# Quadrature approximation to the Magnus exponent for numerical solution of non-autonomous coupled linear differential equations

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Version 17-Apr-2026

Abstract

The Magnus-exponent method of solving non-autonomous (variable-coefficient) coupled linear differential equations is reviewed, and three quadrature approximation formulas are derived with residual errors proportional to the 3rd, 5th, and 7th power of the integration interval size.

## Linear differential equations

A *first-order, linear differential equation* or system of differential equations has the form

$$F'[t] = A[t] \cdot F[t] + B[t], \quad F[0] = F_0 \tag{1}$$

where $F[t]$, $A[t]$, and $B[t]$ are matrix functions of scalar argument $t$, $F_0$ is a specified initial value, and $F[t]$ is to be determined. (The Mathematic notation for bracket-delimited function arguments $[\ldots]$ is used here.) The equation is *autonomous* if $A$ and $B$ are constant, and is *homogeneous* if $B[t]$ is identically zero.

A nonhomogeneous equation can be converted to a homogeneous equation by using an alternative formulation of Eq. 1,

$$\frac{d}{dt}\begin{pmatrix} F[t] \\ \mathbf{I} \end{pmatrix} = \begin{pmatrix} A[t] & B[t] \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \cdot \begin{pmatrix} F[t] \\ \mathbf{I} \end{pmatrix} \tag{2}$$

where $\mathbf{I}$ and $\mathbf{0}$ represent identity and zero matrices, respectively. Therefore, we need only consider homogeneous equations, although Eq. (2) might be implemented to efficiently take advantage of the zeros in the coefficient matrix.

With $B[t] = \mathbf{0}$, the solution of Eq. (1) is a linear function of the initial value $F_0$,

$$F[t] = U[t] \cdot F_0 \tag{3}$$

where $U[t]$ is defined by

$$U'[t] = A[t] \cdot U[t], \quad U[0] = \mathbf{I} \tag{4}$$

## The Magnus exponent

Eq. (4) has an exponential-matrix solution,

$$U[t] = \exp[\Omega[t]], \tag{5}$$

If $A[t]$ commutes with its indefinite integral, then $\Omega[t]$ is the indefinite integral of $A[t]$: $\Omega[t] = \int_0^t dt_1 \cdot A[t_1]$, but we are concerned here with the case where this condition does not hold. In general, $\Omega[t]$ (the *Magnus exponent*) is defined by the conditions

$$\frac{d}{dt}\exp[\Omega[t]] = A[t] \cdot \exp[\Omega[t]], \quad \Omega[0] = \mathbf{0} \tag{6}$$

Commutator algebra

The derivations below are adapted from Ref. [1] and make use of the following definitions and relations: The *commutator* $[\ldots]$ is defined, for square matrix arguments $A$ and $B$, as

$$[A, B] = A \cdot B - B \cdot A, \tag{7}$$

The commutator is antisymmetric and satisfies the Jacobi identity,

$$[B, A] = -[A, B], \tag{8}$$

$$[A,[B,C]] + [B,[C, A]] + [C,[A, B]] = \mathbf{0}, \tag{9}$$

The *adjoint mapping* "$ad$" is defined by

$$ad_\Omega^j[X] = [\overbrace{\Omega,[\Omega,\ldots[\Omega}^{j\text{ times}}, X]]]: \quad ad_\Omega^0[X] = X, \quad ad_\Omega^{j+1}[X] = [\Omega, ad_\Omega^j[X]] \tag{10}$$

$ad$ has the following properties,

$$ad_\Omega^j[a \cdot X + b \cdot Y] = a \cdot ad_\Omega^j[X] + b \cdot ad_\Omega^j[Y] \quad \text{(for scalars } a \text{ and } b) \tag{11}$$

$$ad_{\sigma\cdot\Omega}^j[X] = \sigma^j \cdot ad_\Omega^j[X] \quad \text{(scalar } \sigma) \tag{12}$$

$$ad_\Omega^{j+k}[X] = ad_\Omega^j[ad_\Omega^k[X]] \tag{13}$$

The Magnus theorem

The similarity transformation $\exp[\Omega] \cdot X \cdot \exp[-\Omega]$ has a series expansion of the form

$$\exp[\Omega] \cdot X \cdot \exp[-\Omega] = \sum_j \frac{1}{j!} \cdot ad_\Omega^j[X] \tag{14}$$

This relation is derived as follows: For scalar $\sigma$, the following relation is obtained by induction,

$$\frac{d^j}{d\sigma^j}\left(\exp[\sigma\cdot\Omega]\cdot X\cdot\exp[-\sigma\cdot\Omega]\right)=\exp[\sigma\cdot\Omega]\cdot ad_{\Omega}^{j}[X]\cdot\exp[-\sigma\cdot\Omega] \tag{15}$$

Hence, the expression $\exp[\sigma\cdot\Omega]\cdot X\cdot\exp[-\sigma\cdot\Omega]$ has the Taylor series expansion

$$\exp[\sigma\cdot\Omega]\cdot X\cdot\exp[-\sigma\cdot\Omega]=\sum_j\frac{\sigma^j}{j!}\cdot ad_{\Omega}^{j}[X] \tag{16}$$

Eq. (14) follows from Eq. (16) with $\sigma=1$.

