Aerodynamic Design for Unsteady Flows User Guide

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Contents

1 Introduction

This document is intended to complement the existing user guide for `JETSTREAM` (i.e. on aerodynamic design for steady flows). Only parameters relevant to aerodynamic design for unsteady flows are presented. The reader is referred to the user guide (http://utoronto-comp-aero.wikispaces.com/Jetstream) for additional parameters common to both steady and unsteady flow optimization problems. The following features have been added to `JETSTREAM` to allow for optimization of aerodynamic shapes for unsteady flow:

- solution to adjoint problem at each time step for implicit Euler, BDF (only BDF2 has been thoroughly tested for this class of time-marching methods) and ESDIRK (generalized for all the methods in this class of time marching methods) schemes
- flow can be initialized using an existing solution file (i.e. `results.q0`) or freestream conditions
- for time-marching methods that are not self-starting (e.g. BDF2, BDF2OPT etc.), implicit Euler or ESDIRK schemes can be used as a startup mechanism
- RHS contribution of each time step to last mesh-movement adjoint problem is computed and added to the existing values; only a small number of adjoint solutions are retained (i.e. equivalent to the number of time levels in time-marching scheme)
- objective function contribution of each time step is computed and added to existing value
- gradient contribution for each time step with respect to aerodynamic design variables is computed and added to existing value
- for very long runs, checkpoints are created to restart flow problem or flow adjoint problem from the last point the simulation exited, since the flow and adjoint problems are the most expensive components of a simulation
- restart files are also created for function evaluations during optimization
- both geometric (i.e. B-spline control points) and aerodynamic (i.e. angle of attack and Mach number) design variables can be used for optimization

- for inverse design cases, perturbing the initial geometry (i.e. to get target pressure distribution) and geometry recovery process (i.e. optimization cycle) have been merged into a single simulation

Currently, the added features are **limited** to:

- B-spline geometry control
- storing all flow solution files (i.e. we do not see the merit in traditional checkpointing methods at this stage since one has to trade storage and memory requirements for longer runs due to computing the same time step several times)
- using a fixed time step throughout simulations
- constraints for optimization for steady flows have to be adapted to actual design problems for unsteady flows
- module for checking time left on a job is limited to SciNet's GPC systems

2 Jetstream Parameters

`jtstrm% mean_int_type` - numerical integration scheme for computing objective function. Default is `1`, which is a simple average (i.e. midpoint rule). Option `0` is a summation and `2` uses the weights of trapezoidal method to compute the contribution of each time step.

3 Diablo Parameters

1. `diablo% unsteady` - a logical parameter for selecting steady or unsteady flow option. Default is `.false.`, an option which allows `DIABLO` to solve only steady state problems.
2. `diablo% tdis` - a character parameter for selecting the time-marching method. Default is implicit Euler (i.e. `imp_euler`). Other options include `bdf2`, `bdf2opt`, `bdf3`, `bdf4`, `esdirk2`, `esdirk3`, `esdirk4`.
3. `diablo% tstrup` - an integer parameter for selecting a startup mechanism scheme for time-marching methods that are not self-starting. Default is `1`, which is `imp_euler`. Options `2-4` are `esdirk2`, `esdirk3` and `esdirk4` respectively.
4. `diablo% dt` - a double precision parameter for setting the time step size.
5. `diablo% istep` - an integer parameter for the index of the first time step. Default is `1`.

6. diablo% fstep - an integer parameter for the index of the final time step.

7. diablo% xtrp_type - an integer parameter for the type of extrapolation. Default is 0, which is no extrapolation (use previous solution). Option 1 is extrapolation from past time step solutions and 2 is extrapolation from past stage solutions. Option 1 is recommend.

8. diablo% xtrp - an integer parameter for the number of solution points used in the extrapolation. Default is 1, which is simply the past solution. Higher values correspond to extrapolation using higher degree polynomials, for example option 2 is linear extrapolation and 3 is quadratic extrapolation.

9. diablo% theta - a double precision parameter for variable coefficient time-marching methods like BDF2OPT. Default is 0.d0.

10. diablo% prec_frz - an integer parameter for determining how long to freeze the preconditioner. Default is 0, which uses the default steady logic to determine when the preconditioner is updated. Option 1 freezes the preconditioner over an entire stage and 2 freezes the preconditioner over an entire time step.

11. diablo% surf_press_out - a logical parameter for writing surface pressure distribution to disk at each time step for the purpose of inverse design. Default is .false. (i.e. for all cases except jtstrm% obj_fun='invs' and opt_method='optimize').

12. diablo% use_checkpoint - a logical parameter for creating and restoring checkpoints for very long flow/optimization simulations. Default is .false., but set to .true. for all unsteady optimization problems.

13. diablo% ubckp - a logical parameter for saving flow solutions to disk. Default is .false.. For any run that involves solving an adjoint problem for an unsteady flow set this option to .true..

14. diablo% ubckp_stages - a logical parameter for saving internal stages of multi-stage schemes. Default is .false.. For runs where the adjoint problem for an unsteady flow has to be solved for a multi-stage time-marching method set this option to .true..

15. diablo% ubckp_frq - an integer parameter for how frequently flow solutions are written to disk (e.g. every 100 time steps). For unsteady optimization, set this parameter to 1. Note that this is relative to time step 0 and not diablo% istep.

16. diablo% stats - a logical parameter for writing instantaneous flow properties to disk (unsteady_xxxxxx.istat). This includes Q-criterion, three components of vorticity, and

$\lambda 2$-criterion. All are computed with the high-order SBP operators associated with the current discretization.

17. diablo% mstats - a logical parameter for computing and writing mean-flow statistics to disk (unsteady_xxxxxx.cp, unsteady_xxxxxx.cf, and unsteady_xxxxxx.mstat). This includes time-averaged pressure coefficient in *.cp, time-averaged friction coefficient in *.cf, and time-averaged component velocities (u_i), second-order component velocity products ($u_i u_j$), pressure, viscosity, and friction velocity in *.mstat. All are computed with the high-order SBP operators associated with the current discretization.

18. diablo% stat_frq - an integer parameter for how frequently mean-flow statistics are computed and written to disk (e.g. every 100 time steps). Note that this is relative to time step 0 and not diablo% istep.

19. diablo% acoustic - a logical parameter for acoustic characteristic boundary zones.

20. diablo% abztype - an integer parameter identifying the boundary type where the acoustic characteristic boundary zones are applied. For example, to replace standard type 2 farfield characteristic boundary conditions with the acoustic zonal approach, set this parameter to 2.

21. diablo% abzwdth - an integer parameter for the number of nodes in the boundary normal direction of the acoustic characteristic boundary zones.

22. diablo% use_frstrm - a logical parameter for using freestream conditions. When set to .true., diablo% restart should be set to .false..

