### Structural and Multidisciplinary Optimization Discrete Adjoint for Coupled Conjugate Heat Transfer --Manuscript Draft--

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| Abstract:  | The typical method to solve multi-physics problems such as Conjugate Heat Transfer (CHT) is the partitioned approach which couples separate solvers through boundary conditions. Effective gradient-based optimisation of partitioned CHT problems requires the adjoint of the coupling to maintain the efficiency of the original multi-physics coupling, which is a significant challenge. The use of automatic differentiation (AD) has the potential to ease this burden and leads to generic gradient computation methods. In this paper, we present how to automate the generation of adjoint fluid and solid solvers for a CHT adjoint using Automatic Differentiation (AD). The derivation of the adjoint of the loose coupling algorithms is shown for three fixed-point coupling algorithms. Application is shown to two CHT optimisation benchmark cases for inverse design and shape optimisation. The results demonstrate that Robin-based coupling algorithms have faster runtimes and are an attractive option for CHT optimisation problems |                     |  |
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| Author Comments:                                 | We think we have addressed all the revewiers' concerns.   |                     |  |

#### SAMO-D-22-00194: DISCRETE ADJOINT FOR COUPLED CONJUGATE HEAT TRANSFER

#### IMAM-LAWAL, VERSTRAETE, MÜLLER

Dear Reviewers, thank you for your comments which were very helpful. Below are our responses and relevant changes to the text:

#### 1. Reviewer 1

1.1. p.6, The authors claim that  $\lambda$  is a non-physical quantity which affects the speed of convergence and the stability of the "Temperature Forward Solid Coefficient Back" (TFRB) coupling method. In the referenced paper [13], also by the group of authors, no stability analysis has been carried out for this particular coupling. Should this be addressed in this paper? Presumably, one has to perform the same analysis as for the "Heat-transfer Coefficient Forward Temperature Back" method presented therein.

1.1.1. *Response:* Because the scope of the paper is on optimization rather than on conjugate heat transfer, the authors fear a stability analysis will reduce the focus of the paper, and hence it is left out, but properly referenced in the text. A full stability analysis has been done in [1]

1.1.2. Action: Reference to [1] has been added to the text.

1.2. p.10 The adjoint to the TFFB CHT coupling method, seems to be a "Flux Forward Temperature Back" (FFTB) scheme. According to the stability analysis presented in a previous work of the authors' group [13], the stability of the TFFB method is guaranteed for Biot numbers |Bi| > 1. Otherwise, the use of under-relaxation is needed in order to ensure convergence. However, in the same paper, stability analysis for the FFTB method yields that the scheme is stable if |Bi| < 1. Does this contradictory behavior in stability of the two methods in regards to Bi affect the stability of the discrete adjoint method?

1.2.1. *Response:* The Biot number indeed affects the stability of the primal solver. Both the forward and reverse (adjoint) differentiation linearize the primal solver and inherit the linear stability of the primal solver. In other words, even though the adjoint simulation may have the look of a FFTB scheme, it is a linearizion of the primal and is stable if the primal is stable.

1.2.2. Action: none required

1.3. p.10-13, In tables 3,5,7 the authors validate the sensitivities of dTw/dx, where x=[x,y,z] the coordinates of a node at the bottom surface of the flat plate, using the adjoint method against the two other methods (tangent and central-differences). Why is there a sensitivity with respect to (wrt) the perturbation of the node in the z direction? Is the case 2D or 3D?.

1.3.1. *Response:* The case is 2.5D with only one cell in the z direction.

1.3.2. Action: The following sentence has been added to the first paragraph of Sec 3.1 "A 3D CHT simulation is performed to obtain the interface temperature and heat flux."

#### 1.4. p.13, The authors claim that, in Robin based coupling methods, by reducing the number of reverse-coupling iterations only 0.5% gradient accuracy is lost. Can the authors further expand this comment? Does this 0.5% reduction only refer to the flat plate validation case?

1.4.1. *Response:* This refers to the flat plate validation case. In the results in the table below, 19 coupling iterations were required to converge the primal solution. Performing just 3 reverse coupling iterations as opposed to 19 results in a very similar gradient. This behaviour was observed only for the Robin-based coupling algorithms. More details are provided in [2].

| Primal Its | Adjoint Its | $\frac{dT_w}{dT_b}$ [E-04] | $\frac{dT_w}{dx}$  |
|------------|-------------|----------------------------|--------------------|
| 19         | 19          | 2.593 <b>1768445246677</b> | 12.803442391969877 |
| 19         | 3           | 2.593 <b>2320190671476</b> | 12.803770636795289 |

TABLE 1. hFRB gradients with reverse coupling iterations.

1.4.2. Action: Paragraph 2 of Sec. 3.2. now reads

Furthermore, rather than performing an equal number of primal and reverse coupling iterations, fewer reverse coupling iterations could be performed, at the cost of a slight reduction in gradient accuracy. On the flat plate validation case in Sec. 3.1, for Robin-based coupling algorithms, reducing the number of reverse coupling iterations from 19 to 3 only resulted in a difference of approximately 0.5% in the gradients. This reduction in the number of reverse coupling iterations can also be combined with partial convergence of the fluid adjoint to significantly reduce runtime without great loss of gradient accuracy. However the TFFB algorithm always required the same number of reverse iterations as the primal to obtain accurate gradients.

1.5. p.18, In table 9, the authors show that by using the TFRB coupling method, the optimization converges to the target solution with a much lower computational cost compared to the other two methods, despite the loss in gradient accuracy due to performing less reverse coupling iterations for the

 $\mathbf{2}$ 

#### adjoint. This proves the time savings of this method. Any reason why the authors performed the optimization of the MarkII turbine blade using the hFRB method instead of TFRB?.

1.5.1. *Response:* The hFRB method was used because the TFRB method failed to converge. This was due to extreme interface values at the shocks on the suction side which lead to divergence of the TFRB method. It is possible that a better choice of Robin parameters could solve this issue, however, it is not straightforward to conduct a stability analysis on the irregular geometry and flow field of the blade.

1.5.2. *Action:* The following has been added to paragraph 1 of 4.2: The CHT problem was solved using the hFRB algorithm due to stability reasons.

# 1.6. p.19-20, Is the optimization of the MarkII blade based on mesh adaptation or re-meshing between optimization cycles? In either case, is it somehow guaranteed that conforming/matching meshes will be obtained at the Fluid-Solid interface, as shown in Fig.7(b)?

1.6.1. *Response:* The mesh deformation algorithm used is Inverse Distance Weighted interpolation (IDW). Only the internal mesh nodes are displaced while the boundary nodes are kept fixed. Hence it is guaranteed that the meshes match at the interface

1.6.2. Action: The following has been added to paragraph 1 of 4.2.2:

"The Inverse Distance Weighted (IDW) interpolation method is used to propagate the displacement of the cooling channels to the internal solid mesh nodes. The interface boundary nodes are kept fixed to maintain the match with the fluid domain. The IDW algorithm is also reverse differentiated to obtain fully accurate adjoint gradients of the entire design chain."