The derivative of $\exp[\Omega[t]]$ has the following relationship to $\Omega'[t]$,

$$\frac{d}{dt}\exp[\Omega[t]]=\left(\sum_j\frac{1}{(j+1)!}\cdot ad_{\Omega[t]}^{j}[\Omega'[t]]\right)\cdot\exp[\Omega[t]] \tag{17}$$

This relation is derived by first applying Eq's. (14) and (12) to simplify the following expression.

$$\begin{aligned}&\frac{\partial}{\partial\sigma}\left(\left(\frac{\partial}{\partial t}\exp[\sigma\cdot\Omega[t]]\right)\cdot\exp[-\sigma\cdot\Omega[t]]\right)\\&=\exp[\sigma\cdot\Omega[t]]\cdot\Omega'[t]\cdot\exp[-\sigma\cdot\Omega[t]]\\&=\sum_j\frac{1}{j!}\cdot ad_{\sigma\cdot\Omega[t]}^{j}[\Omega'[t]]=\sum_j\frac{\sigma^j}{j!}\cdot ad_{\Omega[t]}^{j}[\Omega'[t]]\end{aligned} \tag{18}$$

Eq. (18) is integrated over $\sigma$ to obtain Eq. (17),

$$\begin{aligned}&\left(\frac{\partial}{\partial t}\exp[\Omega[t]]\right)\cdot\exp[-\Omega[t]]\\&=\int_0^1 d\sigma\cdot\frac{\partial}{\partial\sigma}\left(\left(\frac{\partial}{\partial t}\exp[\sigma\cdot\Omega[t]]\right)\cdot\exp[-\sigma\cdot\Omega[t]]\right)\\&=\sum_j\frac{1}{(j+1)!}\cdot ad_{\Omega[t]}^{j}[\Omega'[t]]\end{aligned} \tag{19}$$

Eq. (17) is substituted into Eq. (6)

$$A[t]=\sum_j\frac{1}{(j+1)!}\cdot ad_{\Omega[t]}^{j}[\Omega'[t]] \tag{20}$$

This relation is inverted to solve for $\Omega'[t]$, *The Magnus theorem*:

$$\begin{aligned}
\Omega'[t] &= \sum_k \frac{B_k}{k!} \cdot ad^k_{\Omega[t]}[A[t]] \\
&= A[t] - \tfrac{1}{2} \cdot [\Omega[t], A[t]] + \tfrac{1}{12} \cdot [\Omega[t],[\Omega[t], A[t]]] \\
&\quad - \tfrac{1}{720} \cdot [\Omega[t],[\Omega[t],[\Omega[t],[\Omega[t], A[t]]]]] + O\,t^6 \\
&\left(\text{with } \Omega[0] = \mathbf{0},\ \Omega[t] = O\,t\right)
\end{aligned} \tag{21}$$

The $B_k$ factors are the *Bernoulli numbers* defined by

$$\begin{aligned}
&B_0 = 1; \quad \text{For } j > 0,\ B_j = -\sum_{k=0}^{j-1} \frac{j!}{(j-k+1)!\cdot k!} \cdot B_k \\
&\{B_0, B_1, \ldots\} = \{1, -\tfrac{1}{2}, \tfrac{1}{6}, 0, -\tfrac{1}{30}, 0, \tfrac{1}{42}, 0, -\tfrac{1}{30}, 0, \tfrac{5}{66}, 0, -\tfrac{691}{273}, \ldots\}
\end{aligned} \tag{22}$$

(The truncated series residual in Eq. (21) is $O\,t^6$, not $O\,t^5$, because $B_5 = 0$.)

Eq. (21) is obtained by substituting Eq. (20) in Eq. (21) and applying Eq's. (11) and (13),

$$\Omega'[t] = \sum_{j \ge 0,\, k \ge 0} \frac{B_k}{(j+1)!k!} \cdot ad^{j+k}_{\Omega[t]}[\Omega'[t]]] \tag{23}$$

The index $j$ is replaced by $j-k$,

$$\begin{aligned}
\Omega'[t] &= \sum_{j-k \ge 0,\, k \ge 0} \frac{B_k}{(j-k+1)!k!} \cdot ad^{j}_{\Omega[t]}[\Omega'[t]]] \\
&= \sum_{j \ge 0} \left( \sum_{k:\, 0 \le k \le j} \frac{B_k}{(j-k+1)!k!} \right) \cdot ad^{j}_{\Omega[t]}[\Omega'[t]]]
\end{aligned} \tag{24}$$

The coefficients of $ad^{j}_{\Omega[t]}[\Omega'[t]]]$ on both sides of this equation are matched,

$$\sum_{k:\, 0 \le k \le j} \frac{B_k}{(j-k+1)!k!} = \begin{cases} 1, & j = 0 \\ 0, & j > 0 \end{cases} \tag{25}$$

Eq. (25) implies Eq. (22).

<u>The Magnus expansion</u>

The function $\Omega[t]$ determined by Eq. (21) can be represented as a series in progressively higher powers of $A[t]$. To obtain this series, we replace $A[t]$ with $\varepsilon \cdot A[t]$, where $\varepsilon$ is a scalar perturbation parameter, and $\Omega[t]$ is represented as a Taylor series (*Magnus expansion*) in $\varepsilon$,

$$\Omega[t] = \sum_j \Omega_j[t] \cdot \varepsilon^j, \quad \Omega_j[0] = \mathbf{0} \tag{26}$$

(The $\varepsilon$ parameter is used to formally separate powers of $A$ in $\Omega$, but is set to 1 in numerical implementation.) Eq. (21) is replaced by

$$\Omega'[t] = \sum_k \frac{B_k}{k!} \cdot ad^k_{\Omega[t]}[\varepsilon \cdot A[t]] = \sum_k \frac{\varepsilon \cdot B_k}{k!} \cdot ad^k_{\Omega[t]}[A[t]] \tag{27}$$

With $\varepsilon = 0$, Eq. (27) reduces to $\Omega'_0[t] = 0$, and the condition $\Omega_j[0] = \mathbf{0}$ implies that $\Omega_0[t] = 0$,

$$\Omega'_0[t] = 0, \quad \Omega_0[t] = 0 \tag{28}$$

The remaining terms are determined recursively by expanding out Eq. (27),

$$\begin{aligned} &\Omega'_1[t] + \Omega'_2[t] \cdot \varepsilon + \Omega'_3[t] \cdot \varepsilon^2 + \Omega'_4[t] \cdot \varepsilon^3 + \ldots = \\ &\quad A[t] - \tfrac{1}{2} \cdot [\Omega_1[t] + \Omega_2[t] \cdot \varepsilon + \Omega_3[t] \cdot \varepsilon^2 + \ldots, A[t]] \cdot \varepsilon \\ &\quad + \tfrac{1}{12}[\Omega_1[t] + \Omega_2[t] \cdot \varepsilon + \ldots, [\Omega_1[t] + \Omega_2[t] \cdot \varepsilon + \ldots, A[t]]] \cdot \varepsilon^2 \\ &\quad + O\varepsilon^4 \end{aligned} \tag{29}$$

(The residual is $O\varepsilon^4$, not $O\varepsilon^3$, because $B_3 = 0$, Eq. (22).)

