda H_n$. The multiplicities $\alpha_1,\ldots,\alpha_n$ solve the following Vandermonde system, for which an efficient algorithm (relying on Newton polynomial interpolation formula) exists [9],

$$
\begin{bmatrix} 1 & 1 & \cdots & 1\\ z_1 & z_2 & \cdots & z_n\\ \vdots & \vdots & \ddots & \vdots\\ (z_1)^{n-1} & (z_2)^{n-1} & \cdots & (z_n)^{n-1}\end{bmatrix}\begin{bmatrix}\alpha_1\\ \alpha_2\\ \vdots\\ \alpha_n\end{bmatrix} = \begin{bmatrix} s_0\\ s_1\\ \vdots\\ s_{n-1}\end{bmatrix}.
$$

The algorithm starts with computing $N := s_0$ by numerical integration. Then it continues to compute $s_1,\ldots,s_{2N-2}$. Number n of mutually distinct zeros is equal to rank of H_N. Yet, the method has two bottlenecks:

- In practice, it may be difficult to determine rank H_N since the difference between the zero singular values and the least nonzero singular value is often small.
- The approximation of the eigenvalues $z_1,\ldots,z_n$ can be inaccurate, since the matrix pencil $H_n^{(1)} - \lambda H_n$ is usually ill-conditioned.

Example 3. *We consider Example 2 and $\varepsilon_{\mathrm{int}} = 0.01$. The method of FOP now gives accurate zeros*

$$
\begin{aligned}
z_1 &= \underline{1.0000000000000}24 - 2.8968750007\cdot 10^{-16}i,\\
z_2 &= \underline{5.0000000000000}19 - 8.0874999999\cdot 10^{-17}i,
\end{aligned}
$$

as well as their respective multiplicities obtained from the Vandermonde system

$$
\begin{aligned}
\alpha_1 &= 10.00000000000000 + 2.92187499999\cdot 10^{-16}i,\\
\alpha_1 &= 5.00000000006579 + 9.81812500000\cdot 10^{-16}i.
\end{aligned}
$$

The method of FOP works fine for small numbers of distinct zeros regardless their multiplicity. However, the next example documents that the larger numbers of distinct zeros are troublesome.

Example 4. *Let*

$$f(z) := \sum_{j=1}^{10} (z - 0.5 \cdot j), z(t) := 5.5e^{2\pi it}, \text{ and } \varepsilon := 0.01.$$

Matrix pencil $H_{10}^{(1)} - \lambda H_{10}$ *has the following eigenvalues:*

$$\begin{aligned}
z_1 &= -0.482619604959967 - 0.520113046496264i,\\
z_2 &= -0.595622152646554 - 1.443748803 \cdot 10^{-4}i,\\
z_3 &= +0.482619618447490 + 0.520113058046448i,\\
z_4 &= +0.651860357554706 - 1.178169519 \cdot 10^{-5}i,\\
z_5 &= +1.504605605133679 - 1.902167265 \cdot 10^{-5}i,\\
z_6 &= +2.375661289285481 - 1.945767526 \cdot 10^{-5}i,\\
z_7 &= +3.196581772082030 - 1.417457467 \cdot 10^{-5}i,\\
z_8 &= +3.907634470420446 - 6.494754458 \cdot 10^{-6}i,\\
z_9 &= +4.488679268520042 - 1.196308016 \cdot 10^{-6}i,\\
z_{10} &= +4.999754031111922 - 3.592315502 \cdot 10^{-8}i.
\end{aligned}$$

Their respective multiplicities are as follows:

$$\begin{aligned}
\alpha_1 &= 0.006031224859367 + 0.009574773192818i,\\
\alpha_2 &= 0.021388363415923 - 1.976830498 \cdot 10^{-5}i,\\
\alpha_3 &= 0.006031223614133 - 0.009574772225025i,\\
\alpha_4 &= 1.601888235995385 + 2.305237356 \cdot 10^{-5}i,\\
\alpha_5 &= 1.751075490643741 - 7.586842632 \cdot 10^{-6}i,\\
\alpha_6 &= 1.713254640082220 + 5.621126851 \cdot 10^{-6}i,\\
\alpha_7 &= 1.549297289797993 + 1.437335499 \cdot 10^{-5}i,\\
\alpha_8 &= 1.285524904448345 + 1.463574228 \cdot 10^{-5}i,\\
\alpha_9 &= 1.062954316433515 + 5.745175536 \cdot 10^{-6}i,\\
\alpha_{10} &= 1.002554928864612 + 3.541878625 \cdot 10^{-7}i.
\end{aligned}$$

4. Accurate FOP method

The problem with the method of FOP is that matrix pencil $H_n^{(1)} - \lambda H_n$ is ill-conditioned. Therefore, we shall represent φ_n in a monic, but generally non-monomial basis ψ_j,

$$\varphi_n(z) = \psi_n(z) + \sigma_{n-1}\psi_{n-1}(z) + \cdots + \sigma_0\psi_0(z).$$