1.7. p.19 The results section seems rather poor. In specific, there is only one 2D application (the optimization of the MarkII turbine blade) which terminated prematurely due to fact that geometrical constraints for the positions of the cooling channels not to cross the boundary of the blade were not imposed. Even though this is not the subject of this paper, the authors are kindly asked to include these constraints in the optimization to make their results more realistic.

1.7.1. *Response:* Point taken however the focus of this particular paper is the methodology and not the application. The authors are currently working on more challenging test cases which will be published in the near future. Within the timescales of this special issue, we will not be able to redefine and run the cases with additional constraints.

1.7.2. Action: Addressed in the forthcoming paper.

#### 2. Reviewer 2

2.1. Even though adjoint method is a computationally efficient method, it is used to compute sensitives for a gradient-based algorithm which is more prone to result in a local minimum than a gradient-free one. Therefore, I would recommend to add a brief discussion on this matter in the introduction.

2.1.1. *Response:* The merits and downsides of gradient-based approaches are well known and are not the main subject of this paper.

2.1.2. Action: The following has been added to paragraph 3 of Sec. 1

"Although gradient-based approaches are only guaranteed to converge to local minima, they are preferred because they typically require less function evaluations. This is advantageous in applications like CHT where the cost of each function evaluation can be high."

## 2.2. From my point of view, the introduction could be extended with more references on the topics covered.

2.2.1. *Response:* There are a number of papers that summarise the literature of the topic, we have cited the main ones. To add a summary stability analysis to the manuscript, we have added Scholl et al, [1] to the introduction. In our view it would not be best use of the journal pages to repeat the overview.

2.2.2. Action: Reference to [1] has been added to the introductin.

2.3. I suggest to provide more details about the partitioned approach followed. What kind of loosely-coupled scheme did you use? Are the coupling algorithms the loosely-coupled scheme? From my point of view, it is not clear from the text.

2.3.1. *Response:* Yes the coupling algorithms are the loosely-coupled scheme.

2.3.2. Action: The following sentence has been added to the last paragraph above Sec 2.1 These separate solvers are loosely coupled to solve CHT problems.

2.4. A reference to the Spalart-Allmaras turbulence model could be provided to the interested reader.

2.4.1. Response: Thank you for pointing out this omission.

2.4.2. Action: Reference has been included

## 2.5. Why do you have 226 for the inverse optimization problem? I suggest to include more details about the computational model. Did you perform a mesh dependency study?

2.5.1. *Response:* The 226 design variables arise from the number of mesh nodes used to discretise the computational domain. A mesh dependence study using double the number of mesh points showed no significant change in results.

2.5.2. Action: Paragraph 3 of Sec 4.1 has been revised as follows:

Each mesh node at the bottom of the plate has an independent value of  $T_b$  specified as a boundary condition, and is used in this work as a design variable ( $\alpha$ ) that needs to be changed to drive J to zero. The selected mesh following a mesh dependence study results in 226 design variables for the present work.

#### 2.6. Why did you use the BFGS as optimization algorithm?

2.6.1. *Response:* Any gradient-based optimisation algorithm e.g. steepest-descent, conjugate gradient, etc, could be used. The BFGS algorithm is known to have good performance and is the default method for the scipy.optimize.minimize library. It is widely used for unconstrained optimisation.

2.6.2. Action: none required.

#### 2.7. From my point of view, you should present more details about the computational model of the turbine blade.

2.7.1. Response: Thank you for pointing this out.

2.7.2. Action: The following has been added to paragraph 2 of Sec. 4.2

Matching meshes are used for both domains as shown in Figure 7 with 49,532 nodes in the fluid domain and 5,714 nodes in the solid. A near wall spacing  $y^+$  of less than 1 is used for the fluid.

## 2.8. There is a typo on page 19, line 48, where it reads "form", it should read "from".

2.8.1. Response: Thanks for spotting that, this has been changed in the text

2.8.2. Action: Changed in text

#### 2.9. How was the scaling process done for the design optimization problem?

2.9.1. *Response:* The chord length of the turbine blade is only 0.06855 m. Therefore a unit displacement in any direction would take a cooling channel outside the solid domain. As we have no control over the line search and step size used in scipy these large displacements occur. When this happens, a high value of the objective function is returned to the optimiser to indicate that the step is too large.

2.9.2. Action: Revised the following sentence:

"The shallow slopes of the curves in Fig. 10 are due to the scaling performed to prevent the optimiser from taking large steps" to "The irregular shape of the curves in Fig. are a result of the SciPy line search."

#### 2.10. Please include the DOI information of the references.

2.10.1. *Response:* Including the doi is not practised in the recently published papers in the journal.

#### IMAM-LAWAL, VERSTRAETE, MÜLLER

2.10.2. *Action:* none required at this stage, if requested by the editors, can be added during proofreading.

#### References

- Sebastian Scholl, Bart Janssens, and Tom Verstraete. Stability of static conjugate heat transfer coupling approaches using robin interface conditions. Computers & Fluids, 172:209–225, August 2018.
- [2] O.R. Imam-Lawal. Adjoint based optimisation for coupled conjugate heat transfer. PhD thesis, Queen Mary University of London, 2020.

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| 10            | access/download;Manuscript;m2-sn-   |
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| 41            |   |
| 42            | Abstract  |
| 43            | The typical method to solve multi-physics problems such as Conju-   |
| 44            | gate Heat Transfer (CHT) is the partitioned approach which couples  |
| 45            | separate solvers through boundary conditions. Effective gradient-based  |
| 46            | optimisation of partitioned CHT problems requires the adjoint of  |
| 4/            | the coupling to maintain the efficiency of the original multi-physics   |
| 48            | coupling, which is a significant challenge. The use of automatic dif-   |
| 49            | ferentiation (AD) has the potential to ease this burden and leads   |
| 50            | to generic gradient computation methods. In this paper, we present  |
| 51            | how to automate the generation of adjoint fluid and solid solvers for   |
| 52            | a CHT adjoint using Automatic Differentiation (AD). The derivation  |
| 55            | of the adjoint of the loose coupling algorithms is shown for three  |
| 54            | fixed-point coupling algorithms. Application is shown to two CHT opti-  |
| 55            | misation benchmark cases for inverse design and shape optimisation. The   |
| 50            | results demonstrate that Robin-based coupling algorithms have faster  |
| 58            | runtimes and are an attractive option for CHT optimisation problems.  |
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| 59            | reyworus: Gradient-Dased optimisation, adjoint method, conjugate heat transfer. Robin boundary conditions inverse problems shape optimisation |
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#### 1 Introduction

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Conjugate Heat Transfer (CHT) describes the process of heat transfer between a fluid and solid and is ubiquitous in engineering applications such as turbine blade cooling, modelling of heat exchangers, and cooling of electronics.

19 CHT problems may be solved using a monolithic approach in which both 20 fluid and solid equations are solved simultaneously by a single solver. However, 21 the partitioned or segregated approach is often adopted where separate solvers 22 for the fluid and structure are loosely coupled through boundary conditions. 23 These conditions need to be updated iteratively until the temperature and 24 heat flux are continuous between the two domains [1, 2].

