Optimization-Based Design for Fluid Dynamics Application

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Nomenclature

α	thermal diffusivity
$\bar{\tau}_{ij}$	dimensionless deviatoric stress tensor
$\bar{c}$	dimensionless speed of sound
$\bar{p}$	dimensionless pressure
$\bar{T}$	dimensionless temperature
$\bar{t}$	dimensionless time
$\bar{t}_i$	i-th dimensionless traction vector component
$\bar{t}_i^p$	i-th dimensionless pressure component of the traction
$\bar{u}_i$	i-th dimensionless fluid velocity
$\bar{x}_i$	i-th spatial coordinate

$\Delta\mathbf{p}$	pressure increment vector
δ_{ij}	Kronecker delta
Δp	dimensionless pressure increment
ΔT	temperature increment
Δt	dimensionless time increment
Δu_i	i-th velocity increment
Δu_i^{**}	i-th momentum corrector
Δu_i^{*}	i-th momentum predictor
Γ	domain boundary
Γ_C	boundary where $v^h \neq 0$
Γ_F	boundary where $v^h \neq 0$ and Δu_i is not know a-priori
Γ_p	boundary where pressure values are enforced
Γ_t	boundary where tractions are enforced
γ_T	coefficient of thermal expansion
Γ_u	boundary where u_i are prescribed
$\hat{\mathbf{F}}_{\mathbf{Q}}^n$	stabilized plus penalized heat source vector at t^n
$\hat{\mathbf{R}}_{\mathbf{u}}^n$	discrete predictor stabilization at t^n
$\hat{R}_{\bar{T}}^n$	semi-discrete energy equation stabilization at t^n
$\hat{R}_{\bar{u}_i}^n$	semi-discrete predictor stabilization at t^n
κ	permeability coefficient
$\lambda_{\mathbf{p}}$	pressure adjoint vector
$\lambda_{\mathbf{T}}$	temperature adjoint vector
$\lambda_{\mathbf{u}^*}$	predictor adjoint vector
$\lambda_{\mathbf{u}}$	corrector adjoint vector

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$\mathbf{B_u}$	derivatives of the velocity shape functions
$\mathbf{C}_\kappa^n$	stabilized impermeability matrix at t^n
$\mathbf{C_b}^n$	stabilized buoyancy matrix at t^n
$\mathbf{C_p}^n$	stabilized pressure matrix at t^n
$\mathbf{C_u}^n$	momentum advection matrix at t^n
$\mathbf{C_T}^n$	energy advection function at t^n
$\mathbf{D}$	divergence matrix
$\mathbf{F_H}^n$	heat flux vector at t^n
$\mathbf{F_Q}^n$	penalized heat source vector at t^n
$\mathbf{F_p}^n$	dimensionless pressure residual force vector at t^n
$\mathbf{F_u}^n$	dimensionless predictor residual force vector at t^n
$\mathbf{I}_0$	diagonal matrix of coefficients
$\mathbf{K_T}^n$	stabilized diffusion matrix at t^n
$\mathbf{K_u}^n$	stabilized advection matrix at t^n
$\mathbf{K}_\tau$	momentum stiffness matrix
$\mathbf{K_T}$	diffusion matrix
$\mathbf{L}$	Laplacian matrix
$\mathbf{m}$	vector of coefficients
$\mathbf{M}_\kappa$	impermeability mass matrix
$\mathbf{M_b}$	buoyancy mass matrix
$\mathbf{M_u}$	momentum mass matrix
$\mathbf{n}$	normal vector
$\mathbf{N_p}$	pressure shape functions
$\mathbf{N_T}$	temperature shape functions

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$\mathbf{N_u}$	velocity shape functions
$\mathbf{R}_{\mathbf{u}}^{n}$	discrete predictor residual at t^n
$\mathbf{T}$	temperature vector
$\mathbf{T}^n$	discrete dimensionless temperature vector at t^n
$\mathbf{u}^n$	discrete dimensionless velocity vector at t^n
μ	dynamic viscosity
ν	kinematic viscocity
Ω	internal domain
Ω_f	fluid domain
Ω_s	solid domain
π^k	diffusivity penalization function for forced convection problems
π_F^{β}	source term penalization function for forced convection problems
π_N^{β}	source term penalization function for natural convection problems
π_{Pr}^{Br}	Brinkman penalization function for natural convection problems
π_{Re}^{Br}	Brinkman penalization function for forced convection problems
ρ_0	fluid density
τ_{ij}	deviatoric stress tensor
Θ	control vector
$\vartheta_i t$	i-th time level scalar penalty
c	speed of sound
c_p	specific heat capacity at constant pressure
Da	Darcy number
g_i	i-th gravity vector component
Gr_i	i-th Grashof number component

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k_f	fluid thermal conductivity
L_∞	characteristic length
n_i	i-th normal vector component
p	pressure field
p_0	reference pressure
Pr	Prandtl number
Q	heat source
q^h	temperature test function
q_{Br}	convexity parameter for impermeability interpolation function
$R^n_{\bar{T}}$	semi-discrete energy equation residual at t^n
$R^n_{\bar{u}_i}$	semi-discrete predictor residual at t^n
T	temperature
t	time
T_0	reference temperature
u_i	i-th fluid velocity vector component
u_i^0	i-th velocity initial boundary conditions
u_∞	characteristic fluid velocity
v^h	pressure test function
w_i^h	fluid velocity test function
x_i	i-th spatial coordinate

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1 Applications

Incompressible Laminar Flows

Incompressible fluid flows are considered in this section. Incompressible flows are often a good approximation for liquids operating in small Mach number environments. In incompressible flow applications, the density is assumed to be constant throughout the fluid and the mass conservation reduces to $\frac{\partial u_k}{\partial x_k} = 0$.

Natural Convection

Natural convection is a physical process driven by gravity in which fluid motion is created by pressure changes rather than an external source (e.g. fan, pump, etc.). Natural convection driven processes are seen in many science and engineering applications. For instance, electronic devices operating in quiet environments rely on natural convection for cooling.