This translates (6) to

$$\langle \psi_k, \varphi_n \rangle = 0 \quad \text{for all } k \in \{0, 1, \ldots, n-1\}$$

or equivalently

$$G_n \begin{bmatrix} \sigma_0 \\ \vdots \\ \sigma_{n-1} \end{bmatrix} = - \begin{bmatrix} \langle \psi_0, \psi_n \rangle \\ \vdots \\ \langle \psi_{n-1}, \psi_n \rangle \end{bmatrix},$$

where we introduced Gramm matrix

$$G_n := \begin{bmatrix} \langle \psi_0, \psi_0 \rangle & \ldots & \langle \psi_0, \psi_{k-1} \rangle \\ \vdots & \ddots & \vdots \\ \langle \psi_{k-1}, \psi_0 \rangle & \ldots & \langle \psi_{k-1}, \psi_{k-1} \rangle \end{bmatrix}.$$

We further define

$$G_n^{(1)} := \begin{bmatrix} \langle \psi_0, \psi_1\psi_0 \rangle & \ldots & \langle \psi_0, \psi_1\psi_{k-1} \rangle \\ \vdots & \ddots & \vdots \\ \langle \psi_{k-1}, \psi_1\psi_0 \rangle & \ldots & \langle \psi_{k-1}, \psi_1\psi_{k-1} \rangle \end{bmatrix}.$$

Theorem 2. *[5] Let* $t \in \mathbb{N}$.

1. *Then* λ^* *is an eigenvalue of* $H_t^{(1)} - \lambda H_t$ *iff* $\psi_1(\lambda^*)$ *is an eigenvalue of* $G_t^{(1)} - \lambda G_t$.

2. *Let* r *be the largest regular index less or equal* t*. Then the eigenvalues of* $G_r^{(1)} - \lambda G_r$ *are eigenvalues of* $G_t^{(1)} - \lambda G_t$*. We have no information about the remaining* $t - r$ *eigenvalues.*

The theorem suggests to replace the pencil of Hankel matrices by the related pencil of Gramm matrices. For a regular index $t \geq 1$ the zeros $z_1, \cdots, z_t$ of φ_t are shifted eigenvalues $z_1 - \mu, \cdots, z_t - \mu$ of $G_t^{(1)} - \lambda G_t$, where $\mu = \frac{s_1}{s_0}$. In particular, the eigenvalues of $G_n^{(1)} - \lambda G_n$ are $z_1 - \mu, \cdots, z_n - \mu$. When the zeros have positive real parts the condition number of the matrix pencils improves as follows:

$$\kappa\left((G_n)^{-1} G_n^{(1)}\right) = \frac{z_n + \mu}{z_1 + \mu} < \frac{z_n}{z_1} = \kappa\left((H_n)^{-1} H_n^{(1)}\right).$$

The multiplicities can be computed as follows:

$$\begin{bmatrix} \psi_0(z_1) & \ldots & \psi_0(z_n) \\ \vdots & \ddots & \vdots \\ \psi_{n-1}(z_0) & \ldots & \psi_{n-1}(z_n) \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} \langle \psi_0, \psi_0 \rangle \\ \vdots \\ \langle \psi_{n-1}, \psi_0 \rangle \end{bmatrix}.$$

A good choice for the basis turns out to be FOPs φ_j. From now on let $\psi_j := \varphi_j$. In case H_n is strongly regular, meaning that all the leading principal submatrices are regular, then all FOPs $\varphi_0, \varphi_1, ..., \varphi_n$ are regular, G_n is diagonal, and $G_n^{(1)}$ is tridiagonal.

In the other case, H_n is not strongly regular, we establish a set of regular indices $\{i_k\}$, $k = 0, ..., K$, where K is the number of regular blocks in H_n. If $n \geq 1$, then $i_0 = 0$, $i_1 = 1$, and $i_K = n$. We define sequence $\{\varphi_t\}_{t=0}^{\infty}$ of monic polynomials as follows: If t is a regular index, then φ_t is the regular FOP. Otherwise, t is not regular, i.e. $\varphi_t := z^{t-r}\varphi_r(z)$, where r is the largest regular index less than t. In this case φ_t is called an *inner polynomial*. The polynomials are grouped into blocks such that every block starts with a regular polynomial and the remaining polynomials in the block are inner polynomials,

$$\begin{aligned}\Theta^{(0)} &= [\varphi_0],\\ \Theta^{(1)} &= [\varphi_1, \varphi_2, \ldots, \varphi_{i_2-1}],\\ &\vdots\\ \Theta^{(K-1)} &= [\varphi_{i_{K-1}}, \varphi_{i_{K-1}+1}, \ldots, \varphi_{i_K-1}],\\ \Theta^{(K)} &= [\varphi_n, \varphi_{n+1}, \ldots].\end{aligned}$$

The length of $\Theta^{(p)}$, $p < n$, is

$$l_p := i_{p+1} - i_p. \tag{8}$$

For blocks $\Phi := [\phi_0, \ldots, \phi_p]$ and $\Psi = [\psi_0, \ldots, \psi_q]$ we define

$$\langle \Phi, \Psi\rangle := \begin{bmatrix}\langle\phi_0,\psi_0\rangle & \ldots & \langle\phi_0,\psi_q\rangle\\ \vdots & \ddots & \vdots\\ \langle\phi_p,\psi_0\rangle & \ldots & \langle\phi_p,\psi_q\rangle\end{bmatrix}.$$

The following theorem states that G_n is nonsingular, symmetric, and block diagonal.