25 Recent work in CHT has evolved beyond merely solving the CHT problem 26 to an increased interest in shape optimisation [3-6]. This has lead to the need 27 for efficient optimisation methods such as gradient-based approaches. Although 28 gradient-based approaches are only guaranteed to converge to local minima. 29 they are preferred because they typically require less function evaluations. This 30 is advantageous in applications like CHT where the cost of each function eval-31 *uation can be high.* Adjoint methods have been shown to be highly efficient as 32 the cost of obtaining gradients can be made almost independent of the number 33 of design variables. However, for partitioned coupling approaches, the flexibil-34 ity of using different solvers for both domains results in an increased level of 35 complexity with regard to obtaining the required gradients. 36

37 Adjoint methods can be grouped into continuous or discrete methods. In 38 the continuous method the adjoint equations are analytically derived before 39 being discretised while the discrete method discretises the state equations 40 before formulating the discrete adjoint equations<sup>[7]</sup>. Arguments in favour of 41 either approach revolve around stability, accuracy and computational effort. 42 The discrete adjoint is considered to have the advantage with regards to sta-43 bility and accuracy but not with computational effort. However, the use of 44 automatic differentiation (AD) can significantly reduce the implementation 45 effort associated with producing the adjoint code. 46

The majority of the work related to CHT optimisation has favoured the 47 continuous adjoint formulation [3, 4, 6, 8] while Burghardt and Gauger [9] 48 use the discrete adjoint but with a monolithic solver. In the present study, 49 we demonstrate a partitioned/segregated coupling methodology in which the 50 discrete adjoint formulation is achieved through AD. The use of AD has the 51 potential to lead to very generic and less labour intensive implementations 52 of adjoint methods for CHT. We focus on coupling boundary conditions and 53 highlight the advantages Robin boundary conditions in the fluid domain. Fur-54 thermore, the gradient exchange required by partitioned coupling approaches 55 56 is demonstrated using three fixed-point coupling algorithms.

57 This paper is organised as follows: we first describe the CHT problem, 58 governing equations, and the coupling procedure. We then discuss the adjoint 59 procedure for the partitioned approach and gradient verification. Two CHT 60 optimisation problems are then solved using the adjoint method. Finally, a 61 summary is given in the conclusion.

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Fig. 1: Description of primal CHT problem

#### 2 PRIMAL PROBLEM

Consider flow over a flat plate with finite thickness. The free stream flow temperature is  $T_{\infty}$ , while the bottom of the plate is maintained at a lower temperature  $T_b$ . Consequently, heat is transferred at the interface between the solid plate and the fluid. The primal problem is to accurately compute the wall temperature at the interface between the fluid and solid, which is unknown a priori and can only be computed by considering the coupled problem (see Fig 1).

In order to solve the CHT problem using a partitioned approach, the fluid and solid governing equations must be coupled leading to a coupled system of equations

$$F(U^i, W^i) = 0, (1)$$

$$S(U^i, W^{i+1}) = 0, (2)$$

where U denotes the fluid state variables, W the solid state variables, and i the coupling iteration. F represents the Reynolds Averaged Navier-Stokes equations:

$$\frac{\partial}{\partial t} \int_{\Omega_f} \vec{U} d\Omega + \oint_{\partial \Omega_f} (\vec{f_c} - \vec{f_v}) \cdot dS = \int_{\Omega_f} \vec{Q} d\Omega_f, \tag{3}$$

where t denotes pseudo time, Q the source term, and  $x_j$ , j = 1, 2, 3 are the Cartesian coordinates. The state vectors U, and the inviscid and viscous flux vectors  $\vec{f_c}$  and  $\vec{f_v}$  are defined as

$$\vec{U} = \begin{bmatrix} \rho \\ \rho \vec{v} \\ \rho e \\ \tilde{\nu} \end{bmatrix}, \vec{f}_c = \begin{bmatrix} \rho \vec{v} \cdot \vec{n} \\ (\rho \vec{v} \vec{v} + p) \cdot \vec{n} \\ \rho(e+p) \vec{v} \cdot \vec{n} \end{bmatrix}, \vec{f}_v = \begin{bmatrix} 0 \\ \overline{\tau} \cdot \vec{n} \\ \vec{\Theta} \cdot \vec{n} \\ \frac{1}{\sigma} (\nu_L + \tilde{\nu}) (\nabla \nu \cdot \vec{n}) \tilde{\nu} \end{bmatrix},$$
(4)

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Discrete Adjoint for Coupled Conjugate Heat Transfer

$$\vec{\Theta} = \overline{\overline{\tau}} \cdot \vec{v} + \lambda \nabla T. \tag{5}$$

Where,  $\rho$ , p, and  $\vec{v}$  are the fluid density, pressure, and velocity vector respectively,  $\vec{n}$  the surface normal vector, e the internal energy per unit mass,  $\tau$  is the stress tensor for Newtonian fluids and  $\lambda$  is the fluid thermal conductivity,  $\tilde{\nu}$  is the modified eddy viscosity which is obtained using the Spalart-Allmaras turbulence model [10] and S in Eqn. (2) refers to the governing equation of the solid domain  $\Omega_s$ , that is the steady state heat conduction equation

$$\lambda_s \nabla^2 T = 0, \tag{6}$$

25 where  $\lambda_s$  is the conductivity of the solid.

Each domain depends on the other through the boundary conditions specified at the fluid-solid interface. The solid state W, which is the solid's temperature, affects the fluid state U through the viscous flux component of the energy equation and through the heat flux at the non-adiabatic fluid-solid interface which must be specified using a boundary condition. Similarly, the fluid state variables U affect the state of the solid W through the interface boundary conditions specified while solving the heat equation.

Consequently, separate stand alone solvers for the fluid and solid, which are loosely coupled through interface boundary conditions, can be used to solve the primal problem. These boundary conditions are updated iteratively until the temperature and heat flux are continuous between the two domains. That is until

$$T_{sw} = T_{fw},$$

$$\underbrace{\lambda_s \left. \frac{\partial T}{\partial n} \right|_s}_{q_{sw}} = \underbrace{\lambda_f \left. \frac{\partial T}{\partial n} \right|_f}_{q_{fw}}$$

where  $T_{fw}$  is the interface temperature in the fluid domain  $\Omega_f$ ,  $T_{sw}$  the interface temperature in the solid domain  $\Omega_s$ ,  $\lambda_f$  and  $\lambda_s$  the thermal conductivity of the fluid and solid respectively, n the surface normal, and  $q_{fw}$  and  $q_{sw}$  the interface heat flux in the fluid and solid domains respectively (see Figure 1).

In this work, the fluid equations are solved using the in-house mgOpt flow solver, a vertex centered, finite volume solver, which solves the 3-D compressible RANS equation using unstructured grids [11, 12]. The solid equations are solved using the finite element method with open-source solver, CalculiX, developed by Dhondt and Wittig. [13]. These separate solvers are loosely coupled to solve CHT problems.

