Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Higher-Order Split Operator Schemes for Solving the Schrödinger Equation in the Time-Dependent Wave Packet Method: Applications to Triatomic Reactive Scattering Calculations

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The names of the propagators following are named according to its original theoretical orders, the number of stages and the classification in the paper work, such as the 4S5 propagator indicates a 4th-order propagator with 5 stages (one time step needs 5 times action of $\hat{H}$ on the wave function) , which has a symmetric form with respective to the central parameter and the 4A5a propagator has the same stage number as the 4S5 propagator but with different parameters and asymmetric form. The last label "a" in the name of 4A5a is used to distinguish the propagators which fall into same class and have same stage number.

Parameters for all the tested higher-order splitting operators in form of Eq.5 (the Class S, with symmetric form):

4S3 $\omega_1 = 2 + 2^{1/3} + 1/2^{1/3}$, $\omega_0 = 1 - 2\omega_1$ [1]

4S5 $\omega_1 = 1/(4 - 4^{1/3})$, $\omega_2 = \omega_1$, $\omega_0 = 1 - 4\omega_1$ [2]

4S7 $\omega_1 = 1/(6 - 6^{1/3})$, $\omega_2 = \omega_1$, $\omega_3 = \omega_1$, $\omega_0 = 1 - 6\omega_1$ [2]

4S9 $\omega_1 = 1/(8 - 8^{1/3})$, $\omega_2 = \omega_1$, $\omega_3 = \omega_1$, $\omega_4 = \omega_1$, $\omega_0 = 1 - 8\omega_1$ [2]

4S11 $\omega_1 = 1/(10 - 10^{1/3})$, $\omega_2 = \omega_1$, $\omega_3 = \omega_1$, $\omega_4 = \omega_1$, $\omega_5 = \omega_1$ $\omega_0 = 1 - 10\omega_1$ [2]

6S7 $\omega_3 = 0.78451361047755726381949763$, $\omega_2 = 0.23557321335935813368479318$, $\omega_1 = -1.17767998417887100694641568$, $\omega_0 = 1 - 2(\omega_3 + \omega_2 + \omega_1)$, Ref.[1, 3]

6S9a $\omega_4 = 0.39216144400731413927925056$, $\omega_3 = 0.33259913678935943859974864$, $\omega_2 = -0.70624617255763935980996482$, $\omega_1 = 0.08221359629355080023149045$, $\omega_0 = 1 - 2(\omega_4 + \omega_3 + \omega_2 + \omega_1)$, Ref.[3, 4]

6S9b $Y_1 = 1/(2 - 2^{1/5})$, $Y_0 = -2^{1/5}/(2 - 2^{1/5})$, $X_1 = 1/(2 - 2^{1/3})$, $X_0 = -2^{1/3}/(2 - 2^{1/3})$, $\omega_4 = Y_1 * X_1$, $\omega_3 = Y_1 * X_0$, $\omega_2 = Y_1 * X_1$, $\omega_1 = Y_0 * X_1$, $\omega_0 = Y_0 * X_0)$, [2]

6S11a $\omega_5 = 0.1705768865009222157$, $\omega_4 = \omega_5$, $\omega_3 = \omega_5$, $\omega_2 = \omega_5$, $\omega_1 = -0.423366140892658048$, $\omega_0 = 1 - 2(\omega_5 + \omega_4 + \omega_3 + \omega_2 + \omega_1)$, Ref.[5]

6S11b $\omega_5 = 0.21375583945878254555518066964857$,
$\omega_4 = 0.18329381407425713911385974425217$,
$\omega_3 = 0.17692819473098943794898811709929$,
$\omega_2 = -0.44329082681170215849622829626258$,
$\omega_1 = 0.11728560432865935385403585669136$,
$\omega_0 = 1 - 2(\omega_5 + \omega_4 + \omega_3 + \omega_2 + \omega_1)$, Ref.[6]

6S13 $\omega_6 = 0.13861930854051695245808013042625$,
$\omega_5 = 0.13346562851074760407046858832209$,
$\omega_4 = 0.13070531011449225190542755785015$,
$\omega_3 = 0.12961893756907034772505366537091$,
$\omega_2 = -0.35000324893920896516170830911323$,
$\omega_1 = 0.11805530653002387170273438954049$,
$\omega_0 = 1 - 2(\omega_6 + \omega_5 + \omega_4 + \omega_3 + \omega_2 + \omega_1)$, Ref.[6]