Forced Convection

Forced convection us a physical process where fluid motion is driven by an external source such as a pump, fan, etc.. Forced convection problems are seen in many everyday mechanism such as central heating, air conditioning and steam turbines. Forced convection processes are also seen by engineers designing heat exchangers.

Topology Optimization

Topology optimization is a numerical method used to strategically placed material in a free-form manner to create geometries optimized for a set of design intents. Since topology optimization operates on every material point in space, every material point is considered a design variable in the optimization process. Therefore, gradient-based optimization approaches are recommended to solve this class of large-scale optimization problems.

The subsequent sections will introduce the algorithms used in this work to simulate the fluid dynamics in natural and forced convection problems and introduce formulation used to compute the total derivative of the design intents with respect to the design variables.

2 Governing Equations

Natural Convection

The governing conservation equations used in this work to compute optimized designs for natural convection applications via the topology optimization method are given as

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Incompressibility Condition

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

Mass Conservation

$$\frac{1}{c^2}\frac{\partial p}{\partial t} = -\rho_0 \frac{\partial u_i}{\partial x_i} \quad \text{in} \quad \Omega \tag{2}$$

Momentum Conservation

$$\rho_0 \left[\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_j u_i)\right] = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \gamma_T g_i \rho_0 (T - T_0) + \frac{\mu}{\kappa} u_i \quad \text{in} \quad \Omega \tag{3}$$

Energy Conservation

$$c_p \rho_0 \left[\frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i}\right] = \frac{\partial}{\partial x_i}\left(k \frac{\partial T}{\partial x_i}\right) + Q^n + \frac{\partial}{\partial x_i}(\tau_{ij} u_j) - \frac{\partial}{\partial x_j}(u_j p) \quad \text{in} \quad \Omega \tag{4}$$

However, the last two work dissipation terms in (4) are often neglected for fully incompressible flows. Therefore, these two terms will be neglected hereinafter.

In the set of conservation governing equations introduced above, the domain Ω is defined as the union of the fluid and solid domains, i.e. $\Omega = \Omega_f \cup \Omega_s$ and the deviatoric stress tensor is given as

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{5}$$

Recall in (5) that $\frac{\partial u_i}{\partial x_i} = 0$ for fully incompressible flows. The governing conservation equations are completed by defining the initial and boundary conditions for the problem, which are defined as

$$u_i = u_i^0 \quad \text{on} \quad \Gamma_u \tag{6}$$

and

$$t_i = (\tau_{ij} - \delta_{ij} p)\, n_j = t_i^0 \quad \text{on} \quad \Gamma_t \tag{7}$$

Instead of solving Equations (2)-(4) with the corresponding initial and boundary conditions, the dimensionless form of these equations are solved in this work. One advantage of working with the dimensionless form of the conservation equations is that it leads to a reduce number of free parameters, which can reduce the uncertainty in the analyses due to poorly characterized parameters. In addition, working with the dimensionless form of the conservation equations can help identify dominating terms in the equations. This can provide the possibility of simplifying the equations by neglecting the non-dominant terms for the study of certain fluid flows.

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Dimensionless Governing Equations

The scales used in this work to solve the dimensionless conservation equations during the topology optimization iterations are given by

$$\bar{T} = \frac{T - T_0}{\Delta T}, \quad \bar{u}_i = \frac{u_i}{u_\infty}, \quad \bar{x}_i = \frac{x_i}{L_\infty}, \quad \bar{t} = \frac{t u_\infty}{L_\infty}, \quad \bar{p} = \frac{p - p_0}{\rho_0 u_\infty^2} \\ \bar{c}^2 = \frac{c^2}{u_\infty}, \quad u_\infty = \frac{\alpha}{L_\infty} \tag{8}$$

Substituting the dimensionless variables introduced in (8) into (2)-(4) yield the following set of conservation equations

Incompressibility Condition

$$\frac{\partial \bar{u}_i}{\partial \bar{x}_i} = 0 \tag{9}$$

Mass Conservation

$$\left(\frac{1}{\bar{c}^2}\right) \frac{\partial \bar{p}}{\partial \bar{t}} = -\frac{\partial \bar{u}_i}{\partial \bar{x}_i} \quad \text{in} \quad \Omega \tag{10}$$

Momentum Conservation

$$\frac{\partial \bar{u}_i}{\partial \bar{t}} + \frac{\partial}{\partial \bar{x}_j}(\bar{u}_j \bar{u}_i) = -\frac{\partial \bar{p}}{\partial \bar{x}_i} + \frac{\partial \bar{\tau}_{ij}}{\partial \bar{x}_j} + Gr_i Pr^2 \bar{T} + \pi_{Pr}^{Br}(\theta) \bar{u}_i \quad \text{in} \quad \Omega \tag{11}$$

Energy Conservation

$$\frac{\partial \bar{T}}{\partial \bar{t}} + \bar{u}_i \frac{\partial \bar{T}}{\partial \bar{x}_i} = \frac{\partial^2 \bar{T}}{\partial \bar{x}_i^2} + \pi_N^{\beta}(\theta) Q^n \quad \text{in} \quad \Omega \tag{12}$$

The last two work dissipation terms introduced in (4) are neglected in (12) for incompressible flow applications. The dimensionless deviatoric stress tensor in (11) is defined as

$$\tau_{ij} = Pr \left(\frac{\partial \bar{u}_i}{\partial \bar{x}_j} + \frac{\partial \bar{u}_j}{\partial \bar{x}_i} \right) \tag{13}$$

The *dimensionless heat equation* used in the solid domain is given by

$$\frac{\partial \bar{T}}{\partial \bar{t}} - \frac{\partial^2 \bar{T}}{\partial \bar{x}_i^2} = 0 \quad \text{in} \quad \Omega_s \tag{14}$$

Equation (14) is derived by substituting the dimensionless expressions for T, t, and x_i introduced in (8) in the dimension-aware form of the heat equation. The effective impermeability $\pi_{Pr}^{Br}(\theta) \to 0$ in Ω_f and $\pi_{Pr}^{Br}(\theta) \to \infty$ in Ω_s to ensure the fluid velocities are

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nonzero and zero inside the fluid and solid domains, respectively. If x_i is in Ω_s, the fluid velocities tend to zero and the heat equation is directly obtained from (12). Therefore, no additional interpolation function is introduced in this work to interpolate the material properties in the diffusion term since the heat equation is implicitly modeled by (12) when the fluid velocities are zero, *i.e.* $x_i \in \Omega_s$.