Theorem 3. *[5]*

$$\left\langle\Theta^{(p)}, \Theta^{(q)}\right\rangle = \begin{cases} 0_{l_p\times l_q} & \textit{if} \quad p \neq q\\ \delta_p & \textit{if} \quad p = q\end{cases}$$

for $p, q = 0, ..., K-1$, where $\delta_p \in \mathbb{C}^{l_p\times l_p}$ is nonsingular and symmetric. The entries of δ_p vanish above the main antidiagonal and they are equal to $\left\langle z^{i_p+l_p-1}, \varphi_{i_p}\right\rangle$ along the main antidiagonal.

The following theorem states that $G_n^{(1)}$ is nonsingular, symmetric and block tridiagonal.

Theorem 4. *[5]*

$$\left\langle\Theta^{(p)}, \varphi_1\Theta^{(q)}\right\rangle = \begin{cases} 0_{l_p\times l_q} & \textit{if} \quad |p-q| > 1\\ \varrho_p & \textit{if} \quad p = q+1\\ \varrho_q^T & \textit{if} \quad p = q-1\\ \delta_p^{(1)} & \textit{if} \quad p = q\end{cases}$$

for $p, q = 0, ..., K-1$, where $\delta_p^{(1)} \in \mathbb{C}^{l_p\times l_p}$ is symmetric and lower anti-Hessenberg. The entries of $\delta_p^{(1)}$ are equal to $\left\langle z^{i_p+l_p-1}, \varphi_{i_p}\right\rangle$ along the first antidiagonal and they vanish above it. Matrix ϱ_p vanishes up to the entry in the south-east corner, which is equal to $\left\langle z^{i_p+l_p-1}, \varphi_{i_p}\right\rangle$.

For instance, assume $n = 10$ and the following blocks

$$\begin{aligned}\Theta^{(0)} &= [\varphi_0],\\ \Theta^{(1)} &= [\varphi_1, \varphi_2, \varphi_3, \varphi_4],\\ \Theta^{(2)} &= [\varphi_5, \varphi_6, \varphi_7],\\ \Theta^{(3)} &= [\varphi_8, \varphi_9].\end{aligned}$$

Then the structure of G_n and $G_n^{(1)}$ is as follows:

$$G_n = \begin{bmatrix}\odot &&&&&&&&&\\ & 0 & 0 & 0 & \odot &&&&&\\ & 0 & 0 & \odot & \oplus &&&&&\\ & 0 & \odot & \oplus & \oplus &&&&&\\ & \odot & \oplus & \oplus & \oplus &&&&&\\ &&&&& 0 & 0 & \odot &&\\ &&&&& 0 & \odot & \oplus &&\\ &&&&& \odot & \oplus & \oplus &&\\ &&&&&&&& 0 & \odot\\ &&&&&&&& \odot & \oplus\end{bmatrix}$$

$$G_n^{(1)} = \begin{bmatrix}0 &&&& \odot &&&&&\\ & 0 & 0 & \odot & \oplus &&&&&\\ & 0 & \odot & \oplus & \oplus &&&&&\\ & \odot & \oplus & \oplus & \oplus &&&&&\\ \odot & \oplus & \oplus & \oplus & \oplus &&& \odot &&\\ &&&&& 0 & \odot & \oplus &&\\ &&&&& \odot & \oplus & \oplus &&\\ &&&& \odot & \oplus & \oplus & \oplus && \odot\\ &&&&&&&& \odot & \oplus\\ &&&&&&& \odot & \oplus & \oplus\end{bmatrix}$$

The entries marked $\odot$ are nonzero and in each block they are all equal.

We call a regular FOP to be well-conditioned if the corresponding system (7) is well-conditioned, otherwise, the regular FOP is referred to as ill-conditioned. To obtain a numerically stable algorithm, it is crucial to generate only well-conditioned regular FOPs and replace the ill-conditioned regular FOPs by inner polynomials.

The algorithm takes three entries on the input: the bilinear form $\langle\cdot,\cdot\rangle$, $\varepsilon_{\mathrm{cond}}$, and $\varepsilon_{\mathrm{stop}}$ with $\varepsilon_{\mathrm{stop}} < \varepsilon_{\mathrm{cond}}$. The value $\varepsilon_{\mathrm{cond}}$ determines the length of block l_p in (8) and $\varepsilon_{\mathrm{stop}}$ is a stopping criterion.