The first four derivative terms $\Omega'_j[t]$ are obtained from Eq. (29),

$$\Omega'_1[t] = A[t] \tag{30}$$

$$\Omega'_2[t] = -\tfrac{1}{2} \cdot [\Omega_1[t], A[t]] \tag{31}$$

$$\Omega'_3[t] = -\tfrac{1}{2} \cdot [\Omega_2[t], A[t]] + \tfrac{1}{12}[\Omega_1[t], [\Omega_1[t], A[t]]] \tag{32}$$

$$\Omega'_4[t] = -\tfrac{1}{2} \cdot [\Omega_3[t], A[t]] + \tfrac{1}{12} \cdot \left([\Omega_1[t], [\Omega_2[t], A[t]]] + [\Omega_2[t], [\Omega_1[t], A[t]]]\right) \tag{33}$$

Eq's. (30)-(33) are integrated to obtain the $\Omega_j[t]$ coefficients ($\Omega_j[t] = \int_0^t dt_1 \cdot \Omega'_j[t_1]$),

$$\Omega_1[t] = \int_0^t dt_1 \cdot A[t_1] \tag{34}$$

$$\Omega_2[t] = \tfrac{1}{2} \cdot \int_0^t dt_1 \cdot \int_0^{t_1} dt_2 \cdot [A[t_1], A[t_2]] \tag{35}$$

$$\Omega_3[t] = \tfrac{1}{6} \cdot \int_0^t dt_1 \cdot \int_0^{t_1} dt_2 \cdot \int_0^{t_2} dt_3 \cdot \left([A[t_1], [A[t_2], A[t_3]]] + [[A[t_1], A[t_2]], A[t_3]]\right) \tag{36}$$

$$\Omega_4[t] = \tfrac{1}{12} \cdot \int_0^t dt_1 \cdot \int_0^{t_1} dt_2 \cdot \int_0^{t_2} dt_3 \cdot \int_0^{t_3} dt_4 \cdot \begin{pmatrix} [[[A[t_1], A[t_2]], A[t_3]], A[t_4]] \\ +[A[t_1],[[A[t_2], A[t_3]], A[t_4]]] \\ +[A[t_1],[A[t_2],[A[t_3], A[t_4]]]] \\ +[A[t_2],[A[t_3],[A[t_4], A[t_1]]]] \end{pmatrix} \tag{37}$$

Eq's. (36) and (37) are derived in the Appendix.

The Magnus expansion has limited practical utility for numerical implementation because the nested integrals are not easily evaluated and higher-order coefficients are algebraically intractable. A straightforward Taylor-series expansion of $\Omega[t]$ is simpler and more practicable.

<u>Series expansion of the Magnus exponent</u>

Rather than representing the Magnus exponent $\Omega[t]$ as a Taylor series in the $A$ scaling factor $\varepsilon$ (Eq. (26)), it can alternatively be expanded as a series in the function argument $t$,

$$\Omega[t] = \sum_k \frac{\Omega^{[k]}[0]}{k!} \cdot t^k \tag{38}$$

This series is applied in Eq. (21) to determine the first few series coefficients,