23. diablo% restart - a logical parameter for starting flow problem from an existing solution file (i.e. results.q0). When set to.true., diablo% use_frstrm should be set to .false..

4 Checkpoint Parameters

These parameters are assigned in a new input file called checkpoint.param when diablo% use_checkpoint=.true.. The only parameter to be set by the user is chk_pt% pbs_time_limit. When the program creates a checkpoint, the appropriate values for the other parameters are written to checkpoint.param.

See the sample checkpoint.param file for an initial job submission

```
&CHECKPOINT
    chk_pt% pbs_time_limit =     1800,
&END
```

The parameters are defined as follows:

1. chk_pt% restart - a logical parameter indicating whether the current run is to continue from a previous run that was checkpointed. The default is .false..
2. chk_pt% perturbed - a logical parameter indicating whether the pressure distribution at all time steps for the target geometry (i.e. perturbed geometry) have been written to disk. The default is .false.. The program writes the appropriate value after the first and subsequent checkpoints.
3. chk_pt% fstep - an integer parameter indicating the last flow time step completed before checkpoint was created. Default is 0.
4. chk_pt% astep - an integer parameter indicating the last adjoint time step completed before checkpoint was created. Default is 0.
5. chk_pt% nfun - an integer parameter indicating the last function evaluation completed before checkpoint. Default is 0.
6. chk_pt% pbs_time_left - an integer parameter which stores the value of the time left for a job to finish.
7. chk_pt% pbs_time_limit - an integer parameter indicating time below which a checkpoint needs to be created so a job can be resubmitted. This is the only parameter the user sets. Default is 3600 seconds.

Once a checkpoint is created, the string 555 is written to results.scr. The submission script reads the last line of results.scr and if the string matches the above string, it automatically resubmits the job. This approach has been used to successfully run a job continuously for 9 days on SciNet. See the sample script below for automatic job resubmission.

```
#!/bin/bash
#PBS -l nodes=2:ppn=8,walltime=00:03:00:00
#PBS -N test_restart



# job submission script
# ---------------------
echo "************************"
echo "SUBMISSION NO :: " $(($NUM+1))
echo "************************"
```

```
cd $PBS_O_WORKDIR
mpirun -r ssh -np 12 ~/bin/jetstream_x86_64 >& screen


# check end of screen file and use it to restart job
# ---------------------------------------------------
efile=$(tail -1 results.scr)
counter=$NUM

if [ $efile -eq 555 ] && [ $counter -lt 30 ]; then
  counter=$(($counter+1))
  ssh gpc03 "cd $PBS_O_WORKDIR; qsub run_checkpoint.pbs -v NUM=$counter";
  efile=$(tail -1 results.scr)
else
  echo "************************"
  echo "JOB COMPLETED OR CRASHED"
  echo "************************"
fi
```

To automatically resubmit the script above after a checkpoint is created, the following command is used:

```
qsub run_checkpoint.pbs -v NUM=0
```

where `run_checkpoint.pbs` is the file name of the submission script above.

The following files are created after a checkpoint is created:

- `checkpoint.fsol` - last flow/adjoint solution before checkpoint
- `checkpoint.fadj#` - stored adjoint solutions before checkpoint (# $\Rightarrow n = 1, \ldots, r$. See Section 8.1 for the definition and value of r)
- `checkpoint.djdg` - sum of all time step contributions to RHS to the last mesh movement adjoint problem at checkpoint
- `checkpoint.fval` - sum of all time step contributions to objective function and gradient for aerodynamic design variables at checkpoint
- `checkpoint.xdvs` - design variables for which checkpoint was created

The module `common/PBS_Mod.f90` contains functions for making a system call and then estimating the time left for a job to complete. The functions in the module might have to be modified if the program is to be run on a different HPC system.

5 Data Types

5.1 Jetstream Parameters: OptimizeOpts Data Type

See Table 1.

Derived Type	Parameter	Data Type
`jtstrm%`	`mean_int_type`	`integer`

Table 1: optimization option data type

5.2 Checkpoint Parameters: CheckOpts Data Type

See Table 2.

Derived Type	Parameter	Data Type
`chk_pt%`	`restart`	`logical`
	`perturbed`	`logical`
	`fstep`	`integer`
	`astep`	`integer`
	`nfun`	`integer`
	`pbs_time_left`	`integer`
	`pbs_time_limit`	`integer`

Table 2: Checkpoint options data type

5.3 Diablo Parameters: SolverOpts Data Type

See Table 3.

6 Tests and Related Files

The following options (i.e. `opt_method='option'`) can be used to check the new features added:

- `adjsolve` - tests adjoint solution for unsteady flows

Derived Type	Parameter	Data Type
diablo%	unsteady	logical
	restart	logical
	use_frstrm	logical
	acoustic	logical
	ubckp	logical
	ubckp_stages	logical
	surf_press_out	logical
	use_checkpoint	logical
	stats	logical
	mstats	logical
	tstrup	integer
	istep	integer
	fstep	integer
	xtrp_type	integer
	xtrp	integer
	prec_frz	integer
	ubck_frq	integer
	stat_frq	integer
	abztype	integer
	abzwdth	integer
	dt	double precision
	theta	double precision
	tdis	character

Table 3: Solver options data type

- `testdrdg` - compares the analytical values of the contribution of a time step to the RHS of the last mesh-movement adjoint problem with complex-step values
- `testgrad` - tests the computation of the gradient for a specified objective function
- `fdgrad` - compares the analytical gradient with finite-difference gradient for one design variable (sweeps through step sizes)
- `dirderiv` - compares the analytical gradient with finite-difference gradient using a directional derivative approach (sweeps through step sizes)
- `optimize` - tests optimization framework for unsteady flows (constraints are yet to come)

New features added to `JETSTREAM` are in the following `FORTRAN` modules:

- `common/Common_Mod.f90`
- `common/PBS_Mod.f90`

- diablo/IO_Mod.f90
- diablo/Partition_Mod.f90
- diablo/Verify_Mod.f90
- optimize/Optimizer_Mod.f90
- jetstream.f90

7 Miscellaneous - Fully-Discrete Equations

A semi-discrete form of the discretized equations is given as

$$\frac{d\hat{\mathcal{Q}}}{dt} + \hat{\mathcal{R}}(\hat{\mathcal{Q}}) = \tilde{\mathcal{R}}(\hat{\mathcal{Q}}) + \hat{\mathcal{R}}(\hat{\mathcal{Q}}) = \mathbf{0} \tag{1}$$

after applying a time-marching method to time derivative component, a fully-discrete form of the governing equations can be written as

$$\tilde{\mathcal{R}}(\hat{\mathcal{Q}}) + \hat{\mathcal{R}}(\hat{\mathcal{Q}}) = \mathbf{0} \tag{2}$$

where $\tilde{\mathcal{R}}$ and $\hat{\mathcal{R}}$ are the temporal and spatial residuals respectively. The variable $\hat{\mathcal{Q}}$ is the conserved flow variables in curvilinear coordinates (i.e. $\hat{\mathcal{Q}} = J^{-1}\mathcal{Q}$ where J is the grid Jacobian and $\mathcal{Q}$ is the conserved flow variable in Cartesian coordinates).