If $|\langle\varphi_r,\varphi_r\rangle| \geq \varepsilon_{\mathrm{cond}}$ for some regular index r, then φ_{r+1} is generated as an FOP. Otherwise, we search for the smallest t such that $t \leq N-1-r$ and $|\langle z^t\varphi_r,\varphi_r\rangle| > \varepsilon_{\mathrm{cond}}$. If we succeed, $t+1$ is the length of the block and t is the number of inner polynomials in the block. If we fail to find such t we shall check $|\langle z^t\varphi_r,\varphi_r\rangle| < \varepsilon_{\mathrm{stop}}$ for all $t \in \{0, \cdots, N-1-r\}$. In case the latter condition holds true then $n := r$ and we shall compute the zeros of φ_r. Otherwise, if $|\langle z^t\varphi_r,\varphi_r\rangle| \geq \varepsilon_{\mathrm{stop}}$ for some t, then the length of the block is $t := \underset{0\leq s\leq N-1-r}{\arg\max} |\langle z^t\varphi_r,\varphi_r\rangle|$.

Example 5. *Let*

$$f(z) := \sum_{j=1}^{10}(z - 0.5\cdot j), \quad z(t) := \frac{11}{2}\mathrm{e}^{2\pi i t},$$

$\varepsilon_{\mathrm{int}} := 0.01$, $\varepsilon_{\mathrm{cond}} := 1$, and $\varepsilon_{\mathrm{stop}} := 10^{-12}$. The algorithm generates only regular FOPs, the approximated zeros are

Algorithm 1 Accurate FOP method [5].

Require: $\langle \cdot, \cdot \rangle$, $\varepsilon_{\text{cond}}$, $\varepsilon_{\text{stop}}$ with $\varepsilon_{\text{cond}} > \varepsilon_{\text{stop}}$
Ensure: n, zeros

$N \leftarrow \langle 1, 1 \rangle$
if $N = 0$ **then**
  $n \leftarrow 0$ zeros $\leftarrow \emptyset$
else
  $\varphi_0(z) \leftarrow 1$
  $\mu \leftarrow \langle z, 1 \rangle / N$; $\varphi_1(z) \leftarrow z - \mu$
  $r \leftarrow 1$
  while $r < N$ **do**
    if $|\langle \varphi_r, \varphi_r \rangle| \geq \varepsilon_{\text{cond}}$ **then**
      generate φ_{r+1} *as a regular FOP*
      $r \leftarrow r + 1$
    else
      all_small $\leftarrow$ 1; t_notfound $\leftarrow$ 1; maximum $\leftarrow 0$; $t \leftarrow 0$
      while t_notfound $= 1$ **and** $t \leq N - 1 - r$ **do**
        el $\leftarrow |\langle z^t \varphi_r(z), \varphi_r(z) \rangle|$
        if all_small $= 1$ **and** (el $< \varepsilon_{\text{stop}}$) **then**
          all_small $\leftarrow 1$
        else
          all_small $\leftarrow 0$
        end if
        if (el $\geq \varepsilon_{\text{cond}}$) **then**
          t_notfound $\leftarrow 0$; t_large $\leftarrow t$
        end if
        if (el $>$ maximum) **then**
          maximum $\leftarrow$ el; t_max $\leftarrow t$
        end if
        $t \leftarrow t + 1$
      end while
      if t_notfound $= 1$ **then**
        if all_small $= 1$ **then**
          $n \leftarrow r$; zeros $\leftarrow$ zeros(φ_r); **stop**
        else
          length_block $\leftarrow$ t_max
        end if
      else
        length_block $\leftarrow$ t_large
      end if
      for $i = 1$: length_block **do**
        $\varphi_{r+i}(z) \leftarrow z^i \varphi_r(z)$
      end for
      generate $\varphi_{r+\text{length\_block}+1}$ *as a regular FOP*
      $r \leftarrow r +$ length_block $+ 1$
    end if
  end while
  $n \leftarrow N$; zeros $\leftarrow$ zeros(φ_N); **stop**
end if

$$
\begin{aligned}
z_1 &= +\underline{0.499999}245442022 - 2.244735174 \cdot 10^{-8} i, \\
z_2 &= +\underline{0.999999}450552922 + 3.132766752 \cdot 10^{-7} i, \\
z_3 &= +\underline{1.49999}1282809416 + 5.566390567 \cdot 10^{-6} i, \\
z_4 &= +\underline{1.9999999}75589223 + 2.338471947 \cdot 10^{-7} i, \\
z_5 &= +\underline{2.49999}8509456637 + 5.817851659 \cdot 10^{-6} i, \\
z_6 &= +\underline{2.999999}378380768 + 9.865733004 \cdot 10^{-6} i, \\
z_7 &= +\underline{3.49999}2478820148 + 2.404739788 \cdot 10^{-6} i, \\
z_8 &= +\underline{3.99999}5491446401 + 8.779757908 \cdot 10^{-6} i, \\
z_9 &= +\underline{4.4999999}38630227 - 4.909355538 \cdot 10^{-9} i, \\
z_{10} &= +\underline{4.9999999}67711271 - 2.464430622 \cdot 10^{-9} i.
\end{aligned}
$$

