

**SUPPLEMENTARY MATERIALS: EIGENVALUE ANALYSIS FOR
SUMMATION-BY-PARTS FINITE DIFFERENCE TIME
DISCRETIZATIONS***

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Appendix A. Coefficients and auxiliary polynomials for the sixth order approximation.

The coefficients of S in (5.1) are [SM1]

$$\begin{aligned} s_{0,1} &= x - \frac{953}{16200}, & s_{0,2} &= -4x + \frac{715489}{259200}, & s_{0,3} &= 6x - \frac{62639}{14400} \\ s_{0,4} &= -4x + \frac{147127}{51840}, & s_{0,5} &= x - \frac{89387}{129600}, & s_{1,2} &= 10x - \frac{57139}{8640}, \\ s_{1,3} &= -20x + \frac{745733}{51840}, & s_{1,4} &= 15x - \frac{18343}{1728}, & s_{1,5} &= -4x + \frac{240569}{86400}, \\ s_{2,3} &= 20x - \frac{176839}{12960}, & s_{2,4} &= -20x + \frac{242111}{17280}, & s_{2,5} &= 6x - \frac{182261}{43200}, \\ s_{3,4} &= 10x - \frac{165041}{25920}, & s_{3,5} &= -4x + \frac{710473}{259200}, & s_{4,5} &= x, \end{aligned}$$

The centrosymmetric matrix $P = \Delta t \cdot \text{diag}(p_{0,0}, p_{1,1}, p_{2,2}, p_{3,3}, p_{4,4}, p_{5,5}, 1, \dots)$ have coefficients

$$\begin{aligned} p_{0,0} &= \frac{13649}{43200}, & p_{1,1} &= \frac{12013}{8640}, & p_{2,2} &= \frac{2711}{4320}, \\ p_{3,3} &= \frac{5359}{4320}, & p_{4,4} &= \frac{7877}{8640}, & p_{5,5} &= \frac{43801}{43200}. \end{aligned}$$

The polynomials $w_j(\xi, x)$ and $z_j(\xi, x)$ with $j = 6, \dots, 11$ are given by

$$\begin{aligned} w_6(\xi, x) &= \frac{4}{\psi_x} \left(85968164649369600000ix^2\xi \right. \\ &\quad + 34601523051479040000x^2\xi^2 - 130925704210304486400i\xi x \\ &\quad - 34514642471761495429 - 52760948337434131200x\xi^2 \\ &\quad + 49521812834468080661i\xi - 60045408811745280000x^2 \\ &\quad \left. + 19985164192464163800\xi^2 + 91347425343271180800x \right), \end{aligned}$$

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$$\begin{aligned}
w_7(\xi, x) = & \frac{4}{\psi_x} (1065056293548195840000ix^2\xi \\
& + 413132758434201600000x^2\xi^2 - 1614594755100447129600i\xi x \\
& - 412120665819592531057 - 627263956804040582400x\xi^2 \\
& + 608395474600054186485i\xi - 717030630940999680000x^2 \\
& + 236709838471838695412\xi^2 + 1090612145284761715200x),
\end{aligned}$$

$$\begin{aligned}
w_8(\xi, x) = & \frac{4}{\psi_x} (5920623284184023040000ix^2\xi \\
& + 2443936759048028160000x^2\xi^2 - 8951692427837922585600i\xi x \\
& - 2110499233697581321519 - 3693390408357925420800x\xi^2 \\
& + 3365816289578040654493i\xi - 3671907973017108480000x^2 \\
& + 1388166602591785744486\xi^2 + 5584453258245090854400x),
\end{aligned}$$

$$\begin{aligned}
w_9(\xi, x) = & \frac{24}{\psi_x} (346015230514790400000ix^2\xi^3 \\
& - 527609483374341312000ix\xi^3 + 260404207587164160000ix^2\xi \\
& + 199851641924641638000i\xi^3 - 292272196178165760000x^2\xi^2 \\
& - 356607105447971289600i\xi x + 473651105596461100800x\xi^2 \\
& + 122756596536943142108i\xi - 98023449664880640000x^2 \\
& - 18829201299579240547\xi^2 + 148233252115973260800x \\
& - 56360803784096215047),
\end{aligned}$$

$$\begin{aligned}
w_{10}(\xi, x) = & \frac{48}{\psi_x} (3622732329487564800000ix^2\xi^3 \\
& - 5510562459204738816000ix\xi^3 - 24289959255094149120000ix^2\xi \\
& + 2082881581020080848060i\xi^3 - 15675513485529784320000x^2\xi^2 \\
& + 36921230363424734726400i\xi x + 23856764225763152937600x\xi^2 \\
& - 13942452595064941719821i\xi + 13100048842656890880000x^2 \\
& - 9019971825478792684617\xi^2 - 19927030424828770771200x \\
& + 7529401904282397341322),
\end{aligned}$$