The dimensionless interpolation functions $\pi_{Pr}^{Br}(\theta)$ and $\pi_N^{\beta}(\theta)$ in (10)-(12) are defined as

$$\pi_{Pr}^{Br}(\theta) = \frac{Pr}{Da}\left(\frac{1-\theta}{1+q_{Br}\theta}\right) \tag{15}$$

$$\pi_N^{\beta}(\theta) = \theta\beta \tag{16}$$

where the dimensionless constant β is defined as

$$\beta = \frac{L_\infty^2}{\alpha_f(T-T_0)(c_p\rho)_f} = \frac{L_\infty^2}{k_f\Delta T}$$

where the fluid thermal diffusivity $\alpha_f = \frac{k_f}{(c_p\rho)_f}$ was substituted to derived the final expression for β.

The dimensionless parameter Pr in (13) is the Prandtl number. The Prandtl number is defined as

$$Pr = \frac{\nu}{\alpha} \tag{17}$$

where ν is the momentum diffusivity (kinematic viscosity). Small Prandtl numbers, $Pr \ll 1$, indicate that thermal diffusivity dominates the behavior of the flow. Large Prandtl number indicate that momentum diffusivity dominates the behavior of the flow. Prandtl numbers close to 1 indicate that both momentum and heat dissipate about the same rate.

The dimensionless parameter Gr in Equation (11) is known as the Grashof number. The Grashof number is defined as

$$Gr_i = \frac{g_i\gamma_T\Delta T L_\infty^3}{\nu^2} \tag{18}$$

where γ_T is the coefficient of thermal expansion The Grashof number approximates the ratio of the buoyancy and viscous forces acting on the fluid. The Grashof number appears in natural convection applications and it is analogous to the Reynold number. The transition to turbulent flows occurs when the Grashof number is in the $10^8 < Gr < 10^9$ range. Turbulence occurs at higher Grashof numbers, $Gr > 10^9$, and laminar flow occurs in the $10^3 < Gr < 10^6$ range.

The dimensionless parameter Da in (15) denotes the Darcy number. The Darcy number represents the relative effect of the permeability of the medium versus the cross-sectional area. The Darcy number is defined as

$$Da = \frac{\kappa}{L_\infty^2} \tag{19}$$

where κ is the permeability coefficient.

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Forced Convection

The governing conservation equations used in this work to design optimized geometries for forced convection applications via the topology optimization method are given as

Incompressibility Condition

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{20}$$

Mass Conservation

$$\frac{1}{c^2}\frac{\partial p}{\partial t} = -\rho_0 \frac{\partial u_i}{\partial x_i} \quad \text{in} \quad \Omega \tag{21}$$

Momentum Conservation

$$\rho_0 \left[\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(u_j u_i)\right] = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\mu}{\kappa} u_i \quad \text{in} \quad \Omega \tag{22}$$

Energy Conservation

$$c_p \rho_0 \left[\frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i}\right] = \frac{\partial}{\partial x_i}\left(k \frac{\partial T}{\partial x_i}\right) + Q^n \quad \text{in} \quad \Omega \tag{23}$$

Notice the momentum (22) and energy (23) conservation equations are only coupled through the velocity field. The momentum conservation equation does not depend on the previous temperature field as is the case in natural convection applications.

Dimensionless Governing Equations

The scales used in this work to derive the dimensionless conservation equations for forced convection applications are given by

$$\bar{T} = \frac{T - T_0}{\Delta T}, \quad \bar{u}_i = \frac{u_i}{u_\infty}, \quad \bar{x}_i = \frac{x_i}{L_\infty}, \quad \bar{t} = \frac{t u_\infty}{L_\infty}, \quad \bar{p} = \frac{p - p_0}{\rho_0 u_\infty^2}, \quad \bar{c}^2 = \frac{c^2}{u_\infty^2} \tag{24}$$

Substituting the dimensionless variables introduced in (24) into (20)-(23) yield the following set of conservation equations

Incompressibility Condition

$$\frac{\partial \bar{u}_i}{\partial \bar{x}_i} = 0 \tag{25}$$

Mass Conservation

$$\left(\frac{1}{\bar{c}^2}\right)\frac{\partial \bar{p}}{\partial \bar{t}} = -\frac{\partial \bar{u}_i}{\partial \bar{x}_i} \quad \text{in} \quad \Omega \tag{26}$$

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Momentum Conservation

$$\frac{\partial \bar{u}_i}{\partial \bar{t}} + \frac{\partial}{\partial \bar{x}_j}(\bar{u}_j \bar{u}_i) = -\frac{\partial \bar{p}}{\partial \bar{x}_i} + \frac{\partial}{\partial \bar{x}_j}\left(\frac{1}{Re}\left(\frac{\partial \bar{u}_i}{\partial \bar{x}_j} + \frac{\partial \bar{u}_j}{\partial \bar{x}_i}\right)\right) + \pi_{Re}^{Br}(\theta)\bar{u}_i \quad \text{in} \quad \Omega \tag{27}$$

Energy Conservation

$$\frac{\partial \bar{T}}{\partial \bar{t}} + \bar{u}_i \frac{\partial \bar{T}}{\partial \bar{x}_i} = \frac{\partial}{\partial \bar{x}_i}\left(\frac{1}{Pe}\frac{\partial \bar{T}}{\partial \bar{x}_i}\right) + \pi_F^{\beta}(\theta) Q^n \quad \text{in} \quad \Omega \tag{28}$$

The dimensionless parameter Pe is the Peclet number and is defined as

$$Pe = RePr \tag{29}$$

where the dimensionless parameter Re is the Reynolds number and is defined as

$$Re = \frac{\rho_0 u_\infty L_\infty}{\mu} = \frac{u_\infty L_\infty}{\nu} \tag{30}$$

and the Prandtl number, Pr, is given by (17).