Their respective multiplicities are as follows:

$$
\begin{aligned}
\alpha_1 &= 1.000000618154602 - 4.983054260 \cdot 10^{-13} i, \\
\alpha_2 &= 0.999999999999204 + 4.042968493 \cdot 10^{-13} i, \\
\alpha_3 &= 0.999999999980970 - 2.452072579 \cdot 10^{-10} i, \\
\alpha_4 &= 0.999999999969353 + 2.056473775 \cdot 10^{-11} i, \\
\alpha_5 &= 0.999999999893328 - 2.457023087 \cdot 10^{-10} i, \\
\alpha_6 &= 0.999999999782027 + 2.177804928 \cdot 10^{-10} i, \\
\alpha_7 &= 0.999999999993874 - 7.316470179 \cdot 10^{-10} i, \\
\alpha_8 &= 0.999999999667719 + 7.005704794 \cdot 10^{-10} i, \\
\alpha_9 &= 1.000000000472861 - 4.924484795 \cdot 10^{-10} i, \\
\alpha_{10} &= 1.000000000241296 + 3.854785554 \cdot 10^{-10} i.
\end{aligned}
$$

If we set $\varepsilon_{\text{cond}} := 100$ and $\varepsilon_{\text{stop}} := 10^{-12}$, then the algorithm finds that $n = 10$. Polynomials φ_0, φ_1, φ_4, φ_6, φ_8, φ_{10} are regular FOPs, while φ_2, φ_3, φ_5, φ_7, φ_9 are inner polynomials. We obtain the following approximations of zeros:

$$
\begin{aligned}
z_1 &= +\underline{0.49999}2655471288 - 4.909355538 \cdot 10^{-9} i, \\
z_2 &= +\underline{0.999999}731282809 - 3.829294804 \cdot 10^{-7} i, \\
z_3 &= +\underline{1.499999}155892237 + 6.585363951 \cdot 10^{-7} i, \\
z_4 &= +\underline{1.999}668509456421 + 5.301649119 \cdot 10^{-6} i, \\
z_5 &= +\underline{2.49999}5221584756 + 9.634758534 \cdot 10^{-6} i, \\
z_6 &= +\underline{2.999999}333486939 + 7.586897789 \cdot 10^{-7} i, \\
z_7 &= +\underline{3.49999}5491446401 + 8.239161142 \cdot 10^{-6} i, \\
z_8 &= +\underline{3.999999}534505529 + 5.399356928 \cdot 10^{-7} i, \\
z_9 &= +\underline{4.4999999}29381452 + 2.412660883 \cdot 10^{-9} i, \\
z_{10} &= +\underline{4.9999999}55911479 - 7.916055092 \cdot 10^{-9} i,
\end{aligned}
$$

and their respective multiplicities

$$
\begin{aligned}
\alpha_1 &= 1.000000618155972 - 4.770149241 \cdot 10^{-13} i, \\
\alpha_2 &= 1.000000000050812 - 2.483233141 \cdot 10^{-13} i, \\
\alpha_3 &= 0.999999999997617 + 8.870071758 \cdot 10^{-10} i, \\
\alpha_4 &= 1.000000000628639 - 2.704259704 \cdot 10^{-11} i, \\
\alpha_5 &= 0.999999999890872 + 3.965002577 \cdot 10^{-10} i, \\
\alpha_6 &= 1.000000002331731 - 9.066519915 \cdot 10^{-10} i, \\
\alpha_7 &= 1.000000002276952 - 7.928159608 \cdot 10^{-10} i, \\
\alpha_8 &= 0.999999998987094 + 3.653664083 \cdot 10^{-10} i, \\
\alpha_9 &= 0.999999998571259 + 5.855344274 \cdot 10^{-10} i, \\
\alpha_{10} &= 0.999999997264284 + 1.003765461 \cdot 10^{-10} i.
\end{aligned}
$$

This approximation of the zeros is less accurate. The higher $\varepsilon_{\text{cond}}$ gives rise to a higher number of inner polynomials. However, this does not improve the accuracy since the polynomials $\varphi_0, \cdots, \varphi_{10}$ are well-conditioned.

Example 6. *Let*

$$f(z) = \mathrm{e}^{3z} + 2z\cos(z) - 1, \quad z(t) := 2\mathrm{e}^{2\pi i t},$$

$\varepsilon_{\text{int}} := 0.01$, $\varepsilon_{\text{cond}} := 0.1$, *and* $\varepsilon_{\text{stop}} = 10^{-12}$. *The algorithm generates only regular FOPs and decides that* $n = 4$. *We obtain the following approximations of zeros:*

$$\begin{aligned}
z_1 &= -\underline{1.8}155999675277674 - 5.841490757 \cdot 10^{-13} i,\\
z_2 &= +\underline{0.5}092879144652833 + \underline{1.3}02159022859336 i,\\
z_3 &= +\underline{0.5}092879144652846 - \underline{1.3}02159022859335 i,\\
z_4 &= +\underline{0.0}168080197763903 - 4.448060308 \cdot 10^{-12} i
\end{aligned}$$

and their respective multiplicities

$$\begin{aligned}
\alpha_1 &= 1.055230342613981 + 1.1861760144 \cdot 10^{-11} i,\\
\alpha_2 &= 1.074677398053296 - 0.00975786847219671 i,\\
\alpha_3 &= 1.074677398053296 + 0.00975786847219344 i,\\
\alpha_4 &= 0.795420084097749 - 4.45121734260 \cdot 10^{-11} i.
\end{aligned}$$