The fully discrete residual (the emphasis here is on the temporal component $\tilde{\mathcal{R}}_n$) for the BDF2 time-marching method is given as

$$\mathcal{R}_n = \tilde{\mathcal{R}}_n + \hat{\mathcal{R}}_n \quad \text{for } n = 1, \ldots, N \tag{3}$$

where

$$\tilde{\mathcal{R}}_n = \frac{3\hat{\mathcal{Q}}_n - 4\hat{\mathcal{Q}}_{n-1} + \hat{\mathcal{Q}}_{n-2}}{2\Delta t}$$

The variable N is the number of time steps, and Δt is a non-dimensional time step. For the ESDIRK4 scheme, the discrete residual is given as

$$\mathcal{R}_j^{(n)} = \frac{1}{a_{jj}}\tilde{\mathcal{R}}_j^{(n)} + \hat{\mathcal{R}}_j^{(n)} + \sum_{k=1}^{j-1} \frac{a_{jk}}{a_{jj}}\hat{\mathcal{R}}_k^{(n)} \quad \text{for } n = 1, \ldots, N \quad j = 2, \ldots, 6 \tag{4}$$

where

$$\tilde{\mathcal{R}}_j^{(n)} = \frac{\hat{\mathcal{Q}}_j^{(n)} - \hat{\mathcal{Q}}_6^{(n-1)}}{\Delta t}$$

The explicit first stage is specified as $\mathcal{Q}_1^{(n)} = \mathcal{Q}_6^{(n-1)}$, and the solution at time step n is given as $\mathcal{Q}^{(n)} = \mathcal{Q}_6^{(n)}$.

8 Miscellaneous - Flow and Mesh Adjoint Details

The relevant expressions required for the computation of the adjoint variables are presented. For BDF2, see Sections 8.4 and 8.5 for the derivation of the adjoint problem using implicit Euler and ESDIRK4 startup mechanisms. The derivation of the adjoint problem for ESDIRK4 is presented

in Section 8.6. In addition, further details on the computation of the mesh adjoint right-hand side (RHS) contribution from the unsteady flow are presented in Section 8.3.

8.1 BDF2 Time-Marching Method

The discrete adjoint problem for the BDF2 method is given as

$$\left[\frac{\partial \mathcal{R}_n}{\partial \mathcal{Q}_n}\right]^T \boldsymbol{\psi}_n = -\left[\omega_n \frac{\partial \mathcal{J}_n}{\partial \mathcal{Q}_n}\right]^T \quad \text{for } n = N \tag{5}$$

$$\left[\frac{\partial \mathcal{R}_n}{\partial \mathcal{Q}_n}\right]^T \boldsymbol{\psi}_n = -\left[\omega_n \frac{\partial \mathcal{J}_n}{\partial \mathcal{Q}_n} + \sum_{i=1}^{p} \boldsymbol{\psi}_{n+i}^T \frac{\partial \mathcal{R}_{n+i}}{\partial \mathcal{Q}_n}\right]^T \quad \text{for } n = N-1, \ldots, 1 \ , \ p = \min\left[N-n, r\right] \tag{6}$$

$$\left[\frac{\partial \mathcal{M}_j}{\partial \mathcal{B}_j}\right]^T \boldsymbol{\lambda}_j = -\underbrace{\left[\sum_{n=1}^{N} \left(\omega_n \frac{\partial \mathcal{J}_n}{\partial \mathcal{B}_j} + \boldsymbol{\psi}_n^T \frac{\partial \mathcal{R}_n}{\partial \mathcal{B}_j}\right)\right]^T}_{\text{last mesh-movement increment RHS}} \quad \text{for } j = m \tag{7}$$

$$\left[\frac{\partial \mathcal{M}_j}{\partial \mathcal{B}_j}\right]^T \boldsymbol{\lambda}_j = -\left[\boldsymbol{\lambda}_{j+1}^T \frac{\partial \mathcal{M}_{j+1}}{\partial \mathcal{B}_j}\right]^T \quad \text{for } j = m-1, \ldots, 1 \tag{8}$$

where r is the number of time levels of previous solutions required for the time-marching method. For BDF2, r is equal to 2 (r can be varied to generalize the above expressions for any linear multi-step time-marching methods). Equations (5) and (6) constitute the flow adjoint, while Equations (7) and (8) constitute the mesh adjoint equations.

8.2 EDIRK4 Time-Marching Method

The adjoint equations for the ESDIRK4 time-marching method are given as

$$\left[\frac{\partial \mathcal{R}_k^{(n)}}{\partial \mathcal{Q}_k^{(n)}}\right]^T \boldsymbol{\psi}_k^{(n)} = -\left[\omega_n \frac{\partial \mathcal{J}_n}{\partial \mathcal{Q}_k^{(n)}}\right]^T \quad \text{for } n = N\ , \quad k = 6 \tag{9}$$

$$\left[\frac{\partial \mathcal{R}_k^{(n)}}{\partial \mathcal{Q}_k^{(n)}}\right]^T \boldsymbol{\psi}_k^{(n)} = -\left[\sum_{i=k+1}^{6} \left(\boldsymbol{\psi}_i^{(n)}\right)^T \frac{\partial \mathcal{R}_i^{(n)}}{\partial \mathcal{Q}_k^{(n)}}\right]^T \quad \text{for } n = N\ , \quad k = 5, \ldots, 2 \tag{10}$$

$$\left[\frac{\partial \mathcal{R}_k^{(n)}}{\partial \mathcal{Q}_k^{(n)}}\right]^T \boldsymbol{\psi}_k^{(n)} = -\left[\omega_n \frac{\partial \mathcal{J}_n}{\partial \mathcal{Q}_k^{(n)}} + \sum_{i=2}^{6} \left(\boldsymbol{\psi}_i^{(n+1)}\right)^T \frac{\partial \mathcal{R}_i^{(n+1)}}{\partial \mathcal{Q}_k^{(n)}} - \boldsymbol{\psi}_1^{(n+1)}\right]^T \quad \text{for } n = N-1, \ldots, 1\ , \quad k = 6 \tag{11}$$

$$\left[\frac{\partial \mathcal{R}_k^{(n)}}{\partial \mathcal{Q}_k^{(n)}}\right]^T \boldsymbol{\psi}_k^{(n)} = -\left[\sum_{i=k+1}^{6} \left(\boldsymbol{\psi}_i^{(n)}\right)^T \frac{\partial \mathcal{R}_i^{(n)}}{\partial \mathcal{Q}_k^{(n)}}\right]^T \quad \text{for } n = N-1, \ldots, 1\ , \quad k = 5, \ldots, 2 \tag{12}$$