#### 2.1 Coupling Algorithms

In the present work, an implicit coupling method is used to solve the primal problem with a partitioned approach. Different coupling algorithms exist depending on which type of boundary conditions are exchanged between both

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domains. In both domains, boundary conditions could be specified as Dirichlet, Neumann, or Robin, leading to a total of 7 different types of coupling algorithms [14]. In this work, we use the three different fixed-point coupling algorithms described in the following sections.

#### 2.1.1 Temperature Forward Flux Back (TFFB)

In the TFFB method [15], the solid interface heat flux distribution,  $q_{sw}^i$ , where i is the current coupling iteration, is imposed as a boundary condition to the fluid domain. The fluid solver  $\mathbf{F}$  solves the flow equations resulting in a fluid interface temperature distribution,  $T^i_{fw}$ . This temperature is then imposed as boundary condition for the solid domain and the solid conduction solver,  $\mathbf{S}$ , provides an updated heat flux distribution  $q_{sw}^{i+1}$ . This loop is continued until there is no change in the boundary conditions exchanged by both solvers (see Figure 2), 

$$T_{fw}^i = \mathbf{F}(q_{sw}^i),\tag{7}$$

$$q_{sw}^{i+1} = \mathbf{S}(T_{fw}^i).$$
 (8)



Fig. 2: CHT coupling algorithms. Left:TFFB, Centre: TFRB, Right:hFRB.

#### 2.1.2 Temperature Forward Solid Coefficient Back (TFRB)

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$$q_{sw}^i = \mathbf{S}(T_{sw}^i),\tag{9}$$

$$\tilde{T}_s^i = \frac{q_{sw}^i}{\tilde{R}} + T_{sw}^i, \implies (\text{calc. } \tilde{T}_s)$$
(10)

$$\Gamma_{fw}^{i} = \mathbf{F}(\tilde{T}_{s}^{i}, \tilde{R}), \tag{11}$$

$$q_{fw}^{i} = \tilde{R}(\tilde{T}_{s}^{i} - T_{fw}^{i}), \Longrightarrow \text{ (Robin BC in } \Omega_{f})$$
(12)

$$T_{sw}^{i+1} = T_{fw}^i. (13)$$

Assuming the algorithm begins in the solid domain, an initial guess for the wall temperature  $T_{sw}^i$  is imposed on the solid and used to obtain the heat flux  $q_{sw}^i$ . Next, the virtual solid sink temperature  $\tilde{T}_s^i$  is calculated using Eqn. (10). The virtual conductivity and solid sink temperature are used for a Robin boundary condition in the fluid domain (Eqn. (12)). The flow solver then returns an update of the interface temperature which is given to the solid as a Dirichlet boundary condition (see Figure 2).

#### 2.1.3 Heat Transfer Coefficient Forward Solid Coefficient Back (hFRB)

The hFRB method uses Robin boundary conditions in both domains and is the same as TFRB on the fluid side (see Figure 2). Similar to the TFRB method, the algorithm can start with an initial guess of the interface temperature on the solid side. Next, the virtual solid temperature  $\tilde{T}_s$  is then calculated and passed to the flow solver along with the virtual conductivity  $\tilde{R}$ .

$$q_{sw}^i = \mathbf{S}(T_{sw}^i), \tag{14}$$

$$\tilde{T}_{s}^{i} = \frac{q_{sw}^{i}}{\tilde{R}} + T_{sw}^{i}, \implies (\text{calc. } \tilde{T}_{s})$$
(15)

$$T^i_{fw}, q^i_{fw} = \mathbf{F}(\tilde{T}^i_s, \tilde{R}), \tag{16}$$

$$T_{sink}^{i} = T_{fw}^{i} - \frac{q_{fw}^{i}}{\tilde{h}}, \implies (\text{calc. } T_{sink})$$
(17)

$$q_{sw}^{i+1}, T_{sw}^{i+1} = \mathbf{S}(T_{sink}^{i}, \tilde{h}).$$
(18)

The outputs from the flow solver are the interface temperature and heat flux  $(T_{fw}, q_{fw})$ . These are used in Eqn. (17) to calculate the ambient fluid temperature  $(T_{sink}^i)$  for a user specified value of the virtual heat transfer coefficient  $(\tilde{h})$ . The solid solver then returns an update on the interface temperature and heat flux and the exchange is continued until convergence [14, 16].

#### **3 DISCRETE ADJOINT**

For gradient-based CHT optimisation, we require the gradient of the objective function I w.r.t the design variables  $\alpha$ 

$$\frac{dI}{d\alpha} = \frac{\partial I}{\partial \alpha} + \begin{bmatrix} \frac{\partial I}{\partial U} & \frac{\partial I}{\partial W} \end{bmatrix} \begin{bmatrix} \frac{dU}{d\alpha} \\ \frac{dW}{d\alpha} \end{bmatrix},\tag{19}$$

$$\frac{dI}{d\alpha} = \frac{\partial I}{\partial \alpha} + g^T u, \tag{20}$$

where U and W represent the fluid and solid state variables respectively. The term  $g^T u$  is expensive to solve hence it is advantageous to use the adjoint formulation. The derivatives of the state variables for fluid and solid with respect to the design variables  $\left(\frac{dU}{d\alpha}, \frac{dW}{d\alpha}\right)$  can be obtained from the state equations

$$F(\alpha, U, W) = 0, \tag{21}$$

$$S(\alpha, U, W) = 0. \tag{22}$$

Where F is used to represent the RANS equations, and S represents the heat equation. The derivative of the state equations with respect to the design variables which are required to solve Eqn. (19) are obtained from

$$\begin{bmatrix} \frac{\partial F}{\partial U} & \frac{\partial F}{\partial W} \\ \frac{\partial S}{\partial U} & \frac{\partial S}{\partial W} \end{bmatrix} \begin{bmatrix} \frac{dU}{\partial \alpha} \\ \frac{dW}{\partial \alpha} \end{bmatrix} = \begin{bmatrix} -\frac{\partial F}{d\alpha} \\ -\frac{\partial S}{d\alpha} \end{bmatrix}, \qquad (23)$$
$$\mathbf{A}u = f.$$