If we set $\varepsilon_{\text{cond}} := 1$ *and* $\varepsilon_{\text{stop}} := 10^{-12}$, *the algorithm decides that* $n = 4$, *the polynomials* φ_0, φ_1, φ_3, φ_4 *are regular FOPs, while* φ_2 *is an inner polynomial. The approximation of the zeros is as follows:*

$$\begin{aligned}
z_1 &= -\underline{1.844233953262216} - 3.189796250 \cdot 10^{-16} i,\\
z_2 &= +\underline{0.530894930292931} - \underline{1.331791876751123} i,\\
z_3 &= +\underline{0.530894930292938} + \underline{1.331791876751128} i,\\
z_4 &= -1.21 \cdot 10^{-14} - 5.681456752 \cdot 10^{-15} i.
\end{aligned}$$

This approximation of the zeros is more accurate. Here the higher $\varepsilon_{\text{cond}}$ *leads to a better accuracy as we are replacing ill-conditioned regular FOPs by the inner polynomials. We do not observe a remarkable rise of computational time.*

5. Local eigenvalue analysis

The theory and algorithm presented in this section can be found in [1, 4].

Theorem 5. *(Weierstrass Canonical Form) Let* $(zB - A) \in \mathbb{C}^{n\times n}$ *be a regular pencil. Then there exist nonsingular matrices* $P, Q \in \mathbb{C}^{n\times n}$ *such that*

$$P(zB - A)Q = \begin{bmatrix} zI_{k_1} - J_1 & & & & & \\ & \ddots & & & & \\ & & zI_{k_d} - J_d & & & \\ & & & zN_{d+1} - I_{k_d+1} & & \\ & & & & \ddots & \\ & & & & & zN_r - I_{k_r} \end{bmatrix} \tag{9}$$

where $J_i, N_i \in \mathbb{C}^{k_i\times k_i}$ *are Jordan blocks,* N_i *is nilpotent and* $I_{k_i} \in \mathbb{C}^{k_i\times k_i}$ *is the identity matrix.*

According to the structure of the Jordan blocks we divide P and Q into block rows $P_i \in \mathbb{C}^{k_i\times n}$ and block columns $Q_i \in \mathbb{C}^{n\times k_i}$, respectively, for $i = 1, 2, \cdots, r$. By (9) we obtain

$$(zB - A)^{-1} = \\ = \sum_{i=1}^{d} Q_i (zI_{k_i} - J_i)^{-1} P_i + \sum_{i=d+1}^{r} Q_i (zN_i - I_{k_i})^{-1} P_i.$$

Let α_i be an eigenvalue of matrix J_i. Then

$$(zI_{k_i} - J_i)^{-1} = \sum_{m=0}^{k_i-1} \frac{(J_i - \alpha_i I_{k_i})^m}{(z - \alpha_i)^{m+1}},$$

and

$$(zN_i - I_{k_i})^{-1} = -\sum_{m=0}^{k_i-1} z^m N_i^m.$$

The regular pencil $(zB - A)^{-1}$ can be decomposed into

$$\begin{aligned}
&(zB - A)^{-1} = \\
&= \sum_{i=1}^{d} Q_i \left(\sum_{m=0}^{k_i-1} \tfrac{(J_i - \alpha_i I_{k_i})^m}{(z-\alpha_i)^{m+1}} \right) P_i \\
&- \sum_{i=d+1}^{r} Q_i \left(\sum_{m=0}^{k_i-1} z^m N_i^m \right) P_i.
\end{aligned}$$

Let γ be a positively oriented closed Jordan curve and G interior of γ. Define

$$M_0 := \frac{1}{2\pi i} \int_\gamma (zB - A)^{-1}\,\mathrm{d}z, \tag{10}$$

and

$$M_1 := \frac{1}{2\pi i} \int_\gamma z(zB - A)^{-1}\,\mathrm{d}z. \tag{11}$$

We can extract Jordan blocks whose eigenvalues are contained in G. The following collective notations are constructed: The Jordan blocks J_i; $\alpha_i \in G$ are collected to form the $k_\gamma \times k_\gamma$ Jordan matrix J_γ, where $k_\gamma = \sum_{i;\alpha_i\in G} k_i$. Similarly, the corresponding Q_i and P_i are collected to form $Q_\gamma \in \mathbb{C}^{n\times k_\gamma}$ and $P_\gamma \in \mathbb{C}^{k_\gamma\times n}$, respectively.

By using the Residue theorem, the matrix in (10) and (11) can be written as

$$M_0 = Q_\gamma J_\gamma^0 P_\gamma,$$

and

$$M_1 = Q_\gamma J_\gamma^1 P_\gamma.$$

Theorem 6. *Let* V *be arbitrary* $n \times k_\gamma$ *matrix. Define a size-reduced moment matrices* $\mathbb{M}_0 = V^T M_0 V \in \mathbb{C}^{k_\gamma\times k_\gamma}$ *and* $\mathbb{M}_1 = V^T M_1 V \in \mathbb{C}^{k_\gamma\times k_\gamma}$. *If ranks of both* $V^T Q_\gamma$ *and* $P_\gamma V$ *are* k_γ, *the size-reduced matrix pencil* $z\mathbb{M}_0 - \mathbb{M}_1$ *is equivalent to* $zI_{k_\gamma} - J_\gamma$.