6S15 $Y_1 = 1/(4 - 4^{1/5})$, $Y_0 = -4^{1/5}/(4 - 4^{1/5})$, $X_1 = 1/(2 - 2^{1/3})$, $X_0 = -2^{1/3}/(2 - 2^{1/3})$, $\omega_7 = Y_1 * X_1$, $\omega_6 = Y_1 * X_0$, $\omega_5 = Y_1 * X_1$, $\omega_4 = Y_1 * X_1$, $\omega_3 = Y_1 * X_0$, $\omega_2 = Y_1 * X_1$, $\omega_1 = Y_0 * X_1$, $\omega_0 = Y_0 * X_0$, Ref. [2]

8S15a $\omega_7 = 0.629030650210433$, $\omega_6 = 0.1369349464166871$,
$\omega_5 = -1.06458714789183$, $\omega_4 = 1.66335809963315$, $\omega_3 = -1.67896928259640$, $\omega_2 = -1.55946803821447$, $\omega_1 = 0.311790812418427$, $\omega_0 = 1 - 2(\omega_7 + \omega_6 + \omega_5 + \omega_4 + \omega_3 + \omega_2 + \omega_1)$, Ref.[7]

8S15b $\omega_7 = 0.74167036435061295344822780$,
$\omega_6 = -0.40910082580003159399730010$, $\omega_5 = 0.19075471029623837995387626$, $\omega_4 = -0.57386247111608226665638773$, $\omega_3 = 0.29906418130365592384446354$, $\omega_2 = 0.33462491824529818378495798$, $\omega_1 = 0.31529309239676659663205666$, $\omega_0 = 1 - 2(\omega_7 + \omega_6 + \omega_5 + \omega_4 + \omega_3 + \omega_2 + \omega_1)$ Ref.[3, 8]

8S17 $\omega_8 = 0.13020248308889008087881763$,
$\omega_7 = 0.56116298177510838456196441$, $\omega_6 = -0.38947496264484728640807860$,

$\omega_5 = 0.15884190655515560089621075$, $\omega_4 = -0.39590389413323757733623154$, $\omega_3 = 0.18453964097831570709183254$, $\omega_2 = 0.25837438768632204729397911$, $\omega_1 = 0.29501172360931029887096624$, $\omega_0 = 1 - 2(\omega_8 + \omega_7 + \omega_6 + \omega_5 + \omega_4 + \omega_3 + \omega_2 + \omega_1)$ Ref.[6]

8S19 $\omega_9 = 0.102369976919196772179472330167 68$,
$\omega_8 = 0.15193719542124150042122517519886$,
$\omega_7 = -0.25758500798800419714675345320434$,
$\omega_6 = 0.22207280907359627745287320824157$,
$\omega_5 = 0.14428079109272857169409977400023$,
$\omega_4 = 0.45902412791454253044738988194508$,
$\omega_3 = -0.35087981035009346255903840093339$,
$\omega_2 = 0.12632969388923674360157818562148$,
$\omega_1 = 0.14951143568721988602249080443402$,
$\omega_0 = 1 - 2(\omega_8 + \omega_7 + \omega_6 + \omega_5 + \omega_4 + \omega_3 + \omega_2 + \omega_1)$, Ref.[3, 4]

Parameters for all the tested higher-order splitting operators in form of Eq.6 (the Class A, with asymmetric form):

4A4a $\alpha_1 = 1/2 - \frac{\sqrt{7/8}}{3}$, $\alpha_2 = -1/3 + \frac{\sqrt{7/8}}{3}$, $\alpha_3 = 1 - 2(\alpha_1 + \alpha_2)$, $\alpha_4 = \alpha_2$, $\alpha_5 = \alpha_1$; $\beta_1 = 1$, $\beta_2 = 1/2 - \beta_1 = -1/2$, $\beta_3 = \beta_2$, $\beta_4 = \beta_1$ Ref.[8]

4A4b $\alpha_1 = 0.13449619927743108 92/2$, $\alpha_2 = -0.22481980307942080 58$, $\alpha_3 = 0.75632000051566829 11$, $\alpha_4 = 0.33400360328632142 55$, $\alpha_5 = \alpha_1$; $\beta_1 = 0.51535283743112293 64$, $\beta_2 = -0.08578201941297364 6$, $\beta_3 = 0.44158302361646652 42$, $\beta_4 = 0.12884615836538418 54$ Ref.[9]

4A5a $\alpha_1 = \frac{14-\sqrt{19}}{108}$, $\alpha_2 = \frac{20-7\sqrt{19}}{108}$, $\alpha_3 = 1/2 - (\alpha_1 + \alpha_2)$, $\alpha_4 = \alpha_3$, $\alpha_5 = \alpha_2$, $\alpha_6 = \alpha_1$; $\beta_1 = 2/5$, $\beta_2 = -1/10$, $\beta_3 = 1 - 2(\beta_1 + \beta_2) = 2/5$, $\beta_4 = \beta_2$, $\beta_5 = \beta_1$ Ref.[3, 8]