$$
\begin{aligned}
&\Omega'[0]+\Omega''[0]\cdot t+\tfrac{1}{2}\cdot\Omega^{[3]}[0]\cdot t^2+\tfrac{1}{6}\cdot\Omega^{[4]}[0]\cdot t^3+\tfrac{1}{24}\cdot\Omega^{[5]}[0]\cdot t^4+\tfrac{1}{120}\cdot\Omega^{[6]}[0]\cdot t^5+Ot^6\\
&=A[0]\\
&+t\cdot\left(A'[0]-\tfrac{1}{2}\cdot[\Omega'[0],A[0]]\right)\\
&+t^2\cdot\left(\tfrac{1}{2}\cdot A''[0]-\tfrac{1}{2}\cdot\left([\Omega'[0],A'[0]]+\tfrac{1}{2}\cdot[\Omega''[0],A[0]]\right)+\tfrac{1}{12}\cdot[\Omega'[0],[\Omega'[0],A[0]]]\right)\\
&+t^3\cdot\begin{pmatrix}\tfrac{1}{6}\cdot A^{[3]}[0]-\tfrac{1}{2}\cdot\left(\tfrac{1}{2}\cdot[\Omega'[0],A''[0]]+\tfrac{1}{2}\cdot[\Omega''[0],A'[0]]+\tfrac{1}{6}\cdot[\Omega^{[3]}[0],A[0]]\right)\\
+\tfrac{1}{12}\cdot\left([\Omega'[0],[\Omega'[0],A'[0]]]+\tfrac{1}{2}\cdot[\Omega''[0],[\Omega'[0],A[0]]]+\tfrac{1}{2}\cdot[\Omega'[0],[\Omega''[0],A[0]]]\right)\end{pmatrix}\\
&+t^4\cdot\begin{pmatrix}\tfrac{1}{24}\cdot A^{[4]}[0]-\tfrac{1}{2}\cdot\left(\tfrac{1}{6}\cdot[\Omega'[0],A^{[3]}[0]]+\tfrac{1}{4}\cdot[\Omega''[0],A''[0]]+\tfrac{1}{6}\cdot[\Omega^{[3]}[0],A'[0]]+\tfrac{1}{24}\cdot[\Omega^{[4]}[0],A[0]]\right)\\
+\tfrac{1}{12}\cdot\begin{pmatrix}[\Omega'[0],\tfrac{1}{2}\cdot[\Omega'[0],A''[0]]+\tfrac{1}{2}\cdot[\Omega''[0],A'[0]]+\tfrac{1}{6}\cdot[\Omega^{[3]}[0],A[0]]]\\
+\tfrac{1}{2}\cdot[\Omega''[0],[\Omega'[0],A'[0]]+\tfrac{1}{2}\cdot[\Omega''[0],A[0]]]\\
+\tfrac{1}{6}\cdot[\Omega^{[3]}[0],[\Omega'[0],A[0]]]\end{pmatrix}\\
-\tfrac{1}{720}\cdot[\Omega'[0],[\Omega'[0],[\Omega'[0],[\Omega'[0],A[0]]]]]\end{pmatrix}\\
&+t^5\cdot\begin{pmatrix}\tfrac{1}{120}\cdot A^{[5]}[0]-\tfrac{1}{2}\cdot\begin{pmatrix}\tfrac{1}{24}\cdot[\Omega'[0],A^{[4]}[0]]+\tfrac{1}{12}\cdot[\Omega''[0],A^{[3]}[0]]+\tfrac{1}{12}\cdot[\Omega^{[3]}[0],A''[0]]\\
+\tfrac{1}{24}\cdot[\Omega^{[4]}[0],A'[0]]+\tfrac{1}{120}\cdot[\Omega^{[5]}[0],A[0]]\end{pmatrix}\\
+\tfrac{1}{12}\cdot\begin{pmatrix}[\Omega'[0],\tfrac{1}{6}\cdot[\Omega'[0],A^{[3]}[0]]+\tfrac{1}{4}\cdot[\Omega''[0],A''[0]]+\tfrac{1}{6}\cdot[\Omega^{[3]}[0],A'[0]]+\tfrac{1}{24}\cdot[\Omega^{[4]}[0],A[0]]]\\
+\tfrac{1}{2}\cdot[\Omega''[0],\tfrac{1}{2}\cdot[\Omega'[0],A''[0]]+\tfrac{1}{2}\cdot[\Omega''[0],A'[0]]+\tfrac{1}{6}\cdot[\Omega^{[3]}[0],A[0]]]\\
+\tfrac{1}{6}\cdot[\Omega^{[3]}[0],[\Omega'[0],A'[0]]+\tfrac{1}{2}\cdot[\Omega''[0],A[0]]]\\
+\tfrac{1}{24}\cdot[\Omega^{[4]}[0],[\Omega'[0],A[0]]]\end{pmatrix}\\
-\tfrac{1}{720}\cdot\begin{pmatrix}[\Omega'[0],[\Omega'[0],[\Omega'[0],[\Omega'[0],A'[0]]]]]+\tfrac{1}{2}\cdot[\Omega'[0],[\Omega'[0],[\Omega'[0],[\Omega''[0],A[0]]]]]\\
+\tfrac{1}{2}\cdot[\Omega'[0],[\Omega'[0],[\Omega''[0],[\Omega'[0],A[0]]]]]+\tfrac{1}{2}\cdot[\Omega'[0],[\Omega''[0],[\Omega'[0],[\Omega'[0],A[0]]]]]\\
+\tfrac{1}{2}\cdot[\Omega''[0],[\Omega'[0],[\Omega'[0],[\Omega'[0],A[0]]]]]\end{pmatrix}\end{pmatrix}\\
&+Ot^6
\end{aligned}
\tag{39}
$$

$$
\begin{aligned}
&\Omega'[0] = A[0] \\
&\Omega''[0] = A'[0] \\
&\Omega^{[3]}[0] = A''[0] + \tfrac{1}{2}\cdot[A'[0], A[0]] \\
&\Omega^{[4]}[0] = A^{[3]}[0] + [A''[0], A[0]] \\
&\Omega^{[5]}[0] = A^{[4]}[0] + \tfrac{3}{2}\cdot[A^{[3]}[0], A[0]] + [A''[0], A'[0]] + \tfrac{1}{6}\cdot[[A''[0], A[0]], A[0]] \\
&\quad + \tfrac{1}{2}\cdot[A'[0],[A'[0], A[0]]] - \tfrac{1}{6}\cdot[[[A'[0], A[0]], A[0]], A[0]] \\
&\Omega^{[6]}[0] = A^{[5]}[0] \\
&\quad + 2\cdot[A^{[4]}[0], A[0]] \\
&\quad + \tfrac{5}{2}\cdot[A^{[3]}[0], A'[0]] \\
&\quad + \tfrac{1}{2}\cdot[[A^{[3]}[0], A[0]], A[0]] \\
&\quad + 2\cdot[[A''[0], A'[0]], A[0]] \\
&\quad - \tfrac{5}{2}\cdot[[A''[0], A[0]], A'[0]] \\
&\quad - \tfrac{1}{2}\cdot[[[A''[0], A[0]], A[0]], A[0]] \\
&\quad - [[[A'[0], A[0]], A'[0]], A[0]]
\end{aligned} \tag{40}
$$

$$
\begin{aligned}
&\Omega[t] = t\cdot A[0] + \tfrac{1}{2}\cdot t^2\cdot A'[0] \\
&\quad + \tfrac{1}{6}\cdot t^3\cdot\left(A''[0] + \tfrac{1}{2}\cdot[A'[0], A[0]]\right) + \tfrac{1}{24}\cdot t^4\cdot\left(A^{[3]}[0] + [A''[0], A[0]]\right) \\
&\quad + \tfrac{1}{120}\cdot t^5\cdot\begin{pmatrix} A^{[4]}[0] + \tfrac{3}{2}\cdot[A^{[3]}[0], A[0]] + \tfrac{1}{6}\cdot[[A''[0], A[0]], A[0]] + [A''[0], A'[0]] \\ \quad + \tfrac{1}{2}\cdot[A'[0],[A'[0], A[0]]] - \tfrac{1}{6}\cdot[[[A'[0], A[0]], A[0]], A[0]] \end{pmatrix} \\
&\quad + \tfrac{1}{720}\cdot t^6\cdot\begin{pmatrix} A^{[5]}[0] \\ \quad + 2\cdot[A^{[4]}[0], A[0]] \\ \quad + \tfrac{5}{2}\cdot[A^{[3]}[0], A'[0]] \\ \quad + \tfrac{1}{2}\cdot[[A^{[3]}[0], A[0]], A[0]] \\ \quad + 2\cdot[[A''[0], A'[0]], A[0]] - \tfrac{5}{2}\cdot[[A''[0], A[0]], A'[0]] \\ \quad - \tfrac{1}{2}\cdot[[[A''[0], A[0]], A[0]], A[0]] \\ \quad - [[[A'[0], A[0]], A'[0]], A[0]] \end{pmatrix} \\
&+ O\,t^7
\end{aligned} \tag{41}
$$