$$\boldsymbol{\psi}_1^{(n)} = -\left[\sum_{i=2}^{6} \left(\boldsymbol{\psi}_i^{(n)}\right)^T \frac{\partial \mathcal{R}_i^{(n)}}{\partial \mathcal{Q}_1^{(n)}}\right]^T \tag{13}$$

$$\left[\frac{\partial \mathcal{M}_j}{\partial \mathcal{B}_j}\right]^T \boldsymbol{\lambda}_j = -\underbrace{\left[\sum_{n=1}^{N} \left(\omega_n \frac{\partial \mathcal{J}_n}{\partial \mathcal{B}_j} + \sum_{k=2}^{6} \left(\boldsymbol{\psi}_k^{(n)}\right)^T \frac{\partial \mathcal{R}_k^{(n)}}{\partial \mathcal{B}_j}\right)\right]^T}_{\text{last mesh-movement increment RHS}} \quad \text{for } j = m \tag{14}$$

$$\left[\frac{\partial \mathcal{M}_j}{\partial \mathcal{B}_j}\right]^T \boldsymbol{\lambda}_j = -\left[\frac{\partial \mathcal{M}_{j+1}}{\partial \mathcal{B}_j} \boldsymbol{\lambda}_{j+1}\right]^T \quad \text{for } j = m-1, \ldots, 1 \tag{15}$$

Equations (9) to (13) constitute the flow adjoint problem, while Equations (14) and (15) constitute the mesh adjoint problem for the ESDIRK4 time-marching scheme.

8.3 Mesh Adjoint RHS Contribution from Flow Problem

At each time step, the right-hand side contribution to the last mesh-movement increment adjoint problem can be computed and stored as already exists for steady flows. Let $\mathcal{Y}(\mathcal{B}_m)$ and $\mathcal{N}(\mathcal{Y})$ represent the grid points and grid metrics respectively of the flow solution mesh. Based on Equation (7), the component of interest is derived as follows:

$$\left[\sum_{n=1}^{N}\left(\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{B}_m}+\boldsymbol{\psi}_n^T\frac{\partial\mathcal{R}_n}{\partial\mathcal{B}_m}\right)\right]^T=\sum_{n=1}^{N}\left[\left(\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{Y}}\bigg|_{\mathcal{N}}+\omega_n\,\frac{\partial\mathcal{J}_n}{\partial\mathcal{N}}\bigg|_{\mathcal{Y}}\frac{\partial\mathcal{N}}{\partial\mathcal{Y}}+\boldsymbol{\psi}_n^T\frac{\partial\mathcal{R}_n}{\partial\mathcal{N}}\frac{\partial\mathcal{N}}{\partial\mathcal{Y}}\right)\frac{\partial\mathcal{Y}}{\partial\mathcal{B}_m}\right]^T$$

$$=\sum_{n=1}^{N}\left[\left\{\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{Y}}\bigg|_{\mathcal{N}}+\left(\omega_n\,\frac{\partial\mathcal{J}_n}{\partial\mathcal{N}}\bigg|_{\mathcal{Y}}+\boldsymbol{\psi}_n^T\frac{\partial\mathcal{R}_n}{\partial\mathcal{N}}\right)\frac{\partial\mathcal{N}}{\partial\mathcal{Y}}\right\}\frac{\partial\mathcal{Y}}{\partial\mathcal{B}_m}\right]^T$$

$$=\frac{\partial\mathcal{Y}}{\partial\mathcal{B}_m}^T\sum_{n=1}^{N}\left[\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{Y}}\bigg|_{\mathcal{N}}+\left(\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{N}}\bigg|_{\mathcal{Y}}+\boldsymbol{\psi}_n^T\frac{\partial\mathcal{R}_n}{\partial\mathcal{N}}\right)\frac{\partial\mathcal{N}}{\partial\mathcal{Y}}\right]^T$$

$$=\frac{\partial\mathcal{Y}}{\partial\mathcal{B}_m}^T\underbrace{\sum_{n=1}^{N}\left[\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{Y}}\bigg|_{\mathcal{N}}+\left\{\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{N}}\bigg|_{\mathcal{Y}}+\boldsymbol{\psi}_n^T\left(\boxed{\frac{\partial\tilde{\mathcal{R}}_n}{\partial\mathcal{N}}}+\frac{\partial\hat{\mathcal{R}}_n}{\partial\mathcal{N}}\right)\right\}\frac{\partial\mathcal{N}}{\partial\mathcal{Y}}\right]^T}_{\text{compute and add contribution for each time step}} \tag{16}$$

The final expression for Equation (16) is used to compute the RHS for the last mesh movement increment for a single stage scheme like BDF2. For ESDIRK4, the expression is modified to

$$\left[\sum_{n=1}^{N}\left(\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{B}_j}+\sum_{k=2}^{6}\left(\boldsymbol{\psi}_k^{(n)}\right)^T\frac{\partial\mathcal{R}_k^{(n)}}{\partial\mathcal{B}_j}\right)\right]^T=$$

$$\frac{\partial\mathcal{Y}}{\partial\mathcal{B}_m}^T\underbrace{\sum_{n=1}^{N}\left[\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{Y}}\bigg|_{\mathcal{N}}+\left\{\omega_n\frac{\partial\mathcal{J}_n}{\partial\mathcal{N}}\bigg|_{\mathcal{Y}}+\sum_{k=1}^{6}\left(\frac{1}{a_{kk}}\left(\boldsymbol{\psi}_k^{(n)}\right)^T\boxed{\frac{\partial\tilde{\mathcal{R}}_k^{(n)}}{\partial\mathcal{N}}}+\sum_{i=k}^{6}\frac{a_{ik}}{a_{kk}}\left(\boldsymbol{\psi}_i^{(n)}\right)^T\frac{\partial\hat{\mathcal{R}}_k^{(n)}}{\partial\mathcal{N}}\right)\right\}\frac{\partial\mathcal{N}}{\partial\mathcal{Y}}\right]^T}_{\text{compute and add contribution for each time step}} \tag{17}$$

with $\frac{1}{a_{11}}=0$ and $\frac{a_{11}}{a_{11}}=0$. $\tilde{\mathcal{R}}$ and $\hat{\mathcal{R}}$ are the temporal and spatial residuals respectively. Besides the boxed expressions (derivatives of the temporal residual) in Equations (16) and (17) all the expressions present are available from the existing optimization framework for steady flows. The derivative of the temporal residual $\tilde{\mathcal{R}}(\hat{\mathcal{Q}})=\tilde{\mathcal{R}}(J^{-1}(\mathcal{N})\mathcal{Q})$ with respect to the grid metrics $\mathcal{N}$ is given as

$$\frac{\partial\tilde{\mathcal{R}}}{\partial\mathcal{N}}=\frac{\partial\tilde{\mathcal{R}}}{\partial J}\frac{\partial J}{\partial\mathcal{N}} \tag{18}$$