The *dimensionless heat equation* is given by (14). In contrast to the natural buoyancy use case, a material interpolation function is introduced in (28) to derive the energy equation in Ω_f, $\theta = 1$, and the heat equation in Ω_s, $\theta = 0$. Equation (28) is thus recast as

$$\frac{\partial \bar{T}}{\partial \bar{t}} + \bar{u}_i \frac{\partial \bar{T}}{\partial \bar{x}_i} = \frac{\partial}{\partial \bar{x}_i}\left(\pi^{\alpha}(\theta)\frac{\partial \bar{T}}{\partial \bar{x}_i}\right) + \pi_F^{\beta}(\theta) Q^n \quad \text{in} \quad \Omega \tag{31}$$

where

$$\pi^{\alpha}(\theta) = \frac{Pe(1-\theta)+\theta}{Pe} \tag{32}$$

$$\pi_F^{\beta}(\theta) = \theta\left(\frac{\alpha L_\infty}{k_f \Delta T u_\infty}\right) = \theta\left(\frac{\alpha L_\infty}{k_f \Delta T u_\infty}\right)\left(\frac{L_\infty}{L_\infty}\right) = \theta\left(\frac{L_\infty^2}{k_f \Delta T Pe}\right) = \theta\beta \tag{33}$$

Finally, the Brinkman interpolation function for forced convection problems is defined as

$$\pi_{Re}^{Br}(\theta) = \frac{1}{ReDa}\left(\frac{1-\theta}{1+q_{Br}\theta}\right) \tag{34}$$

where the dimensionless parameter Da is the Darcy number and is given by (19).

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3 Fractional Step

The fractional time stepping scheme formulation will be derived only for the natural convection use case. The derivation for the forced convection use case follows the same procedure. In its semi-discrete form, Equations 9-11 can be rewritten as

$$\frac{\bar{u}_i^{n+1} - \bar{u}_i^n}{\Delta t} = \bar{u}_j^{n+\vartheta_1} \frac{\partial \bar{u}_i^{n+\vartheta_1}}{\partial \bar{x}_j} - \frac{\partial \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i} + \frac{\partial}{\partial \bar{x}_j}\left(Pr \frac{\partial \bar{u}_i^{n+\vartheta_3}}{\partial \bar{x}_j}\right) + Gr_i Pr \bar{T}^n + \pi_{Pr}^{Br}(\theta) \bar{u}_i^n \quad (35)$$

where ϑ_i determines the time level at which each term is considered and Δt is in its dimensionless form. The projection method works as a two-stage fractional step scheme based on the Helmholtz-Hodge decomposition. The characteristics-based split scheme can be derived using the auxiliary variables Δu_i^* and Δu_i^{**}, which splits Equation 35 into two parts

$$\bar{u}_i^{n+1} - \bar{u}_i^n = \Delta u_i^* + \Delta u_i^{**} \quad (36)$$

$$\frac{\Delta u_i^*}{\Delta t} = \bar{u}_j^{n+\vartheta_1} \frac{\partial \bar{u}_i^{n+\vartheta_1}}{\partial \bar{x}_j} + \frac{\partial}{\partial \bar{x}_j}\left(Pr \frac{\partial \bar{u}_i^{n+\vartheta_3}}{\partial \bar{x}_j}\right) + Gr_i Pr \bar{T}^n + \pi_{Pr}^{Br}(\theta) \bar{u}_i^n \quad (37)$$

$$\frac{\Delta u_i^{**}}{\Delta t} = -\frac{\partial \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i} \quad (38)$$

Taking the divergence of Equation (38) gives

$$\frac{\partial \Delta u_i^{**}}{\partial \Delta t} = -\frac{\partial^2 \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i^2} \quad (39)$$

substituting (36) into 39 gives

$$\frac{\partial \bar{u}_i^{n+1}}{\partial \bar{x}_i} - \frac{\partial \bar{u}_i^n}{\partial \bar{x}_i} - \frac{\partial \Delta u_i^*}{\partial \bar{x}_i} = -\Delta t \frac{\partial^2 \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i^2} \quad (40)$$

The next step is to expand Equation (9) at time level $n + \vartheta_4$, which yields

$$\frac{\partial \bar{u}_i}{\partial \bar{x}_i} \approx \frac{\partial \bar{u}_i^{n+\vartheta_4}}{\partial \bar{x}_i} = 0 \quad (41)$$

Expanding (41) and solving for the partial derivative term at $n + 1$ gives

$$\frac{\partial \bar{u}_i^{n+1}}{\partial \bar{x}_i} = -\frac{(\vartheta_4 - 1)}{\vartheta_4} \frac{\partial \bar{u}_i^n}{\partial \bar{x}_i} \quad (42)$$

After substituting (42) into (40), Equation (40) is recast as

$$-\frac{\partial \bar{u}_i^n}{\partial \bar{x}_i} - \vartheta_4 \frac{\partial \Delta u_i^*}{\partial \bar{x}_i} = -\Delta t \vartheta_4 \frac{\partial^2 \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i^2} \quad (43)$$

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Recall

$$\frac{\partial^2 \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i^2} = \frac{\partial^2 \bar{p}^n}{\partial \bar{x}_i^2} + \vartheta_2 \frac{\partial^2 \Delta p}{\partial \bar{x}_i^2}$$

Thus, substituting the above expression into (43) gives

$$\Delta t \vartheta_4 \vartheta_2 \frac{\partial^2 \Delta p}{\partial \bar{x}_i^2} = \frac{\partial \bar{u}_i^n}{\partial \bar{x}_i} + \vartheta_4 \frac{\partial \Delta u_i^*}{\partial \bar{x}_i} - \Delta t \vartheta_4 \frac{\partial^2 \bar{p}^n}{\partial \bar{x}_i^2} \tag{44}$$

The characteristic-based split method then consist of determining

1. the initial auxiliary variable Δu_i^* using (37),
2. the pressure at t^{n+1} using (44), and
3. obtaining the velocity variable at t^{n+1} by determining the auxiliary variable Δu_i^{**} using (38).

