The basic formulae are

$$
\begin{aligned}
\bar{\phi}_{mg} &= T_{ml}\phi_{lg} \\
\phi_{lg} &= T^{-1}_{lm}\bar{\phi}_{mg} \\
\dot{\bar{\phi}}_{mg} &= \dot{T}_{ml}\phi_{lg} + T_{ml}\dot{\phi}_{lg} \\
&= P_{mg} + T_{ml}\dot{\phi}_{lg}
\end{aligned}
$$

where $P_{mg} = \dot{T}_{ml}\phi_{lg}$, $\bar{\phi}_{mg}$ are the orthogonal states and ϕ_{mg} are the non-orthogonal states.

Manipulation of P_{mg} via the chain rule yields

$$
\begin{aligned}
P_{mg} &= \frac{\partial T_{ml}}{\partial \phi_{jg'}}\dot{\phi}_{jg'}\phi_{lg} \\
&= \frac{\partial T_{ml}}{\partial \phi_{jg'}}\dot{\phi}_{jg'}T^{-1}_{ls}\bar{\phi}_{sg} \\
&= T_{mq}T^{-1}_{qp}\frac{\partial T_{pl}}{\partial \phi_{jg'}}T^{-1}_{ls}\dot{\phi}_{jg'}\bar{\phi}_{sg} \\
&= T_{ml}T^{-1}_{lp}\frac{\partial T_{pq}}{\partial \phi_{jg'}}T^{-1}_{qs}\dot{\phi}_{jg'}\bar{\phi}_{sg} \\
&= -T_{ml}\frac{\partial T^{-1}_{ls}}{\partial \phi_{jg'}}\dot{\phi}_{jg'}\bar{\phi}_{sg} \\
&= -T_{ml}Q_{lg}
\end{aligned}
$$

where

$$
Q_{lg} = \frac{\partial T^{-1}_{ls}}{\partial \phi_{jg'}}\dot{\phi}_{jg'}\bar{\phi}_{sg}
$$

An identity regarding the parametric differentiation of T used above (well known):

$$
\begin{aligned}
\frac{\partial}{\partial \gamma}T_{pq}T^{-1}_{ql} &= 0 \\
\frac{\partial T_{pq}}{\partial \gamma}T^{-1}_{ql} &= -T_{pq}\frac{\partial T^{-1}_{ql}}{\partial \gamma} \\
T^{-1}_{sp}\frac{\partial T_{pq}}{\partial \gamma}T^{-1}_{ql} &= -\frac{\partial T^{-1}_{ql}}{\partial \gamma}
\end{aligned}
$$

Parametric differentiation of T and S can be used to define an iterative procedure in powers of T, T^{-1} that is rapidly convergent when T, T^{-1} are close to unit matrices (likely well known):

$$\begin{aligned}
T^{-1}_{ml} &= S_{mp}T_{pl} \\
\frac{\partial T^{-1}_{ml}}{\partial \gamma} &= \frac{\partial S_{mp}}{\partial \gamma}T_{pl} + S_{mp}\frac{\partial T_{pl}}{\partial \gamma} \\
&= \frac{\partial S_{mp}}{\partial \gamma}T_{pl} - T^{-1}_{mp}\frac{\partial T^{-1}_{pq}}{\partial \gamma}T_{ql}
\end{aligned}$$

Consider the case T, T^{-1}, S are real symmetric for all γ:

$$\frac{\partial T^{-1}_{ml}}{\partial \gamma} = \frac{1}{2}\left[\frac{\partial S_{mp}}{\partial \gamma}T_{pl} + \frac{\partial S_{lp}}{\partial \gamma}T_{pm} - T^{-1}_{mp}\frac{\partial T^{-1}_{pq}}{\partial \gamma}T_{ql} - T^{-1}_{lp}\frac{\partial T^{-1}_{pq}}{\partial \gamma}T_{qm}\right]$$

Let S take on the simple quadratic form:

$$\begin{aligned}
S_{mp} &= \phi_{mg'}\phi_{pg'}w_{g'} \\
\frac{\partial S_{mp}}{\partial \phi_{gk}} &= w_g\left[\phi_{gp}\delta_{mk} + \phi_{gm}\delta_{pk}\right]
\end{aligned}$$

Substitution yields:

$$\frac{\partial T^{-1}_{ml}}{\partial \phi_{gk}} = \frac{1}{2}\left[w_g\left(\bar{\phi}_{gl}\delta_{mk} + \bar{\phi}_{gm}\delta_{lk} + \phi_{gl}T_{km} + \phi_{gm}T_{kl}\right) - T^{-1}_{mp}\frac{\partial T^{-1}_{pq}}{\partial \phi_{gk}}T_{ql} - T^{-1}_{lp}\frac{\partial T^{-1}_{pq}}{\partial \phi_{gk}}T_{qm}\right]$$