8.4 Adjoint Problem for BDF2 with Implicit Euler startup, 3 Mesh-Movement Increments and 5 Time Steps

8.4.1 Jacobian of Forward Problem, $\frac{\partial \mathcal{G}}{\partial \mathcal{V}}$

$$\frac{\partial \mathcal{G}}{\partial \mathcal{V}} = \begin{pmatrix} \frac{\partial \mathcal{M}_1}{\partial \mathcal{B}_1} & & & & & & & & \\ \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_1} & \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_2} & & & & & & & \\ & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_2} & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_3} & & & & & & \\ & & - & \mathcal{I} & & & & & \\ & & \frac{\partial \mathcal{R}^2}{\partial \mathcal{B}_3} & -\frac{1}{\Delta t}\mathcal{I} & \frac{\partial \mathcal{R}^1}{\partial \mathcal{Q}^1} & & & & \\ & & \frac{\partial \mathcal{R}^2}{\partial \mathcal{B}_3} & \frac{1}{2\Delta t}\mathcal{I} & -\frac{4}{2\Delta t}\mathcal{I} & \frac{\partial \mathcal{R}^2}{\partial \mathcal{Q}^2} & & & \\ & & \frac{\partial \mathcal{R}^3}{\partial \mathcal{B}_3} & & \frac{1}{2\Delta t}\mathcal{I} & -\frac{4}{2\Delta t}\mathcal{I} & \frac{\partial \mathcal{R}^3}{\partial \mathcal{Q}^3} & & \\ & & \frac{\partial \mathcal{R}^4}{\partial \mathcal{B}_3} & & & \frac{1}{2\Delta t}\mathcal{I} & -\frac{4}{2\Delta t}\mathcal{I} & \frac{\partial \mathcal{R}^4}{\partial \mathcal{Q}^4} & \\ & & \frac{\partial \mathcal{R}^5}{\partial \mathcal{B}_3} & & & & \frac{1}{2\Delta t}\mathcal{I} & -\frac{4}{2\Delta t}\mathcal{I} & \frac{\partial \mathcal{R}^5}{\partial \mathcal{Q}^5} \end{pmatrix}$$

$\frac{\partial \mathcal{R}^n}{\partial \mathcal{Q}^n} = \frac{3}{2\Delta t}\mathcal{I} + \frac{\partial \hat{\mathcal{R}}^n}{\partial \mathcal{Q}^n}$ for BDF2 (i.e. $n > 1$) $\qquad$ $\frac{\partial \mathcal{R}^n}{\partial \mathcal{Q}^n} = \frac{1}{\Delta t}\mathcal{I} + \frac{\partial \hat{\mathcal{R}}^n}{\partial \mathcal{Q}^n}$ for implicit Euler (i.e. $n = 1$)

8.4.2 Components of the Adjoint Problem

$$\left[\frac{\partial \mathcal{G}}{\partial \mathcal{V}}\right]^T \mathbf{\Lambda} = -\left[\frac{\partial \mathcal{J}}{\partial \mathcal{V}}\right]^T$$

$$\begin{bmatrix}
\frac{\partial \mathcal{M}_1}{\partial \mathcal{B}_1}^T & \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_1}^T & & & & & & & \\
 & \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_2}^T & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_2}^T & & & & & & \\
 & & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_2}^T & - & \mathbf{0} & \frac{\partial \mathcal{R}^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}^2}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}^3}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}^4}{\partial \mathcal{B}_3} & \frac{\partial \mathcal{R}^5}{\partial \mathcal{B}_3} \\
 & & & & \mathcal{I} & -\frac{1}{\Delta t}\mathcal{I} & \frac{1}{2\Delta t}\mathcal{I} & & & \\
 & & & & & \frac{\partial \mathcal{R}^1}{\partial \mathcal{Q}^1}^T & -\frac{4}{2\Delta t}\mathcal{I} & \frac{1}{2\Delta t}\mathcal{I} & & \\
 & & & & & & \frac{\partial \mathcal{R}^2}{\partial \mathcal{Q}^2}^T & -\frac{4}{2\Delta t}\mathcal{I} & \frac{1}{2\Delta t}\mathcal{I} & \\
 & & & & & & & \frac{\partial \mathcal{R}^3}{\partial \mathcal{Q}^3}^T & -\frac{4}{2\Delta t}\mathcal{I} & \frac{1}{2\Delta t}\mathcal{I} \\
 & & & & & & & & \frac{\partial \mathcal{R}^4}{\partial \mathcal{Q}^4}^T & -\frac{4}{2\Delta t}\mathcal{I} \\
 & & & & & & & & & \frac{\partial \mathcal{R}^5}{\partial \mathcal{Q}^5}^T
\end{bmatrix}
\begin{bmatrix}
\boldsymbol{\lambda}_1 \\ \boldsymbol{\lambda}_2 \\ \boldsymbol{\lambda}_3 \\ - \\ \boldsymbol{\psi}^{(1)} \\ \boldsymbol{\psi}^{(2)} \\ \boldsymbol{\psi}^{(3)} \\ \boldsymbol{\psi}^{(4)} \\ \boldsymbol{\psi}^{(5)}
\end{bmatrix}
=
\begin{bmatrix}
\mathbf{0} \\ \mathbf{0} \\ \sum_{n=1}^{5} \omega_n \frac{\partial \mathcal{J}_n}{\partial \mathcal{B}_3} \\ - \\ \omega_1 \frac{\partial \mathcal{J}_1}{\partial \mathcal{Q}_1} \\ \omega_2 \frac{\partial \mathcal{J}_2}{\partial \mathcal{Q}_2} \\ \omega_3 \frac{\partial \mathcal{J}_3}{\partial \mathcal{Q}_3} \\ \omega_4 \frac{\partial \mathcal{J}_4}{\partial \mathcal{Q}_4} \\ \omega_5 \frac{\partial \mathcal{J}_5}{\partial \mathcal{Q}_5}
\end{bmatrix}$$