4A5b $\alpha_1 = 0.81186273854451628884$, $\alpha_2 = -0.67748039953216912289$, $\alpha_3 = 1/2 - (\alpha_1 + \alpha_2)$, $\alpha_4 = \alpha_3$, $\alpha_5 = \alpha_2$, $\alpha_6 = \alpha_1$; $\beta_1 = -0.00758691311877447385$, $\beta_2 = 0.31721827797316981388$, $\beta_3 = 1 - 2(\beta_1 + \beta_2) = 2/5$, $\beta_4 = \beta_2$, $\beta_5 = \beta_1$ Ref.[10]

4S6a $\alpha_1 = 0.0792036964311957$, $\alpha_2 = 0.353172906049774$, $\alpha_3 = -0.0420650803577195$, $\alpha_4 = 1-2(\alpha_1+\alpha_2+\alpha_3)$, $\alpha_5 = \alpha_3$, $\alpha_6 = \alpha_2$, $\alpha_7 = \alpha_1$; $\beta_1 = 0.209515106613362$, $\beta_2 = -0.143851773179818$, $\beta_3 = 1/2 - (\beta_1 + \beta_2)$, $\beta_4 = \beta_3$, $\beta_5 = \beta_2$, $\beta_6 = \beta_1$ Ref.[11]

4A6b $\alpha_1 = 0.0829844064174052$, $\alpha_2 = 0.396309801498368$, $\alpha_3 = -0.0390563049223486$, $\alpha_4 = 1 - 2(\alpha_1 + \alpha_2 + \alpha_3)$, $\alpha_5 = \alpha_3$, $\alpha_6 = \alpha_2$, $\alpha_7 = \alpha_1$; $\beta_1 = 0.245298957184271$, $\beta_2 = 0.604872665711080$, $\beta_3 = 1/2 - (\beta_1 + \beta_2)$, $\beta_4 = \beta_3$, $\beta_5 = \beta_2$, $\beta_6 = \beta_1$ Ref.[11]

6B6S $\alpha_1 = 0.15$, $\alpha_2 = 0.3297455985640361$, $\alpha_3 = -0.049363257050623707$, $\alpha_4 = 1 - 2(\alpha_1 + \alpha_2 + \alpha_3)$, $\alpha_5 = \alpha_3$, $\alpha_6 = \alpha_2$, $\alpha_7 = \alpha_1$; $\beta_1 = 0.316$, $\beta_2 = 0.4312992634164797$, $\beta_3 = 1/2 - (\beta_1 + \beta_2)$, $\beta_4 = \beta_3$, $\beta_5 = \beta_2$, $\beta_6 = \beta_1$ Ref.[5, 11]

6A8 $\alpha_1 = 0.06942944346252987735848865824703402$,

$\alpha_2 = -0.13315519831598209409961309951373512$,

$\alpha_3 = 0.00129038917981078974230481746443284$,

$\alpha_4 = 0.42243536567364142699881962380226825$,

$\alpha_5 = 1 - 2 * (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4)$,

$\alpha_6 = \alpha_4$, $\alpha_7 = \alpha_3$, $\alpha_8 = \alpha_2$, $\alpha_9 = \alpha_1$;

$\beta_1 = 0.28487837717280084052745346456657828$,

$\beta_2 = 0.32783975759612945412054678367325547$,

$\beta_3 = -0.38122104271932629475622784374211274$,

$\beta_4 = 1/2 - (\beta_1 + \beta_2 + \beta_3)$,

$\beta_5 = \beta_4$, $\beta_6 = \beta_3$, $\beta_7 = \beta_2$, $\beta_8 = \beta_1$, Ref.[12]

6A9 $\alpha_1 = 0.09517625454177405267746114335519342$,

$\alpha_2 = -0.12795028552368677941219191621429411$,

$\alpha_3 = 0.10597295345325113143793587608716998$,

$\alpha_4 = 0.44822227660082748416851634186561201$,

$\alpha_5 = 1/2 - (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4)$,

$\alpha_6 = \alpha_5$, $\alpha_7 = \alpha_4$, $\alpha_8 = \alpha_3$, $\alpha_9 = \alpha_2$, $\alpha_{10} = \alpha_1$;