The number of eigenvalues inside γ is given by

$$k_\gamma = \frac{1}{2\pi i} \int_\gamma \operatorname{trace}\left((zB - A)^{-1} B \right) \mathrm{d}z. \tag{12}$$

The trace of $((zB - A)^{-1}B)$ in (12) is approximated by

$$\operatorname{trace}\left((zB - A)^{-1} B\right) \approx$$
$$\approx \left(\frac{1}{L_0}\right) \sum_{i=1}^{L_0} v_i^T (zB - A)^{-1} B v_i,$$

with some integer L_0, where the elements of the sample vectors $v_i \in \mathbb{R}^N$ are taken as -1 or 1 with equal probability.

Algorithm 2 Local generalized eigenvalue analysis [1].

Require: matrices A, B, curve $\gamma := r + \rho\,\mathrm{e}^{2\pi i t}$, number of integration points N

Ensure: eigenvalues of $A - \lambda B$ inside γ

1: set $\omega_j \leftarrow r + \rho\,\mathrm{e}^{2\pi i (j+1/2)/N}$, $j = 0, 1, \cdots, N-1$

2: set $d_j \leftarrow \rho\,\mathrm{e}^{2\pi i (j+1/2)/N}$, $j = 0, 1, \cdots, N-1$

3: compute $w_j^1 \leftarrow (\omega_j B - A)^{-1} B$, $j = 0, 1, \cdots, N-1$

4: set $w_j^2 \leftarrow (1/L_0) \sum_{i=1}^{L_0} v_i^T w_j^1 v_i$, $j = 0, 1, \cdots, N-1$

5: set $k_\gamma \leftarrow (1/N) \sum_{j=0}^{N-1} w_j^2\, d_j$

6: generate $V \in \mathbb{C}^{n \times k_\gamma}$ as random matrix

7: compute $p_j \leftarrow (\omega_j B - A)^{-1} V$, $j = 0, 1, \cdots, N-1$

8: set $\mathbb{M}_0 = (1/N) \sum_{j=0}^{N-1} V^T p_j d_j$, $j = 0, 1, \cdots, N-1$

9: set $\mathbb{M}_1 = (1/N) \sum_{j=0}^{N-1} V^T p_j d_j (r + d_j)$

10: compute the eigenvalues of the matrix pencil $z\mathbb{M}_0 - \mathbb{M}_1$

Example 7. *We consider a matrix pencil $(A, B) \in \mathbb{R}^{800 \times 800}$, where both matrices are real valued and symmetric positive definite. The matrices arise from the coupled FEM-BEM discretization of the eddy current case of Maxwell's equations, which is a parabolic-elliptic system, for simulations of electromagnetic forming of metalic sheets. The matrices determine transient electric field $e(t)$ as follows:*

$$A\,e'(t) + B\,e(t) = b(t), \qquad e(0) = e_0$$

for which the knowledge of the generalized eigenvalues and eigenvectors is essential. For a more detailed description we refer to Fig. 1 and to another paper [6] of this journal issue.

We search for the generalized eigenvalues inside the curve $z(t) := 3000 + 1500\,\mathrm{e}^{2\pi i t}$. The radius of the curve is chosen to locate exactly ten eigenvalues. The number of integration points of the trapezoidal rule is 1000, $L_0 := 30$.

The following eigenvalues are obtained:

$$\lambda_1 = \underline{1611.01159}65023 - 1.9877771483411 \cdot 10^{-7} i,$$
$$\lambda_2 = \underline{1874.608618}7737 + 1.5402843741156 \cdot 10^{-8} i,$$
$$\lambda_3 = \underline{2146.272919}0177 - 5.0784828616292 \cdot 10^{-8} i,$$
$$\lambda_4 = \underline{2426.34918}28614 - 2.0480216079679 \cdot 10^{-7} i,$$
$$\lambda_5 = \underline{2715.154054}8190 + 7.9639855872003 \cdot 10^{-8} i,$$
$$\lambda_6 = \underline{3012.988891}2592 + 1.0031486333536 \cdot 10^{-8} i,$$
$$\lambda_7 = \underline{3320.123753}3950 - 2.6143088082065 \cdot 10^{-8} i,$$
$$\lambda_8 = \underline{3636.802921}3876 + 4.8790280464325 \cdot 10^{-8} i,$$
$$\lambda_9 = \underline{3963.244813}6808 - 2.4008268580193 \cdot 10^{-8} i,$$
$$\lambda_{10} = \underline{4299.644215}1635 + 8.4676432174231 \cdot 10^{-9} i.$$

6. Conclusion

We presented contour integral method for localization of roots of analytic functions and its extensions towards local generalized eigenvalue analysis $Ae = \lambda Be$. For the latter the linear system with perturbed matrix $A - z_j B$ is solved at each integration point z_j. Thus, our further research shall address two essential problems:

- To find a suitable quadrature method to minimize the number of evaluations.
- To find a reasonable way to update the solver when perturbing the matrix.