8.5 Adjoint Problem for BDF2 with ESDIRK4 startup, 3 Mesh-Movement Increments and 5 Time Steps

8.5.1 Jacobian of Forward Problem, $\frac{\partial \mathcal{G}}{\partial \mathcal{V}}$

$$\frac{\partial \mathcal{G}}{\partial \mathcal{V}} = \begin{pmatrix}
\frac{\partial \mathcal{M}_1}{\partial \mathcal{B}_1} & & & & & & & & & & & & & & \\
\frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_1} & \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_2} & & & & & & & & & & & & & \\
 & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_2} & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_3} & & & & & & & & & & & & \\
 & & - & \mathcal{I} & & & & & & & & & & & \\
 & & \mathbf{0} & -\mathcal{I} & \mathcal{I} & & & & & & & & & & \\
 & & \frac{\partial \mathcal{R}_2^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{22}\Delta t}\mathcal{I} & \frac{a_{21}}{a_{22}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{\partial \mathcal{R}_2^1}{\partial \mathcal{Q}_2^1} & & & & & & & & & \\
 & & \frac{\partial \mathcal{R}_3^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{33}\Delta t}\mathcal{I} & \frac{a_{31}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{a_{32}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1} & \frac{\partial \mathcal{R}_3^1}{\partial \mathcal{Q}_3^1} & & & & & & & & \\
 & & \frac{\partial \mathcal{R}_4^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{44}\Delta t}\mathcal{I} & \frac{a_{41}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{a_{42}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1} & \frac{a_{43}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1} & \frac{\partial \mathcal{R}_4^1}{\partial \mathcal{Q}_4^1} & & & & & & & \\
 & & \frac{\partial \mathcal{R}_5^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{55}\Delta t}\mathcal{I} & \frac{a_{51}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{a_{52}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1} & \frac{a_{53}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1} & \frac{a_{54}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_4^1}{\partial \mathcal{Q}_4^1} & \frac{\partial \mathcal{R}_5^1}{\partial \mathcal{Q}_5^1} & & & & & & \\
 & & \frac{\partial \mathcal{R}_6^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{66}\Delta t}\mathcal{I} & \frac{a_{61}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{a_{62}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1} & \frac{a_{63}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1} & \frac{a_{64}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_4^1}{\partial \mathcal{Q}_4^1} & \frac{a_{65}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_5^1}{\partial \mathcal{Q}_5^1} & \frac{\partial \mathcal{R}_6^1}{\partial \mathcal{Q}_6^1} & & & & & \\
 & & \frac{\partial \mathcal{R}^2}{\partial \mathcal{B}_3} & \frac{1}{2\Delta t}\mathcal{I} & & & & & & -\frac{4}{2\Delta t}\mathcal{I} & \frac{\partial \mathcal{R}^2}{\partial \mathcal{Q}^2} & & & & \\
 & & \frac{\partial \mathcal{R}^3}{\partial \mathcal{B}_3} & & & & & & & \frac{1}{2\Delta t}\mathcal{I} & -\frac{4}{2\Delta t}\mathcal{I} & \frac{\partial \mathcal{R}^3}{\partial \mathcal{Q}^3} & & & \\
 & & \frac{\partial \mathcal{R}^4}{\partial \mathcal{B}_3} & & & & & & & & \frac{1}{2\Delta t}\mathcal{I} & -\frac{4}{2\Delta t}\mathcal{I} & \frac{\partial \mathcal{R}^4}{\partial \mathcal{Q}^4} & & \\
 & & \frac{\partial \mathcal{R}^5}{\partial \mathcal{B}_3} & & & & & & & & & \frac{1}{2\Delta t}\mathcal{I} & -\frac{4}{2\Delta t}\mathcal{I} & \frac{\partial \mathcal{R}^5}{\partial \mathcal{Q}^5} &
\end{pmatrix}$$

Due to space limitations, $\mathcal{R}_k^{(n)}$ is represented as $\mathcal{R}_k^n$, i.e. parantheses are omitted.

8.5.2 Components of the Adjoint Problem

$$\left[\frac{\partial \mathcal{G}}{\partial \mathcal{V}}\right]^T \mathbf{\Lambda} = -\left[\frac{\partial \mathcal{J}}{\partial \mathcal{V}}\right]^T$$

$$\left[\frac{\partial \mathcal{G}}{\partial \mathcal{Q}}\right]^T = \begin{pmatrix}
\frac{\partial \mathcal{M}_1}{\partial \mathcal{B}_1}^T & \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_1}^T & & & & & & & & & & & & & \\
 & \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_2}^T & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_2}^T & & & & & & & & & & & & \\
 & & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_2}^T & - & \mathbf{0} & \frac{\partial \mathcal{R}_2^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_3^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_4^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_5^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_6^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}^2}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}^3}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}^4}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}^5}{\partial \mathcal{B}_3}^T \\
 & & & \mathcal{I} & -\mathcal{I} & -\frac{1}{a_{22}\Delta t}\mathcal{I} & -\frac{1}{a_{33}\Delta t}\mathcal{I} & -\frac{1}{a_{44}\Delta t}\mathcal{I} & -\frac{1}{a_{55}\Delta t}\mathcal{I} & -\frac{1}{a_{66}\Delta t}\mathcal{I} & \frac{1}{2\Delta t}\mathcal{I} & & & \\
 & & & & \mathcal{I} & \frac{a_{21}}{a_{22}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & \frac{a_{31}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & \frac{a_{41}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & \frac{a_{51}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & \frac{a_{61}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & & & & \\
 & & & & & \frac{\partial \mathcal{R}_2^1}{\partial \mathcal{Q}_2^1}^T & \frac{a_{32}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1}^T & \frac{a_{42}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1}^T & \frac{a_{62}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1}^T & \frac{a_{62}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1}^T & & & & \\
 & & & & & & \frac{\partial \mathcal{R}_3^1}{\partial \mathcal{Q}_3^1}^T & \frac{a_{43}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1}^T & \frac{a_{53}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1}^T & \frac{a_{63}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1}^T & & & & \\
 & & & & & & & \frac{\partial \mathcal{R}_4^1}{\partial \mathcal{Q}_4^1}^T & \frac{a_{54}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_4^1}{\partial \mathcal{Q}_4^1}^T & \frac{a_{64}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_4^1}{\partial \mathcal{Q}_4^1}^T & & & & \\
 & & & & & & & & \frac{\partial \mathcal{R}_5^1}{\partial \mathcal{Q}_5^1}^T & \frac{a_{65}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_5^1}{\partial \mathcal{Q}_5^1}^T & & & & \\
 & & & & & & & & & \frac{\partial \mathcal{R}_6^1}{\partial \mathcal{Q}_6^1}^T & -\frac{4}{2\Delta t}\mathcal{I} & \frac{1}{2\Delta t}\mathcal{I} & & \\
 & & & & & & & & & & \frac{\partial \mathcal{R}^2}{\partial \mathcal{Q}^2}^T & -\frac{4}{2\Delta t}\mathcal{I} & \frac{1}{2\Delta t}\mathcal{I} & \\
 & & & & & & & & & & & \frac{\partial \mathcal{R}^3}{\partial \mathcal{Q}^3}^T & -\frac{4}{2\Delta t}\mathcal{I} & \frac{1}{2\Delta t}\mathcal{I} \\
 & & & & & & & & & & & & \frac{\partial \mathcal{R}^4}{\partial \mathcal{Q}^4}^T & -\frac{4}{2\Delta t}\mathcal{I} \\
 & & & & & & & & & & & & & \frac{\partial \mathcal{R}^5}{\partial \mathcal{Q}^5}^T
\end{pmatrix}$$