$\beta_1 = 0.66629689399770780134207498907168068$,

$\beta_2 = 0.02461890095210508713078430308713062$,

$\beta_3 = -0.41072553361795113231992873918199025,$

$\beta_4 = 0.65772926205091317768935130009339042,$

$\beta_5 = 1 - 2*(\beta_1 + \beta_2 + \beta_3 + \beta_4),$

$\beta_6 = \beta_4,\ \beta_7 = \beta_3,\ \beta_8 = \beta_2,\ \beta_9 = \beta_1,$ Ref.[12]

6A10 $\alpha_1 = 0.0502627644003922,\ \alpha_2 = 0.413514300428344,$ $\alpha_3 = 0.0450798897943977,\ \alpha_4 = -0.188054853819569,$ $\alpha_5 = 0.541960678450780,\ \alpha_6 = 1 - 2*(\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5),\ \alpha_7 = \alpha_5,$ $\alpha_8 = \alpha_4,\ \alpha_9 = \alpha_3,\ \alpha_{10} = \alpha_2,\ \alpha_{11} = \alpha_1;\ \beta_1 = 0.148816447901042,$ $\beta_2 = -0.132385865767784,\ \beta_3 = 0.067307604692185,\ \beta_4 = 0.432666402578175,$ $\beta_5 = 1/2 - (\beta_1 + \beta_2 + \beta_3 + \beta_4),\ \beta_6 = \beta_5,\ \beta_7 = \beta_4,\ \beta_8 = \beta_3,\ \beta_9 = \beta_2,\ \beta_{10} = \beta_1,$ Ref.[11]

6A11a $\alpha_1 = 0.0596950146437836379,\ \alpha_2 = 0.3494636851912376154,$ $\alpha_3 = -0.0856561791358,\ \alpha_4 = 0.2006347511256767 24,\ \alpha_5 = 0.00535254,\ \alpha_6 = 1/2 - (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5),\ \alpha_7 = \alpha_6,\ \alpha_8 = \alpha_5,\ \alpha_9 = \alpha_4,\ \alpha_{10} = \alpha_3,\ \alpha_{11} = \alpha_2,$ $\alpha_{12} = \alpha_1;\ \beta_1 = 0.16992,\ \beta_2 = -0.0443007,\ \beta_3 = 0.2929282384129810594,$ $\beta_4 = -0.3015196782682459 44,\ \beta_5 = 0.1617903982773488197,\ \beta_6 = 1 - 2*(\beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5),\ \beta_7 = \beta_5,\ \beta_8 = \beta_4,\ \beta_9 = \beta_3,\ \beta_{10} = \beta_2,\ \beta_{11} = \beta_1,$ Ref.[13]

6A11b $\alpha_1 = 0.0414649985182624,\ \alpha_2 = 0.198128671918067,$ $\alpha_3 = -0.0400061921041533,\ \alpha_4 = 0.0752539843015807,$ $\alpha_5 = -0.0115113874206879,\ \alpha_6 = 1/2 - (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5),\ \alpha_7 = \alpha_6,$ $\alpha_8 = \alpha_5,\ \alpha_9 = \alpha_4,\ \alpha_{10} = \alpha_3,\ \alpha_{11} = \alpha_2,\ \alpha_{12} = \alpha_1;\ \beta_1 = 0.123229775946271,\ \beta_2 = 0.290553797799558,\ \beta_3 = -0.127049212625417,\ \beta_4 = -0.246331761062075,$ $\beta_5 = 0.357208872795928,\ \beta_6 = 1 - 2*(\beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5),\ \beta_7 = \beta_5,$ $\beta_8 = \beta_4,\ \beta_9 = \beta_3,\ \beta_{10} = \beta_2,\ \beta_{11} = \beta_1,$ Ref.[11]

6A11c $\alpha_1 = 0.046487454790863130865306186981 7,$

$\alpha_2 = -0.06069167116564293530913254940 96,$

$\alpha_3 = 0.2184665264634068104730525196 99,$

$\alpha_4 = 0.1680535794830927030415174251 35,$

$\alpha_5 = 0.3143923641703534867418171557 44,$

$\alpha_6 = 1/2 - (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5),$

$\alpha_7 = \alpha_6$, $\alpha_8 = \alpha_5$, $\alpha_9 = \alpha_4$, $\alpha_{10} = \alpha_3$, $\alpha_{11} = \alpha_2$, $\alpha_{12} = \alpha_1$;