$$\begin{aligned}
w_{11}(\xi, x) = & \frac{24}{\psi_x} (7407786414809088000000ix^2\xi^3 \\
& - 112381601597419193856000ix\xi^3 - 477798340514167848960000ix^2\xi \\
& + 42380210597670438999940i\xi^3 - 325166633349679595520000x^2\xi^2 \\
& + 724562083605692135692800i\xi x + 492999042336751076025600x\xi^2 \\
& - 273104932981806697334542i\xi + 234925048347263631360000x^2 \\
& - 185799169127337922651951\xi^2 - 357315653928573599500800x \\
& + 135026783702317505775087),
\end{aligned}$$

$$\begin{aligned}
 z_6(\xi, x) = & \frac{1}{\psi_x} (43695367720796160000ix^2\xi \\
 & + 15617202862325760000x^2\xi^2 - 66830266947715891200i\xi x \\
 & - 23296384421857621513 - 23878172962818662400x\xi^2 \\
 & + 25387158792819872968i\xi - 40270212002119680000x^2 \\
 & + 9071486710640233680\xi^2 + 61481685481182950400x),
 \end{aligned}$$

$$\begin{aligned}
 z_7(\xi, x) = & \frac{1}{\psi_x} (601561273785384960000ix^2\xi \\
 & + 186465147442790400000x^2\xi^2 - 905927045191010611200i\xi x \\
 & - 348335310089525885509 - 282923497528708377600x\xi^2 \\
 & + 339545385968289956060i\xi - 627123377100718080000x^2 \\
 & + 106779856825842827824\xi^2 + 936638354766497356800x),
 \end{aligned}$$

$$\begin{aligned}
 z_8(\xi, x) = & \frac{1}{\psi_x} (3778404388294164480000ix^2\xi \\
 & + 1103057113756631040000x^2\xi^2 - 5627137491353217945600i\xi x \\
 & - 2034047000306985377179 - 1658625567833151820800x\xi^2 \\
 & + 2088349011720406798302i\xi - 3733369035290542080000x^2 \\
 & + 621071144802388085816\xi^2 + 5518863448241712307200x),
 \end{aligned}$$

$$\begin{aligned}
 z_9(\xi, x) = & \frac{6}{\psi_x} (156172028623257600000ix^2\xi^3 \\
 & - 238781729628186624000ix\xi^3 + 73868218832535520000ix^2\xi \\
 & + 90714867106402336800i\xi^3 - 180856612393943040000x^2\xi^2 \\
 & - 1010214750110777395200i\xi x + 302290549192744012800x\xi^2 \\
 & + 345221672882333601665i\xi - 854541521679974400000x^2 \\
 & - 123113796918437809636\xi^2 + 1192208719892161996800x \\
 & - 416258564887890370659),
 \end{aligned}$$

$$\begin{aligned}
 z_{10}(\xi, x) = & \frac{12}{\psi_x} (1635099866018611200000ix^2\xi^3 \\
 & - 2489135270970381696000ix\xi^3 - 13815202137502187520000ix^2\xi \\
 & + 942116186108024654720i\xi^3 - 7899560790553313280000x^2\xi^2 \\
 & + 20986177758900952089600i\xi x + 12020245428086150457600x\xi^2 \\
 & - 7923482606911181366279i\xi + 9999335244583895040000x^2 \\
 & - 4546737733818474369172\xi^2 - 15093907545333282163200x \\
 & + 5664846618108190866030i),
 \end{aligned}$$

$$\begin{aligned}
z_{11}(\xi, x) = \frac{6}{\psi_x} & (33434627437854720000000ix^2\xi^3 \\
& - 50645512722529990656000ix\xi^3 - 314802210504889958400000ix^2\xi \\
& + 19086633778180219487120i\xi^3 - 170462527753646407680000x^2\xi^2 \\
& + 471705802315568322969600i\xi x + 256946608933388322278400x\xi^2 \\
& - 175989809585607907698739i\xi + 213800389798992445440000x^2 \\
& - 96397406768479044336336\xi^2 - 31840863043391268403200x \\
& + 118121838276427015819707).
\end{aligned}$$

Appendix B. Proof of Theorem 5.5 for $x = x_2 = 89387/129600$.

We follow the steps of Theorem 5.4. To start with, we observe that also in this case for $N \geq 17$ the first term of $D(\xi, x_2, N)$ in (5.3) is dominant, since

$$|\tau_{1,2}(\xi, x_2)| \gtrsim 7.576 \cdot 10^{77}, \quad |\tau_{1,5}(\xi, x_2)| \lesssim 6.459 \cdot 10^{73},$$

$$|\tau_{1,6}(\xi, x_2)| \lesssim 4.615 \cdot 10^{73}, \quad |\tau_{2,5}(\xi, x_2)| \lesssim 7.648 \cdot 10^{73},$$

$$|\tau_{2,6}(\xi, x_2)| \lesssim 6.459 \cdot 10^{73}, \quad |\tau_{5,6}(\xi, x_2)| \lesssim 1.210 \cdot 10^{54},$$

for $\xi \in I_\xi = [0, 4.21]$. This results in $D(\xi, x_2, N) \neq 0$ for any $N \geq 17$, and for these values the statement is proved due to Lemma 2.5.