Eq. (41) is simplified by sampling $A$ at the integration interval midpoint, $\tfrac{1}{2}\cdot t$,

$$
\begin{aligned}
&A[0] = A[\tfrac{1}{2}\cdot t] - \tfrac{1}{2}\cdot t\cdot A'[\tfrac{1}{2}\cdot t] + \tfrac{1}{8}\cdot t^2\cdot A''[\tfrac{1}{2}\cdot t] \\
&\quad - \tfrac{1}{48}\cdot t^3\cdot A^{[3]}[\tfrac{1}{2}\cdot t] + \tfrac{1}{384}\cdot t^4\cdot A^{[4]}[\tfrac{1}{2}\cdot t] - \tfrac{1}{3840}\cdot t^5\cdot A^{[5]}[\tfrac{1}{2}\cdot t] + O t^6 \\
&A'[0] = A'[\tfrac{1}{2}\cdot t] - \tfrac{1}{2}\cdot t\cdot A''[\tfrac{1}{2}\cdot t] + \tfrac{1}{8}\cdot t^2\cdot A^{[3]}[\tfrac{1}{2}\cdot t] \\
&\quad - \tfrac{1}{48}\cdot t^3\cdot A^{[4]}[\tfrac{1}{2}\cdot t] + \tfrac{1}{384}\cdot t^4\cdot A^{[5]}[\tfrac{1}{2}\cdot t] + O t^5 \\
&A''[0] = A''[\tfrac{1}{2}\cdot t] - \tfrac{1}{2}\cdot t\cdot A^{[3]}[\tfrac{1}{2}\cdot t] + \tfrac{1}{8}\cdot t^2\cdot A^{[4]}[\tfrac{1}{2}\cdot t] - \tfrac{1}{48}\cdot t^3\cdot A^{[5]}[\tfrac{1}{2}\cdot t] + O t^4 \\
&A^{[3]}[0] = A^{[3]}[\tfrac{1}{2}\cdot t] - \tfrac{1}{2}\cdot t\cdot A^{[4]}[\tfrac{1}{2}\cdot t] + \tfrac{1}{8}\cdot t^2\cdot A^{[5]}[\tfrac{1}{2}\cdot t] + O t^3 \\
&A^{[4]}[0] = A^{[4]}[\tfrac{1}{2}\cdot t] - \tfrac{1}{2}\cdot t\cdot A^{[5]}[\tfrac{1}{2}\cdot t] + O t^2 \\
&A^{[5]}[0] = A^{[5]}[\tfrac{1}{2}\cdot t] + O t
\end{aligned}
\tag{42}
$$

$$
\begin{aligned}
&\Omega[t] = t\cdot A[\tfrac{1}{2}\cdot t] \\
&\quad + \tfrac{1}{240}\cdot t^3\cdot \left(\begin{aligned}
&10\cdot A''[\tfrac{1}{2}\cdot t] + \tfrac{1}{8}\cdot t^2\cdot A^{[4]}[\tfrac{1}{2}\cdot t] \\
&\quad + \left[\left(\begin{aligned}&20\cdot A'[\tfrac{1}{2}\cdot t] + \tfrac{1}{2}\cdot t^2\cdot A^{[3]}[\tfrac{1}{2}\cdot t] \\ &+ \tfrac{1}{3}\cdot t^2\cdot [A''[\tfrac{1}{2}\cdot t] - [A'[\tfrac{1}{2}\cdot t], A[\tfrac{1}{2}\cdot t]], A[\tfrac{1}{2}\cdot t]]\end{aligned}\right), A[\tfrac{1}{2}\cdot t]\right] \\
&\quad - \tfrac{1}{2}\cdot t^2\cdot [A''[\tfrac{1}{2}\cdot t], A'[\tfrac{1}{2}\cdot t]] \\
&\quad + t^2\cdot [A'[\tfrac{1}{2}\cdot t], [A'[\tfrac{1}{2}\cdot t], A[\tfrac{1}{2}\cdot t]]]
\end{aligned}\right) \\
&\quad + O t^7
\end{aligned}
\tag{43}
$$

The derivatives can be replaced by finite differences without compromising the accuracy order.

Second-order approximation:

$$
t\cdot A[\tfrac{1}{2}\cdot t] = \tfrac{1}{2}\cdot t\cdot\big(A[0] + A[t]\big) + O t^3 \tag{44}
$$

$$
\Omega[t] = \tfrac{1}{2}\cdot t\cdot\big(A[0] + A[t]\big) + O t^3 \tag{45}
$$

Fourth-order approximation:

$$
\begin{aligned}
&t^3\cdot A'[\tfrac{1}{2}\cdot t] = t^2\cdot\big(A[t] - A[0]\big) + O t^5 \\
&t^3\cdot A''[\tfrac{1}{2}\cdot t] = 4\cdot t\cdot\big(A[0] + A[t] - 2\cdot A[\tfrac{1}{2}\cdot t]\big) + O t^5
\end{aligned}
\tag{46}
$$

$$
\Omega[t] = \tfrac{1}{6}\cdot t\cdot\big(A[0] + 4\cdot A[\tfrac{1}{2}\cdot t] + A[t]\big) + \tfrac{1}{12}\cdot t^2\cdot [A[t] - A[0], A[\tfrac{1}{2}\cdot t]] + O t^5 \tag{47}
$$