The semi-discrete form of the energy equation (12) can be derived similarly by expanding the convective and diffusive terms at time level $n + \vartheta_5$ and $n + \vartheta_6$, respectively. This approach yields the following semi-discrete form for the energy equation

$$\frac{\bar{T}^{n+1} - \bar{T}^n}{\Delta t} = -\bar{u}_i^{n+\vartheta_5} \frac{\partial \bar{T}^{n+\vartheta_5}}{\partial \bar{x}_i} + \frac{\partial}{\partial \bar{x}_i}\left(\frac{\partial \bar{T}^{n+\vartheta_6}}{\partial \bar{x}_i}\right) + \pi_N^{\beta}(\theta) Q^n \tag{45}$$

The approximation of the nonlinear terms may take multiple forms. The convection terms in (37) and (45) are however considered explicitly herein, *i.e.* $\vartheta_1 = 0$ and $\vartheta_5 = 0$ respectively.

4 Stabilization

The stabilized conservation equations will be presented only for the natural convection use case. The derivation of the stabilized conservation equations for the forced convection use case follows the same procedure.

Most convection dominated flows require some form of stabilization. The fractional step scheme is no exception. The stabilization scheme for the fractional step method takes the form of an explicit characteristic-Galerkin procedure. The incompressible Navier-Stokes equation for natural convection applications is stabilized as follows

$$\begin{aligned} \bar{u}_i^{n+1} - \bar{u}_i^n = &\\ &\Delta t \left(-u_j^{n+\vartheta_1} \frac{\partial \bar{u}_i^{n+\vartheta_1}}{\partial \bar{x}_j} - \frac{\partial \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i} + \frac{\partial \bar{\tau}_{ij}^{n+\vartheta_3}}{\partial x_j} + Gr_i Pr \bar{T}^n + \pi_{Pr}^{Br}(\theta) \bar{u}_i^n \right) \\ &+ \frac{\Delta t^2}{2} \bar{u}_k \frac{\partial}{\partial \bar{x}_k} \left(-u_j^n \frac{\partial \bar{u}_i^n}{\partial \bar{x}_j} - \frac{\partial \bar{p}^n}{\partial \bar{x}_i} + \frac{\partial \bar{\tau}_{ij}^n}{\partial \bar{x}_j} + Gr_i Pr \bar{T}^n + \pi_{Pr}^{Br}(\theta) \bar{u}_i^n \right) \end{aligned} \tag{46}$$

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Neglecting higher-order terms in (46) yields the following stabilized form for the incompressible Navier-Stokes equation

$$\begin{aligned}\bar{u}_i^{n+1} - \bar{u}_i^n = \\ \Delta t \left(-u_j^{n+\vartheta_1}\frac{\partial \bar{u}_i^{n+\vartheta_1}}{\partial \bar{x}_j} - \frac{\partial \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i} + \frac{\partial \bar{\tau}_{ij}^{n+\vartheta_3}}{\partial \bar{x}_j} + Gr_i Pr \bar{T}^n + \pi_{Pr}^{Br}(\theta)\bar{u}_i^n\right) \\ + \frac{\Delta t^2}{2}\bar{u}_k \frac{\partial}{\partial \bar{x}_k}\left(-u_j^n \frac{\partial \bar{u}_i^n}{\partial \bar{x}_j} - \frac{\partial \bar{p}^n}{\partial \bar{x}_i} + Gr_i Pr \bar{T}^n + \pi_{Pr}^{Br}(\theta)\bar{u}_i^n\right)\end{aligned} \tag{47}$$

The stabilized characteristic-based split equations utilized to determine auxiliary variables Δu_i^* and Δu_i^{**} are derived from (47) and are respectively given by

$$\begin{aligned}\Delta u_i^* =& \Delta t \left(-u_j^{n+\vartheta_1}\frac{\partial \bar{u}_i^{n+\vartheta_1}}{\partial \bar{x}_j} + \frac{\partial \bar{\tau}_{ij}^{n+\vartheta_3}}{\partial \bar{x}_j} + Gr_i Pr \bar{T}^n + \pi_{Pr}^{Br}(\theta)\bar{u}_i^n\right) \\ &+ \frac{\Delta t^2}{2}\bar{u}_k \frac{\partial}{\partial \bar{x}_k}\left(-u_j^n \frac{\partial \bar{u}_i^n}{\partial \bar{x}_j} + Gr_i Pr \bar{T}^n + \pi_{Pr}^{Br}(\theta)\bar{u}_i^n\right)\end{aligned} \tag{48}$$

$$\Delta u_i^{**} = -\Delta t \frac{\partial \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i} - \frac{\Delta t^2}{2}\bar{u}_k \frac{\partial}{\partial \bar{x}_k}\left(\frac{\partial \bar{p}^n}{\partial \bar{x}_i}\right) \tag{49}$$

The pressure at t^{n+1} is still determined by solving (44).

The characteristic-Galerkin procedure is also applied to (45) to derive the semi-discrete form of the stabilized energy equation, which is given by

$$\begin{aligned}\bar{T}^{n+1} - \bar{T}^n =& \Delta t \left(-\bar{u}_i^{n+\vartheta_5}\frac{\partial \bar{T}^{n+\vartheta_5}}{\partial \bar{x}_i} + \frac{\partial}{\partial \bar{x}_i}\left(\frac{\partial \bar{T}^{n+\vartheta_6}}{\partial \bar{x}_i}\right) + \pi_N^{\beta}(\theta)Q^n\right) \\ &+ \frac{\Delta t^2}{2}\bar{u}_k \frac{\partial}{\partial \bar{x}_k}\left(-\bar{u}_i^{n+\vartheta_5}\frac{\partial \bar{T}^{n+\vartheta_5}}{\partial \bar{x}_i} + \pi_N^{\beta}(\theta)Q^n\right)\end{aligned} \tag{50}$$

The stabilized diffusive term in (50) is neglected since higher-order terms are ignored.