$\beta_1 = 0.184330483502665563472197717881$,

$\beta_2 = -0.041056903297711462374776749004\,0$,

$\beta_3 = 0.133755679666750330706128392342$,

$\beta_4 = 0.203764547132354738209957028584$,

$\beta_5 = -0.011760166914960043722445217921\,6$,

$\beta_6 = 1 - 2 * (\beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5)$,

$\beta_7 = \beta_5$, $\beta_8 = \beta_4$, $\beta_9 = \beta_3$, $\beta_{10} = \beta_2$, $\beta_{11} = \beta_1$, Ref.[12]

6A14 $\alpha_1 = 0.0378593198406116$, $\alpha_2 = 0.102635633102435$, $\alpha_3 = -0.0258678882665587$, $\alpha_4 = 0.314241403071447$, $\alpha_5 = -0.130144459517415$, $\alpha_6 = 0.106417700369543$, $\alpha_7 = -0.00879424312851058$, $\alpha_8 = 1 - 2 * (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6 + \alpha_7)$, $\alpha_9 = \alpha_7$, $\alpha_{10} = \alpha_6$, $\alpha_{11} = \alpha_5$, $\alpha_{12} = \alpha_4$, $\alpha_{13} = \alpha_3$, $\alpha_{14} = \alpha_2$, $\alpha_{15} = \alpha_1$; $\beta_1 = 0.09171915262446165$, $\beta_2 = 0.183983170005006$, $\beta_3 = -0.05653436583288827$, $\beta_4 = 0.004914688774712854$, $\beta_5 = 0.143761127168358$, $\beta_6 = 0.328567693746804$, $\beta_7 = 1/2 - (\beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5 + \beta_6)$, $\beta_8 = \beta_7$, $\beta_9 = \beta_6$, $\beta_{10} = \beta_5$, $\beta_{11} = \beta_4$, $\beta_{12} = \beta_3$, $\beta_{13} = \beta_2$, $\beta_{14} = \beta_1$, Ref.[11]

8A17a $\alpha_1 = 0.0402075762629562729665392145489236\,7$,

$\alpha_2 = 0.170237595648858947062574539066635\,63$,

$\alpha_3 = 0.243702339985034323531956334868953\,07$,

$\alpha_4 = 0.566019637953660460198995997019395\,48$,

$\alpha_5 = -0.581696957624970395185299997976200\,05$,

$\alpha_6 = -0.241386398304779874531714820292386\,17$,

$\alpha_7 = 0.361150975697931273730140003215996\,16$,

$\alpha_8 = -0.532254504603771652840254469334539\,53$,

$\alpha_9 = 11/2 - (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6 + \alpha_7 + \alpha_8)$,

$\alpha_{10} = \alpha_9$, $\alpha_{11} = \alpha_8$, $\alpha_{12} = \alpha_7$, $\alpha_{13} = \alpha_6$, $\alpha_{14} = \alpha_5$, $\alpha_{15} = \alpha_4$,

$\alpha_{16} = \alpha_3$, $\alpha_{17} = \alpha_2$, $\alpha_{18} = \alpha_1$;

$\beta_1 = 0.109682521400819958808521114521314\,55$,

$\beta_2 = 0.367561588063370064331497573690262\,77$,

$\beta_3 = -0.045441314197580656614373759630888864,$

$\beta_4 = 0.000221671621698640396438221855570309,$

$\beta_5 = 0.055199270980923287596797628295263777,$

$\beta_6 = -0.125139299816180235240503707453217227,$

$\beta_7 = -0.042843893529376102559143087343243331,$

$\beta_8 = -0.003933672993291574105104560948580013,$

$\beta_9 = 1 - 2 * (\beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5 + \beta_6 + \beta_7 + \beta_8),$

$\beta_{10} = \beta_8,\ \beta_{11} = \beta_7,\ \beta_{12} = \beta_6,\ \beta_{13} = \beta_5,\ \beta_{14} = \beta_4,\ \beta_{15} = \beta_3,\ \beta_{16} = \beta_2,$

$\beta_{17} = \beta_1,$ Ref.[12]

8A17b $\alpha_1 = 0.036766803899123373026661549294292911,$

$\alpha_2 = 0.160404293742555602193953812145097800,$

$\alpha_3 = -0.004728776439412879186394124360886645,$

$\alpha_4 = 0.029830984893350569548844405587633334,$

$\alpha_5 = 0.191358443110910979848857561752072225,$

$\alpha_6 = -0.037819681457451286777236357614173776,$

$\alpha_7 = 0.003518459963780936055184438702293885,$

$\alpha_8 = 0.130670138672716186765145806083032776,$

$\alpha_9 = 1/2 - (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6 + \alpha_7 + \alpha_8),$