The diagonal terms are the Jacobians of each discipline while the offdiagonal terms show how the states of one discipline affect the state of the other e.g. how the fluid temperature affects the solid flux and vice-versa. Therefore the sensitivity of the cost function, Eqn. (19), for the coupled problem can be

written as

$$\frac{dI}{d\alpha} = \frac{\partial I}{\partial \alpha} + \begin{bmatrix} \frac{\partial I}{\partial U} & \frac{\partial I}{\partial W} \end{bmatrix} \begin{bmatrix} \frac{\partial F}{\partial U} & \frac{\partial F}{\partial W} \\ \frac{\partial S}{\partial S} & \frac{\partial S}{\partial S} \end{bmatrix}^{-1} \begin{bmatrix} -\frac{\partial F}{\partial \alpha} \\ \frac{\partial S}{\partial S} \end{bmatrix}$$

$$\frac{dI}{d\alpha} = \frac{\partial I}{\partial \alpha} + \begin{bmatrix} \frac{\partial I}{\partial U} & \frac{\partial I}{\partial W} \end{bmatrix} \begin{bmatrix} \frac{\partial I}{\partial U} & \frac{\partial W}{\partial W} \\ \frac{\partial S}{\partial U} & \frac{\partial S}{\partial W} \end{bmatrix} \begin{bmatrix} -\frac{\partial \alpha}{\partial \alpha} \\ -\frac{\partial S}{\partial \alpha} \end{bmatrix}$$
(24)

$$\frac{dI}{d\alpha} = \frac{\partial I}{\partial \alpha} + (g^T \mathbf{A}^{-1})f.$$
(25)

The cost of calculating the gradient can be reduced through the adjoint method. The adjoint variables are the solution to the adjoint equation

$$\begin{bmatrix} \frac{\partial F}{\partial U} & \frac{\partial F}{\partial W} \\ \frac{\partial S}{\partial U} & \frac{\partial S}{\partial W} \end{bmatrix}^{T} \begin{bmatrix} \psi \\ \phi \end{bmatrix} = \begin{bmatrix} \frac{\partial I}{\partial U} \\ \frac{\partial I}{\partial W} \end{bmatrix}, \qquad (26)$$
$$\mathbf{A}^{T} v = g.$$

Where  $v^T = [\psi, \phi]$  represents the fluid and solid adjoint variables respectively and

$$v = (\mathbf{A}^T)^{-1}g,\tag{27}$$

$$v^T = g^T(\mathbf{A}^{-1}). \tag{28}$$

Therefore, after only one solve of Eqn. (26) for the adjoint variable v, the sensitivity can be calculated as

$$\frac{dI}{d\alpha} = \frac{\partial I}{\partial \alpha} + v^T f, \tag{29}$$

$$\frac{dI}{d\alpha} = \frac{\partial I}{\partial \alpha} + \begin{bmatrix} \psi & \phi \end{bmatrix} \begin{bmatrix} -\frac{\partial F}{\partial \alpha} \\ -\frac{\partial S}{\partial \alpha} \end{bmatrix}.$$
(30)

In the partitioned coupling approach, the Jacobian of the coupled system in Eqn. (26) is not calculated. Instead, the adjoint solution is obtained through an iterative approach, similar to the primal coupling, to compensate for the missing off-diagonals. The adjoint of system of each discipline is solved using the adjoint solution of the other discipline from the previous iteration [17]

$$\left(\frac{\partial F}{\partial U}^{T}\right)\psi^{i} = \left(\frac{\partial I}{\partial U}^{T}\right) - \left(\frac{\partial S}{\partial U}^{T}\phi^{i-1}\right)$$
(31)

$$\left(\frac{\partial S}{\partial W}^{T}\right)\phi^{i} = \left(\frac{\partial I}{\partial W}^{T}\right) - \left(\frac{\partial F}{\partial W}^{T}\psi^{i}\right),\tag{32}$$

where *i* is the current coupling iteration. The partial derivatives  $\left(\frac{\partial S}{\partial U}, \frac{\partial F}{\partial W}\right)$ in equations (31) and (32) depend on the type of coupling algorithm used (see Table 1) and are obtained by differentiating the solvers w.r.t. the coupling boundary conditions and coordinates. Reverse mode automatic differentiation is applied to the fluid and heat conduction solvers [18] using Tapenade [19], a source-transformation AD tool. The use of AD significantly reduces the effort required to obtain the adjoint solvers and in the case of the fluid solver, the procedure was fully automated. This allows for easy implementation of new coupling boundary conditions and optimisation objective functions. 

|                                 | Coupling algorithm                        |  |  |  |
|---------------------------------|---|--|--|--|
| Partial derivative              | TFFB                                      | TFRB   | hFRB   |  |
| $rac{\partial S}{\partial U}$  | $\frac{\partial q_{sw}}{\partial T_{fw}}$ | $\frac{\partial q_{sw}}{\partial T_{fw}}$      | $\frac{\partial q_{sw}}{\partial T_{sink}}, \frac{\partial q_{sw}}{\partial h}, \frac{\partial T_{sw}}{\partial T_{sink}}, \frac{\partial T_{sw}}{\partial h}$ |  |
| $\frac{\partial F}{\partial W}$ | $\frac{\partial T_{fw}}{\partial q_{sw}}$ | $\frac{\partial T_{fw}}{\partial \tilde{T}_s}$ | $rac{\partial T_{sink}}{\partial 	ilde{T}_s}, \ rac{\partial h}{\partial 	ilde{T}_s}$  |  |

 Table 1: Description of multidisciplinary partial derivative terms

The iterative approach shown in equations (31) and (32) results in a reversed/inverted version of each coupling algorithm. The total sensitivity in Eqn. (30) is then obtained by accumulating the gradients output after each solid adjoint iteration.

#### 3.1 Gradient Calculation and Verification

We demonstrate accuracy of the partitioned adjoint methodology using a flat plate test case. The plate has a fixed temperature  $T_b$  at the bottom and comes in contact with fluid of a different temperature (see Fig 3). A 3D CHT sim-ulation is performed to obtain the interface temperature and heat flux. A perturbation in the temperature of a red node at the bottom results in a change in the heat flux into the fluid domain. This perturbation travels through the coupling and results in a new interface temperature  $T_w$  at the blue node. Sim-ilarly, a coordinate perturbation (x, y, z) changes the volume of the plate and leads to a change in the heat flux at the fluid-solid interface and consequently alters the solution of the coupled problem. Therefore, the effect of these per-turbations on the interface temperature is described by two gradients  $\frac{dT_w}{dT_h}$  and  $\frac{dT_w}{d\vec{x}}$  where  $\vec{x} = [x, y, z]$ . 

The partitioned adjoint approach to solving equations (31) and (32) is now described.