$$\mathbf{\Lambda} = \begin{bmatrix} \boldsymbol{\lambda}_1 & \boldsymbol{\lambda}_2 & \boldsymbol{\lambda}_3 & - & \boldsymbol{\psi}_1^{(1)} & \boldsymbol{\psi}_2^{(1)} & \boldsymbol{\psi}_3^{(1)} & \boldsymbol{\psi}_4^{(1)} & \boldsymbol{\psi}_5^{(1)} & \boldsymbol{\psi}_6^{(1)} & \boldsymbol{\psi}^{(2)} & \boldsymbol{\psi}^{(3)} & \boldsymbol{\psi}^{(4)} & \boldsymbol{\psi}^{(5)} \end{bmatrix}^T$$

$$\left[\frac{\partial \mathcal{J}}{\partial \mathcal{V}}\right]^T = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \sum_{n=1}^{5} \omega_n \frac{\partial \mathcal{J}_n}{\partial \mathcal{B}_3} & - & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \omega_1 \frac{\partial \mathcal{J}_1}{\partial \mathcal{Q}_1} & \omega_2 \frac{\partial \mathcal{J}_2}{\partial \mathcal{Q}_2} & \omega_3 \frac{\partial \mathcal{J}_3}{\partial \mathcal{Q}_3} & \omega_4 \frac{\partial \mathcal{J}_4}{\partial \mathcal{Q}_4} & \omega_5 \frac{\partial \mathcal{J}_5}{\partial \mathcal{Q}_5} \end{bmatrix}^T$$

8.6 Adjoint Problem for ESDIRK4, 3 Mesh-Movement Increments and 2 Time Steps

8.6.1 Jacobian of Forward Problem, $\frac{\partial \mathcal{G}}{\partial \mathcal{V}}$

$$
\frac{\partial \mathcal{G}}{\partial \mathcal{V}} = \left(\begin{array}{cccccccccccc}
\frac{\partial \mathcal{M}_1}{\partial \mathcal{B}_1} & & & & & & & & & & & \\
\frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_1} & \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_2} & & & & & & & & & & \\
 & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_2} & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_3} & & & & & & & & & \\
 & & - & \mathcal{I} & & & & & & & & \\
 & & \mathbf{0} & -\mathcal{I} & \mathcal{I} & & & & & & & \\
 & & \frac{\partial \mathcal{R}_2^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{22}\Delta t}\mathcal{I} & \frac{a_{21}}{a_{22}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{\partial \mathcal{R}_2^1}{\partial \mathcal{Q}_2^1} & & & & & & \\
 & & \frac{\partial \mathcal{R}_3^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{33}\Delta t}\mathcal{I} & \frac{a_{31}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{a_{32}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1} & \frac{\partial \mathcal{R}_3^1}{\partial \mathcal{Q}_3^1} & & & & & \\
 & & \frac{\partial \mathcal{R}_4^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{44}\Delta t}\mathcal{I} & \frac{a_{41}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{a_{42}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1} & \frac{a_{43}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1} & \frac{\partial \mathcal{R}_4^1}{\partial \mathcal{Q}_4^1} & & & & \\
 & & \frac{\partial \mathcal{R}_5^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{55}\Delta t}\mathcal{I} & \frac{a_{51}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{a_{52}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1} & \frac{a_{53}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1} & \frac{a_{54}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_4^1}{\partial \mathcal{Q}_4^1} & \frac{\partial \mathcal{R}_5^1}{\partial \mathcal{Q}_5^1} & & & \\
 & & \frac{\partial \mathcal{R}_6^1}{\partial \mathcal{B}_3} & -\frac{1}{a_{66}\Delta t}\mathcal{I} & \frac{a_{61}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1} & \frac{a_{62}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1} & \frac{a_{63}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1} & \frac{a_{64}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_4^1}{\partial \mathcal{Q}_4^1} & \frac{a_{65}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_5^1}{\partial \mathcal{Q}_5^1} & \frac{\partial \mathcal{R}_6^1}{\partial \mathcal{Q}_6^1} & & \\
 & & \mathbf{0} & & & & & & -\mathcal{I} & \mathcal{I} & & \\
 & & \frac{\partial \mathcal{R}_2^2}{\partial \mathcal{B}_3} & & & & & & -\frac{1}{a_{22}\Delta t}\mathcal{I} & \frac{a_{21}}{a_{22}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2} & \frac{\partial \mathcal{R}_2^2}{\partial \mathcal{Q}_2^2} & \\
 & & \frac{\partial \mathcal{R}_3^2}{\partial \mathcal{B}_3} & & & & & & -\frac{1}{a_{33}\Delta t}\mathcal{I} & \frac{a_{31}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2} & \frac{a_{32}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_2^2}{\partial \mathcal{Q}_2^2} & \frac{\partial \mathcal{R}_3^2}{\partial \mathcal{Q}_3^2} \\
 & & \frac{\partial \mathcal{R}_4^2}{\partial \mathcal{B}_3} & & & & & & -\frac{1}{a_{44}\Delta t}\mathcal{I} & \frac{a_{41}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2} & \frac{a_{42}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_2^2}{\partial \mathcal{Q}_2^2} & \frac{a_{43}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_3^2}{\partial \mathcal{Q}_3^2} \\
 & & \frac{\partial \mathcal{R}_5^2}{\partial \mathcal{B}_3} & & & & & & -\frac{1}{a_{55}\Delta t}\mathcal{I} & \frac{a_{51}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2} & \frac{a_{52}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_2^2}{\partial \mathcal{Q}_2^2} & \frac{a_{53}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_3^2}{\partial \mathcal{Q}_3^2} \\
 & & \frac{\partial \mathcal{R}_6^2}{\partial \mathcal{B}_3} & & & & & & -\frac{1}{a_{66}\Delta t}\mathcal{I} & \frac{a_{61}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2} & \frac{a_{62}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_2^2}{\partial \mathcal{Q}_2^2} & \frac{a_{63}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_3^2}{\partial \mathcal{Q}_3^2}
\end{array}\right.
$$