$\alpha_{10} = \alpha_9,\ \alpha_{11} = \alpha_8,\ \alpha_{12} = \alpha_7,\ \alpha_{13} = \alpha_6,\ \alpha_{14} = \alpha_5,\ \alpha_{15} = \alpha_4,$

$\alpha_{16} = \alpha_3,\ \alpha_{17} = \alpha_2,\ \alpha_{18} = \alpha_1;$

$\beta_1 = 0.110726550037397841757547973122797745,$

$\beta_2 = 0.611012678251715236279627186077854228,$

$\beta_3 = -0.192028090690325353968383340493795558,$

$\beta_4 = -0.259790739298116602571628335448612286,$

$\beta_5 = 0.383845640668820937542744994212362298,$

$\beta_6 = 0.326616648867781201359729217618729954,$

$\beta_7 = -0.534634433748970256786633982427421774,$

$\beta_8 = -0.399356320810782813548068423496356698,$

$\beta_9 = 1 - 2 * (\beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5 + \beta_6 + \beta_7 + \beta_8),$

$\beta_{10} = \beta_8,\ \beta_{11} = \beta_7,\ \beta_{12} = \beta_6,\ \beta_{13} = \beta_5,\ \beta_{14} = \beta_4,\ \beta_{15} = \beta_3,\ \beta_{16} = \beta_2,$

$\beta_{17} = \beta_1,$ Ref.[12]

8A17c $\alpha_1 = 0.044637950523590227559139996257335 90,$

$\alpha_2 = 0.21988440427147072254445535069606167,$

$\alpha_3 = 0.10250365693975069608261241007779814,$

$\alpha_4 = -0.00477482916916881658022489063962934,$

$\alpha_5 = -0.03886264282111817697737420875189743,$

$\alpha_6 = 0.18681583743297155471526153503972746,$

$\alpha_7 = -0.02405084735747361993573587982407554,$

$\alpha_8 = -0.05897433015592386914575323926766330,$

$\alpha_9 = 1/2 - (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6 + \alpha_7 + \alpha_8),$

$\alpha_{10} = \alpha_9,\ \alpha_{11} = \alpha_8,\ \alpha_{12} = \alpha_7,\ \alpha_{13} = \alpha_6,\ \alpha_{14} = \alpha_5,\ \alpha_{15} = \alpha_4,$

$\alpha_{16} = \alpha_3,\ \alpha_{17} = \alpha_2,\ \alpha_{18} = \alpha_1;$

$\beta_1 = 0.13593258071690959145543264213495574,$

$\beta_2 = 0.13024946780523828601621193778196846,$

$\beta_3 = 0.43234521869358547487983257884877035,$

$\beta_4 = -0.58253476904040845493112837930861212,$

$\beta_5 = 0.31548728537940479698273603797274199,$

$\beta_6 = 0.26500275499062083398346002963079872,$

$\beta_7 = -0.45040492499772251180922896712151891,$

$\beta_8 = -0.02168476171861335324934388684707580,$

$\beta_9 = 1 - 2 * (\beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5 + \beta_6 + \beta_7 + \beta_8),$

$\beta_{10} = \beta_8,\ \beta_{11} = \beta_7,\ \beta_{12} = \beta_6,\ \beta_{13} = \beta_5,\ \beta_{14} = \beta_4,\ \beta_{15} = \beta_3,\ \beta_{16} = \beta_2,$

$\beta_{17} = \beta_1$, Ref.[12]

For more details about the meaning of the parameters in the following table, please see Ref.[14].