#### 3.1.1 Temperature Forward Flux Back (TFFB)

The adjoint run of the TFFB algorithm, starts with seeding a vector  $\overline{T}_{fw}^i$ which is set to 1 for the blue node in Figure 3 while all others are set to 0.  $\overline{T}_{fw}$  is used by the adjoint flow solver (**F**<sub>b</sub>) to obtain the adjoint heat flux  $\overline{q}_{sw}$ . This is then passed directly to the adjoint solid (**S**<sub>b</sub>) solver to obtain an update of the adjoint temperature.

$$\overline{q}_{sw}^i = \mathbf{F}_{\mathbf{b}}(\overline{T}_{fw}^i), \tag{33}$$

$$\overline{\vec{x}}^{i}, \overline{T}^{i}_{b}, \overline{T}^{i-1}_{fw} = \mathbf{S}_{\mathbf{b}}(\overline{q}^{i}_{sw}).$$
(34)

The reverse loop is performed for the same number of iterations as for the primal solution and at the end of each coupling iteration, the gradient  $\overline{T}_b$  is accumulated. This single adjoint solve obtains the gradient of the interface temperature at the blue node w.r.t to all design variables (red nodes). A block structure representation of the reverse differentiated coupling algorithm is shown in Figure 4. In fact, both  $\frac{dT_w}{dT_b}$  and  $\frac{dT_w}{dx}$  are obtained in one reverse solve highlighting the advantage and cost savings of the adjoint method.

|                                   | Design variable            |                            |                            |
|-----------------------------------|----------------------------|----------------------------|----------------------------|
| Gradient method                   | $1 [\times 10^{-4}]$       | $2 [\times 10^{-2}]$       | $3 [\times 10^{-4}]$       |
| Tangent                           | 3.57424996556775 <b>86</b> | 1.0915639124275244         | 6.2298230582871 <b>555</b> |
| Adjoint                           | 3.57424996556775 <b>91</b> | 1.09156391242752 <b>37</b> | 6.2298230582871 <b>479</b> |
| $CD [\Delta = 10^{-4} \text{ K}]$ | 3.5665266295836773         | 1.0898488085331337         | 6.2618937590741552         |
|                                   |                            |                            |                            |

**Table 2:** TFFB gradient of interface temperature  $T_w$  w.r.t bottom temperature  $T_b \left(\frac{dT_w}{dT_b}\right)$ 

Table 2 shows gradients for  $\frac{dT_w}{dT_b}$  while Table 3 shows the gradients for  $\frac{dT_w}{d\vec{x}}$ . Both Tables show good agreement between the tangent, adjoint, and central difference (CD) methods.

|                             | Design variable            |                             |                             |
|-----------------------------|----------------------------|-----------------------------|-----------------------------|
| Gradient method             | x                          | y                           | z                           |
| Tangent                     | 16.3537546 <b>63042668</b> | -13.270758 <b>597756023</b> | 0.410171858 <b>55131066</b> |
| Adjoint                     | 16.353754647042667         | -13.270758 <b>610753868</b> | 0.410171858 <b>29135394</b> |
| $CD \ [\Delta = 10^{-7} m]$ | 16.3 <b>21095586135925</b> | -13.244326737549272         | 0.40858196825865889         |

**Table 3**: TFFB gradient of interface temperature  $T_w$  w.r.t coordinates



**Fig. 4**: Reverse differentiated CHT coupling algorithms; Left:TFFB, Centre: TFRB, Right:hFRB.

#### 3.1.2 Temperature Forward Solid Coefficient Back (TFRB)

The adjoint TFRB run is started by seeding a vector of the adjoint fluid temperature  $\overline{T}_{fw}$  to the flow solver to obtain  $\tilde{T}_{sb}$ . The reverse differentiated routine for Eqn. (10) is also required to obtain the adjoint heat flux and temperature as shown in equations (36). The solid solver then uses the adjoint heat flux

to obtain  $\overline{T}_{sw}$ . The two adjoint interface temperatures are then summed to provide an update for the next iteration.

$$\tilde{T}^{i}_{sb} = \mathbf{F}_{\mathbf{b}}(\overline{T}^{i}_{fw}), \tag{35}$$

$$\overline{q}_{sw}^i, \overline{T}_{sw} = f(\tilde{T}_{sb}^i, \tilde{R}) \implies (\text{calc. } \tilde{T}_{sb}), \tag{36}$$

$$\overline{\vec{x}}^{i}, \overline{T}^{i}_{b}, \overline{T}^{i}_{fw} = \mathbf{S}_{\mathbf{b}}(\overline{q}^{i}_{sw}), \tag{37}$$

$$\overline{T}_{fw}^{i-1} = \overline{T}_{fw}^i + \overline{T}_{sw}.$$
(38)

The loop is done for the same number of coupling iterations and  $\overline{T}_b$  and  $\overline{\vec{x}}$  are accumulated. The final result returns  $\frac{dT_w}{dT_b}$  and  $\frac{dT_w}{d\vec{x}}$  and is shown in Tables 4 and 5. Good agreement is seen between the tangent, adjoint, and central difference (CD) methods.

|                                   | Design variable            |                            |                            |
|-----------------------------------|----------------------------|----------------------------|----------------------------|
| Gradient method                   | $1 [\times 10^{-4}]$       | $2 [\times 10^{-2}]$       | $3 [\times 10^{-4}]$       |
| Tangent                           | 3.57355505580010 <b>70</b> | 1.091430424038719 <b>9</b> | 6.2333366050062 <b>219</b> |
| Adjoint                           | 3.57355505580010 <b>43</b> | 1.091430424038719 <b>6</b> | 6.2333366050062 <b>176</b> |
| CD $[\Delta = 10^{-4} \text{ K}]$ | 3.5 <b>665607356349938</b> | 1.0898481832555262         | 6.2 <b>619392338092439</b> |

**Table 4**: TFRB gradient of interface temperature  $T_w$  w.r.t bottom temperature  $T_b$ 

|                                  | Design variable            |                             |                             |
|----------------------------------|----------------------------|-----------------------------|-----------------------------|
| Gradient method                  | x                          | y                           | <i>z</i>                    |
| Tangent                          | 16.370061472907469         | -13.2839935 <b>73142387</b> | 0.410965932 <b>85022071</b> |
| Adjoint                          | 16.370061462907479         | -13.2839935 <b>81266039</b> | 0.41096593268774745         |
| CD $[\Delta = 10^{-7} \text{m}]$ | 16.3 <b>21095586135925</b> | -13.244325032246707         | 0.40858196825865889         |

**Table 5**: TFRB gradient of interface temperature  $T_w$  w.r.t coordinates

#### 3.1.3 Heat Transfer Coefficient Forward Solid Coefficient Back (hFRB)

For the hFRB adjoint, the adjoint wall temperature  $\overline{T}_{fw}$  is used by the flow solver to obtain the adjoint solid sink temperature  $\overline{T}_s$ . This is then converted into an adjoint heat flux  $\overline{q}_{sw}$  and adjoint temperature  $\overline{T}_{sw}$  using the differen-tiated routine which calculates the Robin parameters  $T_{sink}$  and  $\hat{h}$  for the solid domain. The solid solver then returns an adjoint sink temperature  $\overline{T}_{sink}$  and adjoint virtual heat transfer coefficient  $\overline{h}$ . The differentiated Robin preprocess-ing step uses the virtual heat transfer coefficient  $\overline{h}$  to calculate the adjoint wall temperature  $\overline{T}_{fw}$  while the adjoint sink temperature  $\overline{T}_{sink}$  is assigned to the first off wall node, as shown in Eqn. (42). 