In the limit T^{-1}, T are diagonally dominent, three natural zero order approximations can be formed by taking $T_{km} \approx \delta_{mk}$ and $\phi_{gl} \approx \bar{\phi}_{gl}$,

$$\begin{aligned}
\frac{\partial T^{-1}_{ml}}{\partial \phi_{gk}} &= w_g\left(\bar{\phi}_{gl}\delta_{mk} + \bar{\phi}_{gm}\delta_{lk}\right) + \mathcal{O}(T) \\
\frac{\partial T^{-1}_{ml}}{\partial \phi_{gk}} &= w_g\left(\phi_{gl}\delta_{mk} + \phi_{gm}\delta_{lk}\right) + \mathcal{O}(T) \\
\frac{\partial T^{-1}_{ml}}{\partial \phi_{gk}} &= \frac{w_g}{2}\left(\bar{\phi}_{gl}\delta_{mk} + \bar{\phi}_{gm}\delta_{lk} + \phi_{gl}\delta_{mk} + \phi_{gm}\delta_{lk}\right) + \mathcal{O}(T)
\end{aligned}$$

A 1st order approximation in T, T^{-1} is

$$\frac{\partial T^{-1}_{ml}}{\partial \phi_{gk}} = \frac{w_g}{2}\left(\bar{\phi}_{gl}\delta_{mk} + \bar{\phi}_{gm}\delta_{lk} + \phi_{gl}T_{km} + \phi_{gm}T_{kl}\right) + \mathcal{O}(T^2)$$

Higher order approximations are formed by inserting the above into the self-consistent equation and iterating.

The above results allow progressively more accurate approximations to be made to the quantity of interest, Q_{lg},

$$
\begin{aligned}
Q_{lg}^{(1,l)} &= \left(\Lambda_{ls}+\Lambda_{sl}\right)\bar{\phi}_{sg}\\
Q_{lg}^{(1,\hat{l})} &= \left(\hat{\Lambda}_{ls}+\hat{\Lambda}_{sl}\right)\bar{\phi}_{sg}\\
Q_{lg}^{(1,h)} &= \frac{1}{2}\left(\Lambda_{ls}+\Lambda_{sl}+\hat{\Lambda}_{ls}+\hat{\Lambda}_{sl}\right)\bar{\phi}_{sg}\\
Q_{lg}^{(2)} &= \frac{1}{2}\left(\Lambda_{ls}+\Lambda_{sl}+\bar{\Lambda}_{ls}+\bar{\Lambda}_{sl}\right)\bar{\phi}_{sg}\\
\Lambda_{ls} &= w_g\bar{\phi}_{lg}\dot{\phi}_{sg}\\
\hat{\Lambda}_{ls} &= w_g\phi_{lg}\dot{\phi}_{sg}\\
\bar{\Lambda}_{ls} &= w_g\phi_{lg}T_{sj}\dot{\phi}_{jg}
\end{aligned}
$$

where the sum of the components of the Λ matrices are related to time derivatives of S matrix elements as might be expected.

In this way, a hierarchy of approximations to the state velocities is developed

$$
\begin{aligned}
\dot{\bar{\phi}}_{mg}^{(1)} &= T_{ml}\dot{\phi}_{lg}\\
\dot{\bar{\phi}}_{mg}^{(2,l)} &= T_{ml}\left[\dot{\phi}_{lg}-Q_{lg}^{(1,l)}\right]\\
\dot{\bar{\phi}}_{mg}^{(2,\hat{l})} &= T_{ml}\left[\dot{\phi}_{lg}-Q_{lg}^{(1,\hat{l})}\right]\\
\dot{\bar{\phi}}_{mg}^{(2,h)} &= T_{ml}\left[\dot{\phi}_{lg}-Q_{lg}^{(1,h)}\right]\\
\dot{\bar{\phi}}_{mg}^{(3)} &= T_{ml}\left[\dot{\phi}_{lg}-Q_{lg}^{(2)}\right]
\end{aligned}
$$

The two lower accuracy 2nd order formulae labeled $(2,l/\hat{l})$ require less computational work to evaluate than the higher accuracy 2nd order formula labeled $(2,h)$ which itself requires less work to evaluate than the 3rd order formula labeled (3). The low accuracy 2nd order approximation $(2,l)$ has the same structure as the formula employed to generate the forces on the ϕ_{mg}; the function $\bar{f}_{lg}$ is simply replaced by $\dot{\phi}_{lg}$. The $(2,l)$ method has a lower communication overhead than the alternative method, $(2,\hat{l})$ which makes the $(2,l)$ approximation the superior choice for applications on large parallel platforms. Note, in the limit $\phi_{mg}\equiv\bar{\phi}_{mg}$ or T is diagonal and $\hat{\Lambda}_{ls}+\hat{\Lambda}_{sl}=0$, then $\dot{\bar{\phi}}_{mg}\equiv\dot{\phi}_{mg}$ as these two conditions place the system on the surface of constraint, $S_{lm}=\delta_{lm},\dot{S}_{lm}=0$, at time, t.