8.6.2 Components of the Adjoint Problem

$$\left[\frac{\partial \mathcal{G}}{\partial \mathcal{V}}\right]^T \mathbf{\Lambda} = -\left[\frac{\partial \mathcal{J}}{\partial \mathcal{V}}\right]^T$$

$$\left[\frac{\partial \mathcal{G}}{\partial \mathcal{Q}}\right]^T = \begin{pmatrix}
\frac{\partial \mathcal{M}_1}{\partial \mathcal{B}_1}^T & \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_1}^T & & & & & & & & & & & & & & & & \\
 & \frac{\partial \mathcal{M}_2}{\partial \mathcal{B}_2}^T & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_2}^T & & & & & & & & & & & & & & & \\
 & & \frac{\partial \mathcal{M}_3}{\partial \mathcal{B}_2}^T & - & \mathbf{0} & \frac{\partial \mathcal{R}_2^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_3^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_4^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_5^1}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_6^1}{\partial \mathcal{B}_3}^T & \mathbf{0} & \frac{\partial \mathcal{R}_2^2}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_3^2}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_4^2}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_5^2}{\partial \mathcal{B}_3}^T & \frac{\partial \mathcal{R}_6^2}{\partial \mathcal{B}_3}^T \\
 & & & \mathcal{I} & -\mathcal{I} & -\frac{1}{a_{22}\Delta t}\mathcal{I} & -\frac{1}{a_{33}\Delta t}\mathcal{I} & -\frac{1}{a_{44}\Delta t}\mathcal{I} & -\frac{1}{a_{55}\Delta t}\mathcal{I} & -\frac{1}{a_{66}\Delta t}\mathcal{I} & & & & & & \\
 & & & & \mathcal{I} & \frac{a_{21}}{a_{22}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & \frac{a_{31}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & \frac{a_{41}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & \frac{a_{51}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & \frac{a_{61}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_1^1}{\partial \mathcal{Q}_1^1}^T & & & & & & \\
 & & & & & \frac{\partial \mathcal{R}_2^1}{\partial \mathcal{Q}_2^1}^T & \frac{a_{32}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1}^T & \frac{a_{42}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1}^T & \frac{a_{52}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1}^T & \frac{a_{62}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_2^1}{\partial \mathcal{Q}_2^1}^T & & & & & & \\
 & & & & & & \frac{\partial \mathcal{R}_3^1}{\partial \mathcal{Q}_3^1}^T & \frac{a_{43}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1}^T & \frac{a_{53}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1}^T & \frac{a_{63}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_3^1}{\partial \mathcal{Q}_3^1}^T & & & & & & \\
 & & & & & & & \frac{\partial \mathcal{R}_4^1}{\partial \mathcal{Q}_4^1}^T & \frac{a_{54}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_4^1}{\partial \mathcal{Q}_4^1}^T & \frac{a_{64}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_4^1}{\partial \mathcal{Q}_4^1}^T & & & & & & \\
 & & & & & & & & \frac{\partial \mathcal{R}_5^1}{\partial \mathcal{Q}_5^1}^T & \frac{a_{65}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_5^1}{\partial \mathcal{Q}_5^1}^T & & & & & & \\
 & & & & & & & & & \frac{\partial \mathcal{R}_6^1}{\partial \mathcal{Q}_6^1}^T & & & & & & \\
 & & & & & & & & & & -\mathcal{I} & -\frac{1}{a_{22}\Delta t}\mathcal{I} & -\frac{1}{a_{33}\Delta t}\mathcal{I} & -\frac{1}{a_{44}\Delta t}\mathcal{I} & -\frac{1}{a_{55}\Delta t}\mathcal{I} & -\frac{1}{a_{66}\Delta t}\mathcal{I} \\
 & & & & & & & & & & \mathcal{I} & \frac{a_{21}}{a_{22}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2}^T & \frac{a_{31}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2}^T & \frac{a_{41}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2}^T & \frac{a_{51}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2}^T & \frac{a_{61}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_1^2}{\partial \mathcal{Q}_1^2}^T \\
 & & & & & & & & & & & \frac{\partial \mathcal{R}_2^2}{\partial \mathcal{Q}_2^2}^T & \frac{a_{32}}{a_{33}}\frac{\partial \hat{\mathcal{R}}_2^2}{\partial \mathcal{Q}_2^2}^T & \frac{a_{42}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_2^2}{\partial \mathcal{Q}_2^2}^T & \frac{a_{52}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_2^2}{\partial \mathcal{Q}_2^2}^T & \frac{a_{62}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_2^2}{\partial \mathcal{Q}_2^2}^T \\
 & & & & & & & & & & & & \frac{\partial \mathcal{R}_3^2}{\partial \mathcal{Q}_3^2}^T & \frac{a_{43}}{a_{44}}\frac{\partial \hat{\mathcal{R}}_3^2}{\partial \mathcal{Q}_3^2}^T & \frac{a_{53}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_3^2}{\partial \mathcal{Q}_3^2}^T & \frac{a_{63}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_3^2}{\partial \mathcal{Q}_3^2}^T \\
 & & & & & & & & & & & & & \frac{\partial \mathcal{R}_4^2}{\partial \mathcal{Q}_4^2}^T & \frac{a_{54}}{a_{55}}\frac{\partial \hat{\mathcal{R}}_4^2}{\partial \mathcal{Q}_4^2}^T & \frac{a_{64}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_4^2}{\partial \mathcal{Q}_4^2}^T \\
 & & & & & & & & & & & & & & \frac{\partial \mathcal{R}_5^2}{\partial \mathcal{Q}_5^2}^T & \frac{a_{65}}{a_{66}}\frac{\partial \hat{\mathcal{R}}_5^2}{\partial \mathcal{Q}_5^2}^T \\
 & & & & & & & & & & & & & & & \frac{\partial \mathcal{R}_6^2}{\partial \mathcal{Q}_6^2}^T
\end{pmatrix}$$

$$\mathbf{\Lambda} = \begin{bmatrix} \boldsymbol{\lambda}_1 & \boldsymbol{\lambda}_2 & \boldsymbol{\lambda}_3 & - & \boldsymbol{\psi}_1^{(1)} & \boldsymbol{\psi}_2^{(1)} & \boldsymbol{\psi}_3^{(1)} & \boldsymbol{\psi}_4^{(1)} & \boldsymbol{\psi}_5^{(1)} & \boldsymbol{\psi}_6^{(1)} & \boldsymbol{\psi}_1^{(2)} & \boldsymbol{\psi}_2^{(2)} & \boldsymbol{\psi}_3^{(2)} & \boldsymbol{\psi}_4^{(2)} & \boldsymbol{\psi}_5^{(2)} & \boldsymbol{\psi}_6^{(2)} \end{bmatrix}^T$$

$$\left[\frac{\partial \mathcal{J}}{\partial \mathcal{V}}\right]^T = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \omega_1 \frac{\partial \mathcal{J}_1}{\partial \mathcal{B}_3} + \omega_2 \frac{\partial \mathcal{J}_2}{\partial \mathcal{B}_3} & - & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \omega_1 \frac{\partial \mathcal{J}_1}{\partial \mathcal{Q}_1} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \omega_2 \frac{\partial \mathcal{J}_2}{\partial \mathcal{Q}_2} \end{bmatrix}^T$$