 $\overline{T}^i_s, \overline{R}^i \,=\, {f F_b}(\overline{T}^i_{fw})$ 

$$\overline{q}_{sw}^i, \overline{T}_{sw}^i = f(R, \overline{T}_s^i) \implies (\text{calc. } \widetilde{T}_{sb})$$
 (40)

(39)

$$\overline{\vec{x}}^{i}, \overline{T}^{i}_{b}, \overline{T}^{i}_{sink}, \overline{h}^{i} = \mathbf{S}_{\mathbf{b}}(\overline{q}^{i}_{sw}, \overline{T}^{i}_{sw}), \tag{41}$$

$$\overline{T}_{fw}^{i-1}, \overline{T}_{1}^{i} = f(\overline{T}_{sink}^{i}, \overline{h}^{i}) \implies (\text{calc. } \overline{T}_{sink})$$
(42)

$$\overline{T}_{s}^{i-1} = \mathbf{F}_{\mathbf{b}}(\overline{T}_{fw}^{i-1}, \overline{T}_{1}^{i-1}).$$
(43)

Tables 6 and 7 show good agreement between the gradients of  $\frac{dT_w}{dT_b}$  and  $\frac{dT_w}{d\vec{x}}$  obtained using the tangent, adjoint, and central difference (CD) methods.

|                                   | Design variable            |                            |                            |
|-----------------------------------|----------------------------|----------------------------|----------------------------|
| Gradient method                   | $1 [\times 10^{-4}]$       | $2 [\times 10^{-2}]$       | $3 [\times 10^{-4}]$       |
| Tangent                           | 2.57621104676445 <b>55</b> | 1.092538001954116 <b>1</b> | 6.26993861582025 <b>40</b> |
| Adjoint                           | 2.57621104676445 <b>82</b> | 1.0925380019541164         | 6.26993861582025 <b>84</b> |
| CD $[\Delta = 10^{-4} \text{ K}]$ | 2.5761096367205027         | 1.0925347169177257         | 6.2 <b>007757151150145</b> |

**Table 6**: hFRB gradient of interface temperature  $T_w$  w.r.t bottom temperature  $T_b$ 

|                                  | Design variable            |                             |                             |
|----------------------------------|----------------------------|-----------------------------|-----------------------------|
| Gradient method                  | x                          | y                           | z                           |
| Tangent                          | 12.7768341 <b>18125210</b> | -10.5235973 <b>06166273</b> | 0.323839452 <b>81109172</b> |
| Adjoint                          | 12.7768341 <b>08125197</b> | -10.5235973 <b>14289930</b> | 0.323839452 <b>64861863</b> |
| CD $[\Delta = 10^{-7} \text{m}]$ | 12.7 <b>60587537741230</b> | -10.5 <b>09541539249767</b> | 0.32302864383382257         |

**Table 7:** hFRB gradient of interface temperature  $T_w$  w.r.t coordinates

#### 3.2 Advantage of fluid Robin-based coupling algorithms

All the gradients obtained in Tables 2 - 7 were obtained by fully converging the fluid and solid primal and adjoint equations as well as performing an equal number of primal and reverse coupling iterations. However, for all coupling algorithms, significant time savings can be obtained by only partially converging the fluid primal and adjoint equations each time without significantly impacting the accuracy of the gradients [18].

Furthermore, rather than performing an equal number of primal and reverse coupling iterations, fewer reverse coupling iterations could be performed, at the cost of a slight reduction in gradient accuracy. On the flat plate validation case in Sec. 3.1, for Robin-based coupling algorithms, reducing the number of reverse coupling iterations from 19 to 3 only resulted in a difference of approximately 0.5% in the gradients. This reduction in the number of reverse coupling

iterations can also be combined with partial convergence of the fluid adjoint to significantly reduce runtime without great loss of gradient accuracy. However the TFFB algorithm always required the same number of reverse iterations as the primal to obtain accurate gradients.

Consequently, Robin-based coupling algorithms reduce the wall clock time required to obtain reasonably accurate gradients [18]. The Robin-based coupling algorithms have also been shown by Verstraete and Scholl [2, 14] to require less coupling iterations to converge the primal. Therefore, the time saving in both the primal and adjoint coupling runs will significantly speed up the optimisation process.

#### 4 APPLICATION TO OPTIMISATION PROBLEMS

#### 4.1 Inverse Design Optimisation

To demonstrate the efficacy of the partitioned adjoint methodology, we start with a simple inverse problem for which the final solution is known. Inverse problems are solved by providing a desired solution and adjusting design variables in order to achieve the desired target. In this problem, we seek the bottom temperature  $(T_b)$  which results in the best match for a given the interface wall temperature  $(T_{target})$  as shown in Figure 5. Table 8 and Figure 1 show the remaining parameters.



The inverse problem is solved by formulating an optimisation problem, which allows the use of classical direct methods to solve the physics involved. An objective function (J) is defined as the difference between the desired

| Parameter    | Value                | Units        |
|--------------|----------------------|--------------|
| b            | 0.01                 | m            |
| L            | 0.2                  | m            |
| $M_{\infty}$ | 0.1                  |              |
| $P_{\infty}$ | $1.03 \cdot 10^{5}$  | Pa           |
| $T_{\infty}$ | 1000                 | Κ            |
| $T_b$        | 600                  | Κ            |
| $\lambda_s$  | 0.2222               | W/mK         |
| $\lambda_f$  | 0.05568              | W/mK         |
| $\mu$        | $3.95 \cdot 10^{-5}$ | $Pa \cdot s$ |
| $Re_L$       | $1.132 \cdot 10^{5}$ |              |
| Pr           | 0.713                |              |

 Table 8: Table of parameters

interface temperature  $(T_{target})$  and the obtained interface temperature  $(T_w)$ for an estimated bottom temperature  $(\tilde{T}_b)$ .

$$J = \frac{1}{2} \int_0^L (T_{target} - T_w)^2 dx,$$
 (44)

and minimising Eqn. (44) results in an interface temperature which matches the target temperature. The objective function depends implicitly on the bottom temperature  $T_b$  through the solution of the coupled problem. Each mesh node at the bottom of the plate has an independent value of  $T_b$  specified as a boundary condition, and is used in this work as a design variable ( $\alpha$ ) that needs to be changed to drive J to zero. The selected mesh following a mesh dependence study results in 226 design variables for the present work.

The objective is hence to minimise Eqn. (44) subject to the constraints of satisfying both the state equations of both domains and maintain continuity of state variables  $(T_w, q_w)$  across the interface.

A gradient based method is used to reduce the deviation of the current interface wall temperature with the desired one. The gradient of the objective function (sensitivity) w.r.t the control variables,  $\alpha$ , is given as

 $\frac{dJ}{d\alpha} = \int_0^L (T_{target} - T_w) \frac{dT_w}{d\alpha} dx.$ (45)

The gradients of the temperature w.r.t the design variables, i.e. the temperature specified on the bottom of the flat plate, are computed using the adjoint approach for calculating  $\frac{dT_w}{dT_b}$  described in Sec. 3. The target temperature is obtained by solving the primal problem with a bottom temperature of 600K, hence it is guaranteed that a solution to the problem exists.  $\tilde{T}_b$  is initially taken as 400K and refers to the estimated bottom temperature that should yield  $T_{target}$ .