5 Weak Formulation

The weak formulation for the characteristic-based split equations is derived by applying the Galerkin method to Equations (44), (48), (49), and (50).

Momentum Predictor

The weak form of the momentum predictor equation is defined as

$$\int_\Omega w_i^h \left(\frac{\bar{u}_i^* - \bar{u}_i^n}{\Delta \bar{t}}\right) d\Omega = R_{\bar{u}_i}^n(w_i^h) + \frac{\Delta \bar{t}}{2}\int_\Omega \left(\frac{\partial w_i^h}{\partial \bar{x}_k}\bar{u}_k^n\right)\hat{R}_{\bar{u}_i}^n d\Omega \tag{51}$$

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where

$$R^n_{\bar{u}_i}(w^h_i) = -\int_\Omega w^h_i \left(\bar{u}^{n+\vartheta_1}_j \frac{\partial \bar{u}^{n+\vartheta_1}_i}{\partial \bar{x}_j}\right) d\Omega - \int_\Omega \frac{\partial w^h_i}{\partial \bar{x}_j} \bar{\tau}^{n+\vartheta_3}_{ij}\, d\Omega + \int_\Gamma w^h_i \bar{\tau}^{n+\vartheta_3}_{ij} n_j\, d\Gamma$$
$$+ \int_\Omega w^h_i \left(Gr_i Pr^2 \bar{T}^n\right) d\Omega + \int_\Omega w^h_i \left(\pi^{Br}_{Pr}(\theta)\bar{u}^n_i\right) d\Omega$$

and

$$\hat{R}^n_{\bar{u}_i}(w^h_i) = -\bar{u}^n_j \frac{\partial \bar{u}^n_i}{\partial \bar{x}_j} + Gr_i Pr^2 \bar{T}^n + \pi^{Br}_{Pr}(\theta)\bar{u}^n_i$$

In (51) w^h_i is the fluid velocity test function and t_i is the prescribed traction force on Γ_t. The boundary contributions resulting from the integration by parts of the stabilization term are neglected in (51) since their contribution is negligible along the boundary.

Pressure Increment

The weak form for the pressure increment equation in (44) is defined as

$$\begin{aligned}\Delta t \vartheta_4 \vartheta_2 \int_\Omega \frac{\partial v^h}{\partial \bar{x}_i} \frac{\partial \Delta p}{\partial \bar{x}_i}\, d\Omega = \int_\Omega \frac{\partial v^h}{\partial \bar{x}_i} \left(\bar{u}^n_i + \vartheta_4 \left(\Delta u^*_i - \Delta t \frac{\partial \bar{p}^n}{\partial \bar{x}_i}\right)\right) \\ - \int_\Gamma v^h n_i \left(\bar{u}^n_i + \vartheta_4 \left(\Delta u^*_i - \Delta t \frac{\partial \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i}\right)\right) d\Gamma\end{aligned} \tag{52}$$

where v^h is the pressure test function, n_i is the unit normal vector, and

$$\frac{\partial \bar{p}^{n+\vartheta_2}}{\partial \bar{x}_i} = \frac{\partial \bar{p}^n}{\partial \bar{x}_i} + \vartheta_2 \frac{\partial \Delta p}{\partial \bar{x}_i}$$

Momentum Corrector

The weak form for the momentum corrector equation in (38) is defined as

$$\int_\Omega w^h_i \left(\frac{\bar{u}^{n+1}_i - \bar{u}^*_i}{\Delta \bar{t}}\right) d\Omega = -\int_\Omega w^h_i \frac{\partial \bar{p}^{\,n+\theta_2}}{\partial \bar{x}_i} d\Omega + \frac{\Delta \bar{t}}{2} \int_\Omega \frac{\partial w^h_i}{\partial \bar{x}_k} \left(\bar{u}^n_k \frac{\partial \bar{p}^{\,n}}{\partial \bar{x}_i}\right) d\Omega \tag{53}$$

where the boundary contribution resulting from the integration by parts of the stabilization term was neglected from (53) since their contribution is negligible along the boundary.

Temperature Increment

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The weak form for the energy equation in (45) is defined as

$$\int_\Omega q^h \left(\frac{\bar{T}^{n+1} - \bar{T}^n}{\Delta \bar{t}} \right) d\Omega = R^n_{\bar{T}}(q^h) + \frac{\Delta \bar{t}}{2} \int_\Omega \frac{\partial q^h}{\partial \bar{x}_k} \left(\bar{u}^n_k \hat{R}^n_{\bar{T}} \right) d\Omega \tag{54}$$

where

$$\begin{aligned} R^n_{\bar{T}}(q^h) = &- \int_\Omega q^h \left(\bar{u}_i^{n+\vartheta_5} \frac{\partial \bar{T}^{n+\vartheta_5}}{\partial \bar{x}_i} \right) d\Omega - \int_\Omega \frac{\partial q^h}{\partial \bar{x}_i} \frac{\partial \bar{T}^{n+\vartheta_6}}{\partial \bar{x}_i} d\Omega \\ &+ \int_{\Gamma_H} q^h H d\Gamma + \int_\Omega q^h \left(\pi^\beta_N(\theta) Q^n \right) d\Omega \end{aligned}$$

and

$$\hat{R}^n_{\bar{T}}(q^h) = - \bar{u}_i^{n+\vartheta_5} \frac{\partial \bar{T}^{n+\vartheta_5}}{\partial \bar{x}_i} - \frac{\partial^2 \bar{T}^{n+\vartheta_6}}{\partial \bar{x}_i^2} + \pi^\beta_N(\theta) Q^n$$

In Equation (54) q^h denotes the test function associated with the temperature field and H is the total heat flux on Γ_H. The boundary contributions resulting from the integration by parts of the stabilization term in (54) are neglected since these are negligible along the boundary.

6 Boundary Conditions

Traction boundary conditions can be weakly prescribed in (51). Aside from enforcing Dirichlet boundary conditions by prescribing momentum values on Γ_u, the following boundary condition options are also considered:

1. the full traction is prescribed on Γ_t: $-\bar{p} n_i + \bar{\tau}_{ij} n_j = \bar{t}_i$ (given)
2. only the pressure component of the traction is prescribed on Γ_p: $-\bar{p} n_i = \bar{t}^p_i$ (given)
3. no boundary conditions are prescribed on the boundary, i.e. the free part of the boundary Γ_F.