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	$H+H_2$	H+HN	$H+^{32}O_2$	F+HD
Grid/basis range and size	$R \in [0.1, 12.0]$, N_R^1=63, N_R^2=49	$R \in [0.3, 16.0]$, N_R^1=143, N_R^2=63	$R \in [0.015, 14.5]$, N_R^1=179, N_R^2=119	$R \in [0.1, 38.0]$, N_R^1=399, N_R^2=299
	$r \in [0.4, 9.0]$, N_r^1=49, N_r^2=23	$r \in [0.4, 13.5]$, N_r^1=127, N_r^2=31	$r \in [0.7, 13.2]$, N_r^1=255, N_r^2=49	$r \in [0.6, 36.0]$, N_r^1=269, N_r^2=31
	$j_{\min} = 0 \sim j_{\max} = 46$, N_j=24	$j_{\min} = 0 \sim j_{\max} = 46$, N_j=47	$j_{\min} = 0 \sim j_{\max} = 120$, N_j=61	$j_{\min} = 0 \sim j_{\max} = 260$, N_j=261
Initial wavepacket				
$\exp[-\frac{(R-R_0)^2}{2\Delta_R^2} ik_0R]$ or	R_0=8.0	R_0=11.0	R_0=11.0	R_0=17.0
$\exp[-\frac{(R-R_0)^2}{2\Delta_R^2}]\cos(k_0R)$	Δ_R=0.5	Δ_R=0.3	Δ_R=0.5	Δ_R=1.0
	$k_0 = \sqrt{2E_0\mu_R}$ with E_0=0.7eV	$k_0 = \sqrt{2E_0\mu_R}$ with E_0=0.5eV	$k_0 = \sqrt{2E_0\mu_R}$ with E_0=0.7eV	$k_0 = \sqrt{2E_0\mu_R}$ with E_0=0.035eV
Absorbing Potential	$C' = 0.1$, $n' = n = 2$, $R_a = 9.5$	$C' = 0.02$, $n' = n = 1$, $R_a = 12.0$	$C' = 0.012$, $n' = n = 2$, $R_a = 9.2$	$C' = 0.0015$, $n' = n = 1$, $R_a = 22.0$
	$C_a = 0.12$, $C_b = 0.3$, r_a=6.7, r_b=8.9	$C_a = 0.01$, $C_b = 0.03$, r_a=10.5, r_b=12.5	$C_a = 0.003$, $C_b = 0.04$, r_a=10.0, r_b=12.2	$C_a = 0.001$, $C_b = 0.06$, r_a=16.0, r_b=34.0
Total propagation time	10000a.u./ 1200 iterations	150K a.u./ 70K iterations	170K a.u./ 60K iterations	300K a.u./ 150K iterations
Matching Plane	R_0'=5.5	R_0'=10.0	R_0'=10.0	R_0'=13.2

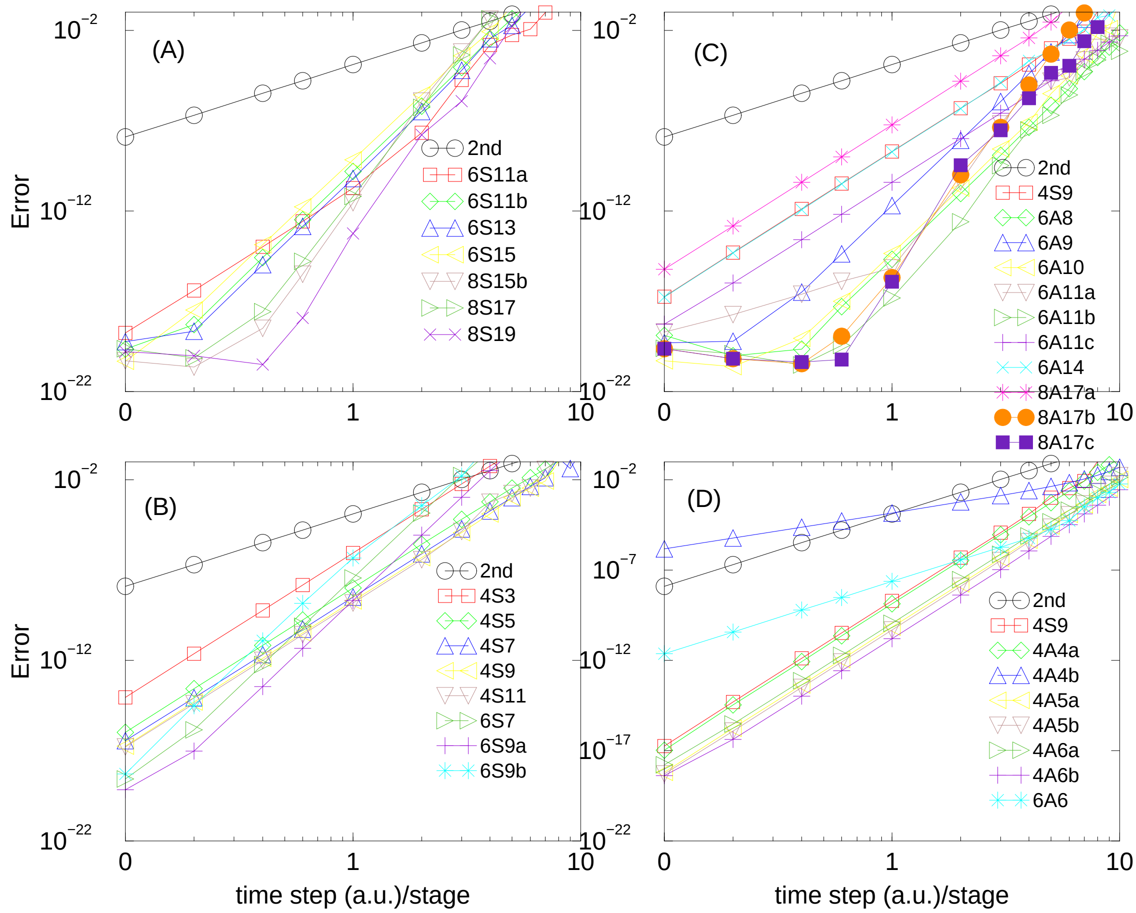

FIG. 1: $\log_{10}(\text{error})$ vs $\log_{10}(\text{effort-time step})$ associated with higher order operator splitting methods implemented in the VTV form on 1D Morse model.