#### 4.1.1 Results

The objective is minimised using the BFGS optimisation algorithm from the SciPy library [20]. The difference between the temperatures obtained from the direct and inverse solution is defined as

$$Error = T_{Target} - T_{Inverse}.$$
 (46)

Figure 6a shows that the reduction in the objective function for all three coupling algorithms. The results for the TFRB algorithm in Fig. 6b show that the inverse solution is significantly closer to the target than the initial guess. Similar results were obtained for the TFFB and hFRB coupling algorithms (omitted for clarity). The successful solution of the inverse problem shows that the partitioned discrete adjoint methodology described is effective for solving CHT optimisation problems.



and this is attributed to needing fewer primal and reverse coupling iterations. Despite the loss of gradient accuracy due to partially converging the fluid adjoint and performing  $\approx 80\%$  less reverse coupling iterations than primal coupling iterations, the Robin-based algorithms solve the inverse problem. This shows that the time savings are worth the sacrifice in gradient accuracy.

|            | Coupling method    |     |     |  |
|------------|--------------------|-----|-----|--|
|            | TFFB   TFRB   HFRB |     |     |  |
| Time[hrs]  | 14.6               | 6.0 | 9.5 |  |
| Iterations | 30                 | 30  | 38  |  |

Table 9: Comparison of optimisation runtimes for all coupling algorithms

#### 4.2 MarkII Turbine Blade

Modern gas turbines are equipped with internal cooling channels which cool the internal structure and prevent damage from high turbine inlet temperatures. Hence, an optimisation problem is formulated to minimise the maximum temperature in a turbine blade by changing only the location of each cooling channel.

channel.
The vane geometry is modelled after the Mark II turbine vane which has
been investigated experimentally by Hylton et al. [21]. The blade is convectively cooled by ten cooling channels and a 2D simulation of the problem is
carried out. Matching meshes are used for both domains as shown in Figure
7 with 49,532 nodes in the fluid domain and 5,714 nodes in the solid. A near
wall spacing y<sup>+</sup> of less than 1 is used for the fluid.



Fig. 7: MarkII turbine blade

In the fluid domain, boundary conditions for the freestream pressure and temperature, as well as the Mach number at inlet are specified, while a gauge pressure of zero is specified at the outlet. In the solid domain, a constant temperature is imposed in each of the cooling channels.

| $P_{T_{in}}[Pa]$ | $T_{T_{in}}$ [K] | $P_{out}[Pa]$ | $M_{in}$ | $M_{out}$ |
|------------------|------------------|---------------|----------|-----------|
| 337100           | 788              | 167000        | 0.19     | 1.04      |

Table 10: MarkII run 5411 fluid boundary conditions

The blade is made of ASTM 310 stainless steel and the thermal conductivity is a function of temperature taken as

$$\lambda_s = 6.811 + 0.020176 \cdot T, \tag{47}$$

where T is the temperature at a point in the solid. The density and heat capacity are taken as 7900 kgm<sup>-3</sup> and 586.5 J kg<sup>-1</sup> K<sup>-1</sup> respectively. We define an objective function (J) as the maximum temperature in the solid domain

$$J = \sqrt[p]{\frac{1}{\Omega_s} \int_{\Omega_s} \left(\frac{T}{T_{ref}}\right)^p d\Omega_s},\tag{48}$$

where p is a user-defined integer taken as 10 currently and  $T_{ref}$  is a userdefined constant. The objective function depends on the solid temperature field which is obtained by solving the CHT problem. The CHT problem was solved using the hFRB algorithm due to stability reasons.

The coordinates (x, y) of each of the cooling channels are taken as control variables  $(\alpha)$  that need to be changed to drive J to zero. As a result, the control variable  $\alpha$  in the discrete problem is an array of size N. Where N is the number of channels (10), times the x & y coordinates leading to a total of 20. The gradients of the objective function w.r.t the design variables are computed using the partitioned adjoint approach described in Sec. 3.

#### 4.2.1 Baseline Analysis

Figures 8 and 9 show the temperature, pressure, and heat transfer coefficient distributions on the baseline geometry. The computational surface tempera-ture distribution deviates from the experiment near the leading edge but this discrepancy reduces closer to the trailing edge. The primary cause of the dis-crepancy on the suction surface of the leading edge is the due to the limitation of the Spalart-Allmaras turbulence model. This model is not well suited for modelling transitional flow and transitional models can be used to better match the experiment [22-24]. 

At the trailing edge where we see good agreement between the experiment and CHT results, the presence of the cooling channels leads to oscillations in the interface temperature and heat transfer coefficient distributions. We also see that the solid temperature is highest at the trailing edge.

#### 4.2.2 Optimisation Results

An unconstrained optimisation is performed using the BFGS optimisation algorithm from the SciPy library [20]. The Inverse Distance Weighted (IDW)



Fig. 8: Temperature distribution at fluid-solid interface and in the computational domain



Fig. 9: Pressure and heat transfer coefficient distribution at the fluid-solid interface

interpolation method is used to propagate the displacement of the cooling channels to the internal solid mesh nodes. The interface boundary nodes are kept fixed to maintain the match with the fluid domain. The IDW algorithm is also reverse differentiated to obtain fully accurate adjoint gradients of the entire design chain.

We achieve approximately 0.9% reduction in the objective function which
corresponds to a 3.14 K drop in the maximum temperature as shown in Fig.
10. The irregular shape of the curves in Fig. 10 are a result of the SciPy line
search.

Figure 11a shows the displacement of the cooling channels. The black lines represent the channels of the optimised blades while the solid surface is the initial geometry and temperature distribution. The optimisation is terminated prematurely as the first cooling channel (channel 1) moves out of the solid domain in the next optimisation step. The channels at the leading edge (chan-nels 1-3) are displaced upwards and outwards towards the higher temperature regions, the trailing edge channels (channels 7-10) are displaced downwards, while the middle channels (channels 4-6) are displaced towards the suction surface. 



#### 5 CONCLUSION

A partitioned discrete adjoint method for the partitioned approach to Conjugate Heat Transfer modelling has been presented. Loose coupling of the fluid

9 Springer Nature 2021 LATEX template 10 11 Discrete Adjoint for Coupled Conjugate Heat Transfer 2112 13 and solid domains with three fixed-point coupling algorithms was presented 14 15 and their adjoints were derived. The discrete adjoint solvers were developed 16 using reverse mode automatic differentiation (AD) which reduces the effort of 17 development and in particular maintenance. The process of developing the fluid 18 adjoint solver was fully automated which provides a strong case for adopting 19 the discrete adjoint over the continuous adjoint for multidisciplinary optimi-20 sation problems. The exchange of sensitivity information between solvers was 21 also described and the gradients verified. The presented methodology was then 22 applied to two CHT optimisation problems involving a flat plate and a turbine 23 blade. It was shown that Robin-based coupling algorithms have lower runtimes 24 as they need fewer coupling iterations to converge the primal and adjoint. Con-25 sequently, partitioned methods with Robin-based coupling algorithms can be 26 an attractive and competitive option for CHT optimisation in comparison to 27 monolithic methods.

#### References

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