However, differently from Theorem 5.4, by using (5.4) it can be verified that the first term of (5.3) ceases to be dominant for $N \leq 15$. For such values of N cancellation errors may occur in the computation of the determinant leading to untrustworthy results. On the other hand, for $N \in \{12, 13, 14, 15\}$ the claim can be verified numerically. Figure SM1 shows the spectrum of \mathcal{D} for the sixth order approximation with

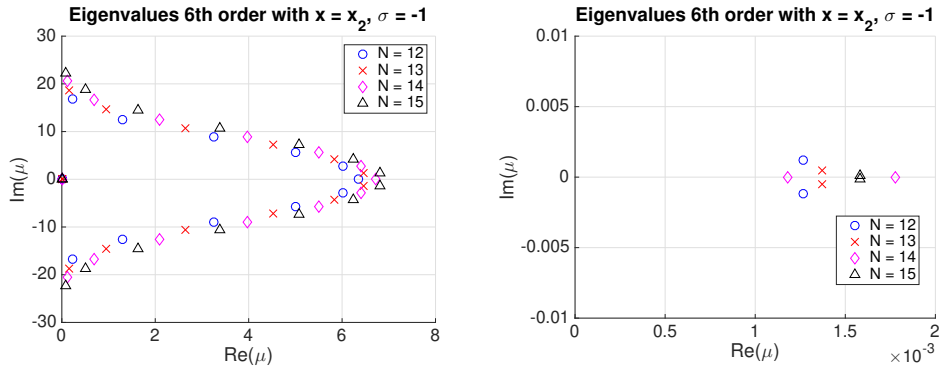


FIG. SM1. The spectrum of the sixth order approximation \mathcal{D} with $x = x_2 = 89387/129600$, $\sigma = -1$, $N \in \{12, 13, 14, 15\}$ and $\Delta t = 1/N$. The right figure is a magnification of the left figure.

$x = x_2$, $\Delta t = 1/N$ and $\sigma = -1$. Note that the minimum value of $\text{Re}(\mu)$ is positive for each N , but extremely close to the imaginary axis. This phenomenon appears to be peculiar for the parameter choice $x = x_2$ when N is small.

Appendix C. Proof of Theorem [Theorem 5.5](#) for $x = x_3 = 0.70127127\dots$

As for [Theorem 5.4](#), for $N \geq 17$ the term with $1/(r_1 r_2)^{N-17}$ in [\(5.3\)](#) is dominant, since

$$|\tau_{1,2}(\xi, x_3)| \gtrsim 1.576 \cdot 10^{83}, \quad |\tau_{1,5}(\xi, x_3)| \lesssim 7.559 \cdot 10^{71},$$

$$|\tau_{1,6}(\xi, x_3)| \lesssim 6.121 \cdot 10^{71}, \quad |\tau_{2,5}(\xi, x_3)| \lesssim 9.728 \cdot 10^{71},$$

$$|\tau_{2,6}(\xi, x_3)| \lesssim 7.559 \cdot 10^{71}, \quad |\tau_{5,6}(\xi, x_3)| \lesssim 2.219 \cdot 10^{52},$$

for $\xi \in I_\xi = [0, 4.21]$. This implies that $D(\xi, x_3, N) \neq 0$ for any $N \geq 17$.

The determinant can not be zero also for smaller values of $N \geq 12$. Indeed, the term with $1/(r_1 r_2)^{N-17}$ dominates even for $N = 12$, value for which we find

$$\left| \frac{\tau_{1,2}(\xi, x_3)}{(r_1 r_2)^{-5}} \right| \gtrsim 9.446 \cdot 10^{73}, \quad \left| \frac{\tau_{1,5}(\xi, x_3)}{(r_1 r_5)^{-5}} \right| \lesssim 7.559 \cdot 10^{71},$$

$$\left| \frac{\tau_{1,6}(\xi, x_3)}{(r_1 r_6)^{-5}} \right| \lesssim 7.828 \cdot 10^{71}, \quad \left| \frac{\tau_{2,5}(\xi, x_3)}{(r_2 r_5)^{-5}} \right| \lesssim 9.728 \cdot 10^{71},$$

$$\left| \frac{\tau_{2,6}(\xi, x_3)}{(r_2 r_6)^{-5}} \right| \lesssim 7.559 \cdot 10^{71}, \quad \left| \frac{\tau_{5,6}(\xi, x_3)}{(r_5 r_6)^{-5}} \right| \lesssim 4.126 \cdot 10^{61},$$

for $\xi \in I_\xi$.

As a result, the determinant $D(\xi, x_3, N) \neq 0$ for $N \geq 12$, $\xi \in I_\xi$. Hence, no eigenvectors of $P^{-1}S$ in [\(5.1\)](#) have first and last component equal to zero, if $x = x_3 = 0.70127127127\dots$. As a result, the eigenvalues μ of \mathcal{D} have strictly positive real parts due to [Lemma 2.5](#).

REFERENCE

[SM1] B. STRAND, *Summation by parts for finite difference approximations for d/dx* , Journal of Computational Physics, 110 (1994), pp. 47–67, <https://doi.org/10.1006/jcph.1994.1005>.