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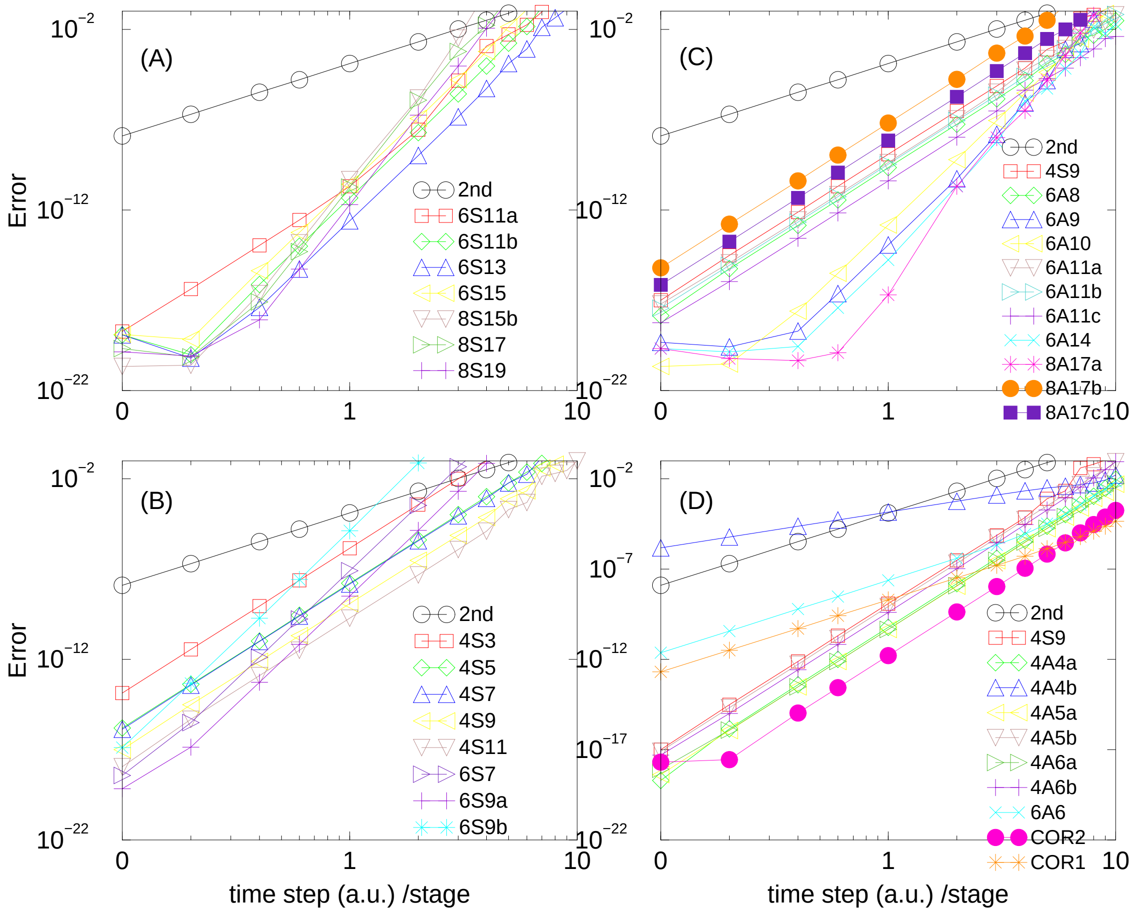

FIG. 2: $\log_{10}$(error) vs $\log_{10}$(effort-time step) associated with higher order operator splitting methods implemented in the TVT form on 1D Morse model. In this TVT form implementation, the accuracy of the 4A4a, 4S9, 6S9b, 6S15, 6A9, 6S11a, 6S11b and 8A17a propagators increases but the accuracy of the 4A6b, 6S13, 6A8, 6A11a, 6A10, 6A11b and 8S19 propagators decrease, comparing with that of those in the VTV form implementation.