Sixth-order approximation is

$$
\begin{aligned}
&t^3 \cdot A'[\tfrac{1}{2}\cdot t] = \tfrac{1}{3}\cdot t^2 \cdot \left(A[0] - 8\cdot A[\tfrac{1}{4}\cdot t] + 8\cdot A[\tfrac{3}{4}\cdot t] - A[t]\right) + O\,t^7 \\
&t^3 \cdot A''[\tfrac{1}{2}\cdot t] = \tfrac{1}{3}\cdot t \cdot \left(-4\cdot A[0] + 64\cdot A[\tfrac{1}{4}\cdot t] - 120\cdot A[\tfrac{1}{2}\cdot t] + 64\cdot A[\tfrac{3}{4}\cdot t] - 4\cdot A[t]\right) + O\,t^7 \\
&t^5 \cdot A''[\tfrac{1}{2}\cdot t] = 4\cdot t^3 \cdot \left(A[0] - 2\cdot A[\tfrac{1}{2}\cdot t] + A[t]\right) + O\,t^7 \\
&t^5 \cdot A^{[3]}[\tfrac{1}{2}\cdot t] = 32\cdot t^2 \cdot \left(-A[0] + 2\cdot A[\tfrac{1}{4}\cdot t] - 2\cdot A[\tfrac{3}{4}\cdot t] + A[t]\right) + O\,t^7 \\
&t^5 \cdot A^{[4]}[\tfrac{1}{2}\cdot t] = 256\cdot t \cdot \left(A[0] - 4\cdot A[\tfrac{1}{4}\cdot t] + 6\cdot A[\tfrac{1}{2}\cdot t] - 4\cdot A[\tfrac{3}{4}\cdot t] + A[t]\right) + O\,t^7 \\
&t^5 \cdot A'[\tfrac{1}{2}\cdot t] = t^4 \cdot \left(A[t] - A[0]\right) + O\,t^7 \\
&t^5 \cdot [A''[\tfrac{1}{2}\cdot t], A'[\tfrac{1}{2}\cdot t]] = 4\cdot t^2 \cdot [A[0] - 2\cdot A[\tfrac{1}{2}\cdot t] + A[t], A[t] - A[0]] + O\,t^7 \\
&t^5 \cdot [A'[\tfrac{1}{2}\cdot t], [A'[\tfrac{1}{2}\cdot t], A[\tfrac{1}{2}\cdot t]]] = t^3 \cdot [A[t] - A[0], [A[t] - A[0], A[\tfrac{1}{2}\cdot t]]] + O\,t^7
\end{aligned}
\tag{48}
$$

$$
\begin{aligned}
\Omega[t] = {}& \tfrac{1}{90}\cdot t \cdot \left(7\cdot A[0] + 32\cdot A[\tfrac{1}{4}\cdot t] + 12\cdot A[\tfrac{1}{2}\cdot t] + 32\cdot A[\tfrac{3}{4}\cdot t] + 7\cdot A[t]\right) \\
& + \tfrac{1}{180}\cdot t^2 \cdot \left[\begin{pmatrix} -7\cdot A[0] - 16\cdot A[\tfrac{1}{4}\cdot t] + 16\cdot A[\tfrac{3}{4}\cdot t] + 7\cdot A[t] \\ + \left[\begin{pmatrix} t\cdot\left(A[0] - 2\cdot A[\tfrac{1}{2}\cdot t] + A[t]\right) \\ -\tfrac{1}{4}\cdot t^2 \cdot [A[t] - A[0], A[\tfrac{1}{2}\cdot t]] \end{pmatrix}, A[\tfrac{1}{2}\cdot t]\right] \end{pmatrix}, A[\tfrac{1}{2}\cdot t]\right] \\
& - \tfrac{1}{120}\cdot t^2 \cdot [A[0] - 2\cdot A[\tfrac{1}{2}\cdot t] + A[t], A[t] - A[0]] \\
& + \tfrac{1}{240}\cdot t^3 \cdot [A[t] - A[0], [A[t] - A[0], A[\tfrac{1}{2}\cdot t]]] \\
& + O\,t^7
\end{aligned}
\tag{49}
$$

The residual errors in Eq's. (45), (47), and (49) ($O\,t^3$, $O\,t^5$, and $O\,t^7$) represent the error scaling with integration step size $t$ for a single integration step. In a multi-step integration process, the number of steps is inversely proportional to the step size, and the cumulative error will typically be increased by a factor of the number of steps relative to the single-step error. Thus, the cumulative error would be expected to be of order $O\,t^2$, $O\,t^4$, or $O\,t^6$ for approximation order 2, 4, or 6, respectively.

Reference

[1] Blanes, Sergio, et al. "The Magnus expansion and some of its applications." *Physics reports* 470.5-6 (2009): 151-238.
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Appendix: Derivation of the third and fourth Magnus coefficients

$\Omega_3[t]$ is derived from Eq. (36) as follows: Eq's. (34) and (35) are substituted in Eq. (32), and the result is integrated,

$$\begin{aligned}\Omega_3[t] &= -\tfrac{1}{4}\cdot\int_0^t dt_1\cdot\int_0^{t_1} dt_2\cdot\int_0^{t_2} dt_3\cdot[[A[t_2],A[t_3]],A[t_1]] \\ &\quad +\tfrac{1}{12}\cdot\int_0^t dt_1\cdot\int_0^{t_1} dt_2\cdot\int_0^{t_1} dt_3\cdot[A[t_2],[A[t_3],A[t_1]]]\end{aligned} \tag{50}$$

The two integrations have different inner integration limits. To facilitate consolidation of the integrals, the inner integral in the second term is split into two integrals:

$$\int_0^{t_1} dt_3\cdot\ldots = \int_0^{t_{12}} dt_3\cdot\ldots + \int_{t_2}^{t_1} dt_3\cdot\ldots \tag{51}$$

Next, the order of integration over $t_2$ and $t_3$ is reversed in the last expression,

$$\int_0^{t_1} dt_2\cdot\int_{t_2}^{t_1} dt_3\cdot\ldots = \int_{0\le t_2\le t_3\le t_1} dt_2\cdot dt_3\cdot\ldots = \int_0^{t_1} dt_3\cdot\int_0^{t_3} dt_2\cdot\ldots \tag{52}$$