The first two conditions are standard and can be easily enforced. However, the third condition is not as clear to enforce as the first two. The third condition is known as the free boundary condition. In other words, no prescribed velocity or tractions are enforced on the free boundary Γ_F. This approach is commonly used in compressible flow applications at supersonic outflows. It can also be present as an outflow boundary condition in flow problems inside large domains.

Momentum Predictor

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The deviatoric traction boundary term $\int_\Gamma w_i^h \bar{\tau}_{ij} n_j \, d\Gamma$ in (51) can be splitted into two parts

$$\int_\Gamma w_i^h \bar{\tau}_{ij} n_j \, d\Gamma = \int_{\Gamma-\Gamma_t} w_i^h \bar{\tau}_{ij}^n n_j \, d\Gamma + \int_{\Gamma_t} w_i^h \left(\bar{t}_i + \bar{p}^n n_i \right) \, d\Gamma \tag{55}$$

The prescribed traction forces could then be used to calculate the deviatoric traction component on Γ_t while the velocity field on $\Gamma - \Gamma_t$ boundary would be used to calculate the deviatoric traction forces on $\Gamma - \Gamma_t$. However, to avoid the difficulties associated with the evaluation of the deviatoric traction over the whole boundary Γ, the predictor velocity values are prescribed in the predictor step. This approach introduces a local error confined to the vicinity of the boundary nodes, this error however is corrected in the corrector step by inserting the correct values for the velocity variables. To avoid the enforcement of the deviatoric tractions on boundary Γ_t, the full traction forces are used instead. Both errors, prescription of the predicted velocity u_i^* and use of the full traction force $\bar{t}_i$, are automatically corrected in the corrector step by using zero boundary velocity and traction boundary conditions. Therefore, the final expression for the weak form of the momentum predictor equation is given by

$$\int_\Omega w_i^h \left(\frac{\bar{u}_i^* - \bar{u}_i^n}{\Delta \bar{t}} \right) d\Omega = \mathcal{R}_{\bar{u}_i}^n (w_i^h) + \frac{\Delta \bar{t}}{2} \int_\Omega \left(\bar{u}_k^n \frac{\partial w_i^h}{\partial \bar{x}_k} \right) \hat{R}_{\bar{u}_i}^n d\Omega \tag{56}$$

where

$$\begin{aligned} \mathcal{R}_{\bar{u}_i}^n (w_i^h) = &- \int_\Omega w_i^h \left(\bar{u}_j^{n+\vartheta_1} \frac{\partial \bar{u}_i^{n+\vartheta_1}}{\partial \bar{x}_j} \right) d\Omega - \int_\Omega \frac{\partial w_i^h}{\partial \bar{x}_j} \bar{\tau}_{ij}^{n+\vartheta_3} \, d\Omega + \int_{\Gamma_t} w_i^h \bar{t}_i \, d\Gamma_t \\ &+ \int_\Omega w_i^h \left(Gr_i Pr^2 \bar{T}^n \right) \, d\Omega + \int_\Omega w_i^h \left(\pi_{Pr}^{Br}(\theta) \bar{u}_i^n \right) \, d\Omega \end{aligned}$$

and

$$\hat{R}_{\bar{u}_i}^n = -\bar{u}_j^n \frac{\partial \bar{u}_i^n}{\partial \bar{x}_j} + Gr_i Pr^2 \bar{T}^n + \pi_{Pr}^{Br}(\theta) \bar{u}_i^n$$

Pressure Increment

These boundary condition options can be enforced in (52)

1. on Γ_t: $\bar{p} = n_i \bar{\tau}_{ij} n_j - n_i \bar{t}_i$
2. on Γ_p: $\bar{p} = n_i \bar{t}_i^p$

These two boundary conditions are of the Dirichlet boundary type. Thus, the pressure test function vanishes (i.e. $v^h = 0$) on Γ_t and Γ_p, leaving $\Gamma_C = \Gamma - \Gamma_t - \Gamma_p$. On the other hand, $\Delta u_i = 0$ on Γ_u. The problem lies on the free boundary Γ_F where $v^h \neq 0$ and Δu_i is not known *a priori*.

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Let's introduce the following relationship

$$n_i \left(\Delta u_i^* - \Delta t \frac{\partial \bar{p}^{n+\theta_2}}{\partial x_i} \right) = n_i \Delta u_i \tag{57}$$

where $\Delta u_i^* = \bar{u}_i^* - \bar{u}_i^n$ and $\Delta u_i = \bar{u}_i^{n+1} - \bar{u}_i^n$. If Equation (57) is used on Γ_F, Equation (52) becomes coupled with Equation (56) through $\bar{u}_i^n$, which is not known yet. To avoid this coupling, $n_i \Delta u_i$ is set to zero on Γ_F. In transient applications, if the normal component of u_i varies on Γ_F, the approximation will be on the order of Δt. However, in steady state applications, the steady state solution (if reached) will be correct.

Using (57) and $n_i \Delta u_i = 0$ on Γ_F, the weak form for Equation (52) is recast as

$$\Delta t \vartheta_4 \vartheta_2 \int_\Omega \frac{\partial v^h}{\partial \bar{x}_i} \frac{\partial \Delta p}{\partial \bar{x}_i} \, d\Omega = \int_\Omega \frac{\partial v^h}{\partial \bar{x}_i} \left(\bar{u}_i^n + \vartheta_4 \left(\Delta u_i^* - \Delta t \frac{\partial \bar{p}^n}{\partial \bar{x}_i} \right) \right) - \int_{\Gamma_u} v^h \left(n_i \bar{u}_i^n \right) d\Gamma \tag{58}$$

Momentum Corrector

Zero boundary velocities and tractions are enforced since the correct velocities and tractions were enforced in (56) and (57).