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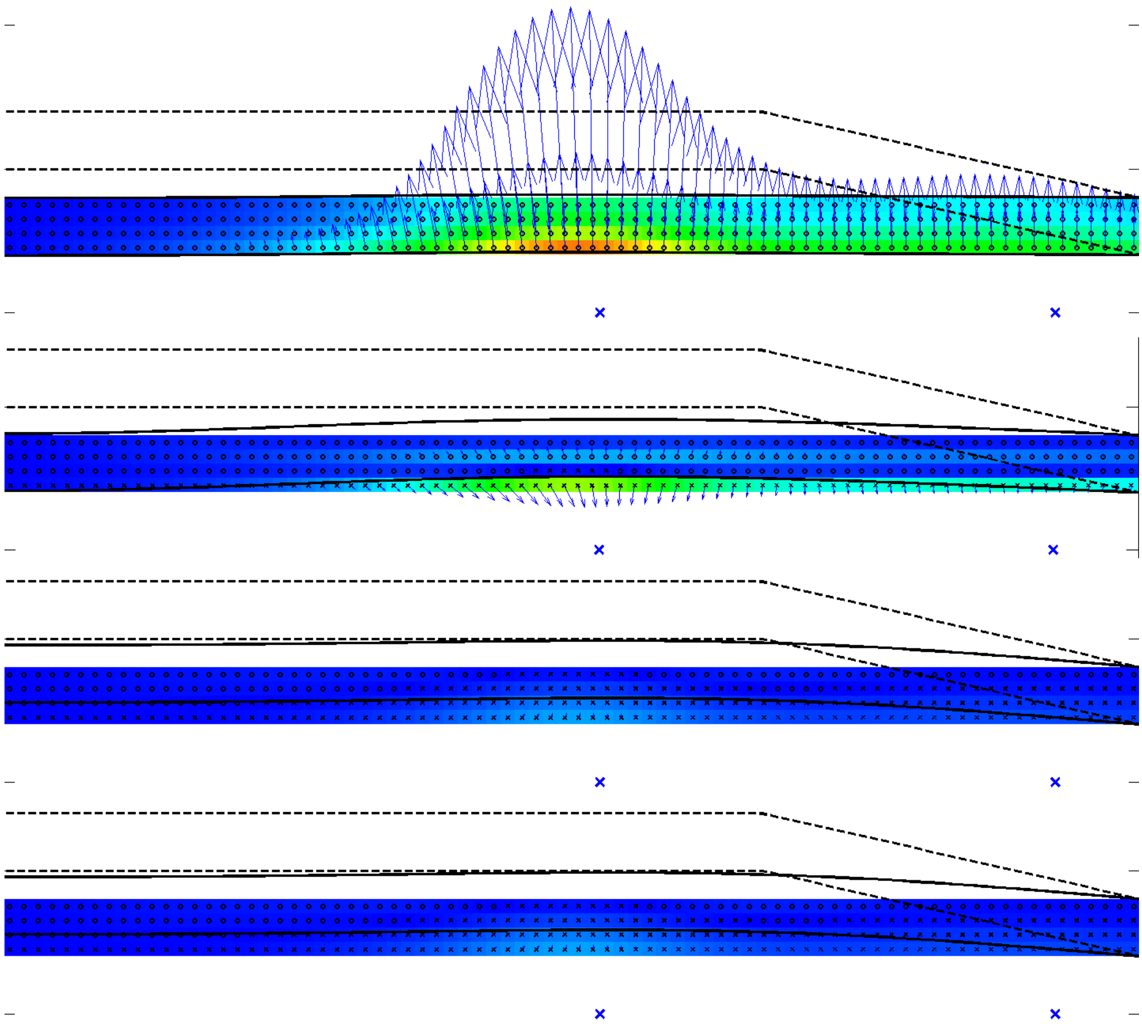

Fig. 1: Snapshots of a simulation of electromagnetic forming of a cylindrical metalic sheet: The electromagnetic field and the mechanical displacements are sketched in the cylindrical coordinates (the axis is on the left hand side) at four times (top-down). Positions of line circular turns of the excitation coil are marked by the blue crosses. The colour map corresponds to the magnitude of the eddy current distribution, the black circles and crosses correspond to the outward and inward orientation, respectively, of the eddy currents. The Lorentz forces are depicted with arrows. The mechanical displacements of the metalic sheet is depicted by the solid lines, while the shape of the form against which the sheet is pressed is depicted with the dashed lines. Note that after the Lorentz forces vanish the deformation of the sheet continues due to the inertial forces.

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About Authors

Erika STRAKOVÁ was born in Námestovo, Slovakia. She received her M.Sc. from VŠB-Technical University of Ostrava in 2016. Her research interests include numerical analysis and linear algebra.

Dalibor LUKÁŠ was born in Ostrava, Czech Republic. He received his Ph.D. from VŠB-Technical University of Ostrava in 2003. His research interests include numerical analysis and optimization for partial differential equations.

Petr VODSTRČIL was born in Svitavy, Czech Republic. He received his Ph.D. from Masaryk University in Brno in 2005. His research interests include calculus and functional analysis.