$t_2$ and $t_3$ are renamed to $t_3$ and $t_2$, respectively, in the last expression to convert this into an integral of the form $\int_0^{t_1} dt_2\cdot\int_0^{t_2} dt_3\cdot\ldots$, which can be consolidated with the other two integral terms to obtain

$$\Omega_3[t] = \int_0^t dt_1\cdot\int_0^{t_1} dt_2\cdot\int_0^{t_2} dt_3\cdot\begin{pmatrix}\tfrac{1}{4}\cdot[A[t_1],[A[t_2],A[t_3]]] + \tfrac{1}{12}\cdot[A[t_2],[A[t_3],A[t_1]]] \\ -\tfrac{1}{12}\cdot[A[t_3],[A[t_1],A[t_2]]]\end{pmatrix} \tag{53}$$

The Jacobi identity (Eq. (9)) is used to eliminate the middle integrand term,

$$[A[t_2],[A[t_3],A[t_1]]] = -[A[t_1],[A[t_2],A[t_3]]] - [A[t_3],[A[t_1],A[t_2]]] \tag{54}$$

With this substitution, Eq. (53) simplifies to Eq. (36).

$\Omega_4[t]$ is derived from Eq. (37) by substituting Eq's. (34), (35), and (36) Eq. (33), and integrating the result,

$$\begin{aligned}\Omega_4[t] &= -\tfrac{1}{2}\cdot\int_0^t dt_1\cdot[\Omega_3[t_1],A[t_1]]\\ &\quad+\tfrac{1}{12}\cdot\int_0^t dt_1\cdot[\Omega_1[t_1],[\Omega_2[t_1],A[t_1]]]+\tfrac{1}{12}\cdot\int_0^t dt_1\cdot[\Omega_2[t_1],[\Omega_1[t_1],A[t_1]]]\\ &= \tfrac{1}{12}\cdot\int_{0<t_4<t_3<t_2<t_1<t} dt_1\cdot dt_2\cdot dt_3\cdot dt_4\cdot\begin{pmatrix}[A[t_1],[A[t_2],[A[t_3],A[t_4]]]]\\ -[A[t_1],[A[t_4],[A[t_2],A[t_3]]]]\end{pmatrix}\\ &\quad+\tfrac{1}{24}\cdot\int_{\substack{0<t_4<t_3<t_1<t\\ 0<t_2<t_1}} dt_1\cdot dt_2\cdot dt_3\cdot dt_4\cdot[A[t_2],[[A[t_3],A[t_4]],A[t_1]]]\\ &\quad+\tfrac{1}{24}\cdot\int_{\substack{0<t_3<t_2<t_1<t\\ 0<t_4<t_1}} dt_1\cdot dt_2\cdot dt_3\cdot dt_4\cdot[[A[t_2],A[t_3]],[A[t_4],A[t_1]]]\end{aligned} \tag{55}$$

The second integral over the range $0<t_2<t_1$ is split into three integrals over subranges $0<t_2<t_4$, $t_4<t_2<t_3$ and $t_3<t_2<t_1$, and the third integration over $0<t_4<t_1$ is similarly split into subranges $0<t_4<t_3$, $t_3<t_4<t_2$, and $t_2<t_4<t_1$:

$$\int_{\substack{0<t_4<t_3<t_1<t\\ 0<t_2<t_1}}\cdots=\int_{0<t_2<t_4<t_3<t_1<t}\cdots+\int_{0<t_4<t_2<t_3<t_1<t}\cdots+\int_{0<t_4<t_3<t_2<t_1<t}\cdots \tag{56}$$

$$\int_{\substack{0<t_3<t_2<t_1<t\\ 0<t_4<t_1}}\cdots=\int_{0<t_4<t_3<t_2<t_1<t}\cdots+\int_{0<t_3<t_4<t_2<t_1<t}\cdots+\int_{0<t_3<t_2<t_4<t_1<t}\cdots \tag{57}$$

The $t_j$ indices in each integral are renumbered to convert all of the integrals to the standard form $\int_{0<t_4<t_3<t_2<t_1<t}\cdots$, and the results are consolidated into a single integral,

$$\Omega_4[t]=\tfrac{1}{24}\cdot\int_{0<t_4<t_3<t_2<t_1<t} dt_1\cdot dt_2\cdot dt_3\cdot dt_4\cdot\begin{pmatrix}2\cdot[A[t_1],[A[t_2],[A[t_3],A[t_4]]]]\\ -2\cdot[A[t_1],[A[t_4],[A[t_2],A[t_3]]]]\\ +[A[t_4],[[A[t_2],A[t_3]],A[t_1]]]\\ +[A[t_3],[[A[t_2],A[t_4]],A[t_1]]]\\ +[A[t_2],[[A[t_3],A[t_4]],A[t_1]]]\\ +[[A[t_2],A[t_3]],[A[t_4],A[t_1]]]\\ +[[A[t_2],A[t_4]],[A[t_3],A[t_1]]]\\ +[[A[t_3],A[t_4]],[A[t_2],A[t_1]]]\end{pmatrix} \tag{58}$$

The integrand terms will be converted to a standard format $[\ldots,[\ldots,[\ldots,\ldots]]]$ with the innermost commutator in lexical order. The last three terms, which are of the form $[[\ldots,\ldots],[\ldots,\ldots]]$, can be transformed by using the Jacobi identities

$$\begin{aligned}&[[U,V],[W,X]]\\ &=[U,[V,[W,X]]]-[V,[U,[W,X]]]\\ &=[[[U,V],W],X]-[[[U,V],X],W]\end{aligned} \tag{59}$$

The commutator order in each of the last three terms in Eq. (58) can be chosen so that $U = A[t_1]$ and $[W, X]$ is in lexical order,

$$\begin{aligned}&[[A[t_1], A[t_2]],[A[t_3], A[t_4]]]\\&=[A[t_1],[A[t_2],[A[t_3], A[t_4]]]]-[A[t_2],[A[t_1],[A[t_3], A[t_4]]]]\\&=[A[t_4],[A[t_3],[A[t_1], A[t_2]]]]-[A[t_3],[A[t_4],[A[t_1], A[t_2]]]]\end{aligned} \tag{60}$$

$$\begin{aligned}&[[A[t_1], A[t_3]],[A[t_2], A[t_4]]]\\&=[A[t_1],[A[t_3],[A[t_2], A[t_4]]]]-[A[t_3],[A[t_1],[A[t_2], A[t_4]]]]\\&=[A[t_4],[A[t_2],[A[t_1], A[t_3]]]]-[A[t_2],[A[t_4],[A[t_1], A[t_3]]]]\end{aligned} \tag{61}$$

$$\begin{aligned}&[[A[t_1], A[t_4]],[A[t_2], A[t_3]]]\\&=[A[t_1],[A[t_4],[A[t_2], A[t_3]]]]-[A[t_4],[A[t_1],[A[t_2], A[t_3]]]]\\&=[A[t_3],[A[t_2],[A[t_1], A[t_4]]]]-[A[t_2],[A[t_3],[A[t_1], A[t_4]]]]\end{aligned} \tag{62}$$

The choice between which of the two reductions to use in Eq. (59) by using a linear combination of both expressions, e.g.,

$$\begin{aligned}&[[U,V],[W,X]]\\&=b\cdot\left([U,[V,[W,X]]]-[V,[U,[W,X]]]\right)\\&\quad+(1-b)\cdot\left([[[U,V],W],X]-[[[U,V],X],W]\right)\end{aligned} \tag{63}$$

($b$ is a scalar.) Additional degrees of freedom will be provided by including scalar multiples of the following Jacobi identities,

$$\begin{aligned}&[A[t_1],[A[t_2],[A[t_3], A[t_4]]]]-[A[t_1],[A[t_3],[A[t_2], A[t_4]]]]\\&\quad+[A[t_1],[A[t_4],[A[t_2], A[t_3]]]]=0\end{aligned} \tag{64}$$

$$\begin{aligned}&[A[t_2],[A[t_1],[A[t_3], A[t_4]]]]-[A[t_2],[A[t_3],[A[t_1], A[t_4]]]]\\&\quad+[A[t_2],[A[t_4],[A[t_1], A[t_3]]]]=0\end{aligned} \tag{65}$$

$$\begin{aligned}&[A[t_3],[A[t_1],[A[t_2], A[t_4]]]]+[A[t_3],[A[t_4],[A[t_1], A[t_2]]]]\\&\quad-[A[t_3],[A[t_2],[A[t_1], A[t_4]]]]=0\end{aligned} \tag{66}$$

$$\begin{aligned}&[A[t_4],[A[t_1],[A[t_2], A[t_3]]]]+[A[t_4],[A[t_3],[A[t_1], A[t_2]]]]\\&\quad-[A[t_4],[A[t_2],[A[t_1], A[t_3]]]]=0\end{aligned} \tag{67}$$

Scalar weighting factors $b_2$, $b_3$, and $b_4$ are used for Eq's. (60)-(62), and factors $c_1$, $c_2$, $c_3$, and $c_4$ is used for Eq's. (64)-(67), leading to the following transformation of Eq. (58),

$$\Omega_4[t] = \tfrac{1}{24} \cdot \int_{0<t_4<t_3<t_2<t_1<t} dt_1 \cdot dt_2 \cdot dt_3 \cdot dt_4 \cdot \begin{pmatrix} (2+b_2+c_1)\cdot[A[t_1],[A[t_2],[A[t_3],A[t_4]]]] \\ +(b_3-c_1)\cdot[A[t_1],[A[t_3],[A[t_2],A[t_4]]]] \\ -(2-b_4-c_1)\cdot[A[t_1],[A[t_4],[A[t_2],A[t_3]]]] \\ -(1+b_2-c_2)\cdot[A[t_2],[A[t_1],[A[t_3],A[t_4]]]] \\ -(1-b_4+c_2)\cdot[A[t_2],[A[t_3],[A[t_1],A[t_4]]]] \\ -(1-b_3-c_2)\cdot[A[t_2],[A[t_4],[A[t_1],A[t_3]]]] \\ -(1+b_3-c_3)\cdot[A[t_3],[A[t_1],[A[t_2],A[t_4]]]] \\ +(1-b_4-c_3)\cdot[A[t_3],[A[t_2],[A[t_1],A[t_4]]]] \\ -(1-b_2-c_3)\cdot[A[t_3],[A[t_4],[A[t_1],A[t_2]]]] \\ -(1+b_4-c_4)\cdot[A[t_4],[A[t_1],[A[t_2],A[t_3]]]] \\ +(1-b_3-c_4)\cdot[A[t_4],[A[t_2],[A[t_1],A[t_3]]]] \\ +(1-b_2+c_4)\cdot[A[t_4],[A[t_3],[A[t_1],A[t_2]]]] \end{pmatrix} \tag{68}$$

The following coefficient choice matches Eq. (37)

$$b_2 = b_3 = b_4 = 0, \quad c_1 = 0, \quad c_2 = c_3 = c_4 = 1 \tag{69}$$

Another Jacobi-equivalent solution is obtained from the coefficient choice $b_2 = b_3 = b_4 = 1$, $c_1 = 1$, $c_2 = c_3 = c_4 = 0$ (with some simplification via Eq. (59)),

$$\Omega_4[t] = \tfrac{1}{12} \cdot \int_{0<t_4<t_3<t_2<t_1<t} dt_1 \cdot dt_2 \cdot dt_3 \cdot dt_4 \cdot \begin{pmatrix} [A[t_1],[A[t_2],[A[t_3],A[t_4]]]] \\ +[[A[t_1],A[t_2]],[A[t_3],A[t_4]]] \\ +[[A[t_1],[A[t_2],A[t_4]]],A[t_3]] \\ +[[A[t_1],[A[t_2],A[t_3]]],A[t_4]] \end{pmatrix} \tag{70}$$