7 Discrete Formulation

The Galerkin finite element method is applied to the weak formulation presented in the previous section. Furthermore, recall from Section 3 that the convective terms are considered explicitly in this work, i.e. $\vartheta_1 = 0$ and $\vartheta_5 = 0$.

Momentum Predictor

The discrete form of the momentum predictor equations in (56) is given by

$$\left(\mathbf{M}_\mathbf{u} - \vartheta_3 \Delta t \mathbf{K}_\tau \right) \mathbf{u}^* = \mathbf{M}_\mathbf{u} \mathbf{u}^n + \Delta \bar{t} \, \mathbf{R}_\mathbf{u}^n + \frac{\Delta \bar{t}^2}{2} \hat{\mathbf{R}}_\mathbf{u}^n \tag{59}$$

where

$$\mathbf{R}_\mathbf{u}^n = -\mathbf{C}_\mathbf{u}^n \mathbf{u}^n + (\vartheta_3 - 1) \mathbf{K}_\tau \mathbf{u}^n + \mathbf{M}_\kappa \mathbf{u}^n + \mathbf{M}_\mathbf{b} \mathbf{T}^n + \mathbf{F}_\mathbf{u}^n$$

and

$$\hat{\mathbf{R}}_\mathbf{u}^n = -\mathbf{K}_\mathbf{u}^n \mathbf{u}^n + \mathbf{C}_\mathbf{b}^n \mathbf{T}^n + \mathbf{C}_\kappa^n \mathbf{u}^n$$

The discrete matrices and vectors in (59) are given by

$$\mathbf{M}_\mathbf{u} = \int_\Omega \mathbf{N}_\mathbf{u}^T \mathbf{N}_\mathbf{u} d\Omega$$

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$$\mathbf{C}^n_{\mathbf{u}} = \int_{\Omega} \mathbf{N}^T_{\mathbf{u}} (\nabla(\mathbf{u}^n \mathbf{N}_{\mathbf{u}})) d\Omega$$

$$\mathbf{M}_{\kappa} = \int_{\Omega} \mathbf{N}^T_{\mathbf{u}} \left(\pi^{Br}_{Pr}(\theta) \mathbf{N}_{\mathbf{u}}\right) d\Omega$$

$$\mathbf{M}_{\mathbf{b}} = \int_{\Omega} \mathbf{N}^T_{\mathbf{u}} \left(Gr_i Pr^2 \mathbf{N}_{\mathbf{T}}\right) d\Omega$$

$$\mathbf{C}^n_{\mathbf{b}} = \int_{\Omega} (\nabla(\mathbf{u}^n \mathbf{N}_{\mathbf{u}}))^T \left(Gr_i Pr^2 \mathbf{N}_{\mathbf{T}}\right) d\Omega$$

$$\mathbf{C}^n_{\kappa} = \int_{\Omega} (\nabla(\mathbf{u}^n \mathbf{N}_{\mathbf{u}})^T) \left(\pi^{Br}_{Pr}(\theta) \mathbf{N}_{\mathbf{u}}\right) d\Omega$$

$$\mathbf{K}^n_{\mathbf{u}} = \int_{\Omega} (\nabla(\mathbf{u}^n \mathbf{N}_{\mathbf{u}})^T)(\nabla(\mathbf{u}^n \mathbf{N}_{\mathbf{u}}))\, d\Omega$$

$$\mathbf{K}_{\tau} = \int_{\Omega} \mathbf{B}^T_{\mathbf{u}} \left(Pr \left(\mathbf{I}_0 - \frac{2}{3} \mathbf{m}\mathbf{m}^T \right) \right) \mathbf{B}_{\mathbf{u}}\, d\Omega$$

$$\mathbf{F}^n_{\mathbf{u}} = \int_{\Gamma_t} \mathbf{N}^T_{\mathbf{u}} \left(\mathbf{n}^T \tau^n\right) d\Gamma$$

In the equations defined above, $\mathbf{I}_0 = \text{diag}(2,\ 2,\ 2,\ 1,\ 1,\ 1)$ and $\mathbf{m} = [1,\ 1,\ 1,\ 0,\ 0,\ 0]$ in three dimensional problems. The gradient operator is defined as $\nabla \phi \equiv \partial \bar{x}_i \phi$, where ϕ is a scalar field.

Pressure Increment

The discrete form of the pressure increment system of equations in (58) is given by

$$\vartheta_4 \vartheta_2 \mathbf{L} \Delta \mathbf{p} = \frac{1}{\Delta \bar{t}} \left[\mathbf{D} \mathbf{u}^n + \theta_4 \mathbf{D} \Delta \mathbf{u}^* - \theta_4 \Delta \bar{t}\, \mathbf{L} \Delta \mathbf{p} - \mathbf{F}^n_{\mathbf{p}} \right] \tag{60}$$

where

$$\mathbf{F}^n_{\mathbf{p}} = \int_{\Gamma_u} \mathbf{N}^T_{\mathbf{p}} \left(\mathbf{n}^T \mathbf{u}^n\right) d\Gamma$$

$$\mathbf{L} = \int_{\Omega} (\nabla \mathbf{N}_{\mathbf{p}})^T \nabla \mathbf{N}_{\mathbf{p}}\, d\Omega$$

$$\mathbf{D} = \int_{\Omega} (\nabla \mathbf{N}_{\mathbf{p}})^T\, \mathbf{N}_{\mathbf{u}}\, d\Omega$$

Momentum Corrector

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The discrete form of the momentum corrector system of equations in (53) is given by

$$\mathbf{M_u}\left(\mathbf{u}^{n+1}-\mathbf{u}^*\right)=-\Delta\bar{t}\left[\mathbf{D}^T\left(\mathbf{p}^n+\vartheta_2\Delta\mathbf{p}\right)+\frac{\Delta\bar{t}}{2}\mathbf{C}^n_{\mathbf{p}}\mathbf{p}^n\right] \tag{61}$$

where

$$\mathbf{C}^n_{\mathbf{p}}=\int_\Omega\left(\nabla(\mathbf{u}^n\mathbf{N_u})\right)^T\nabla\mathbf{N_p}\,d\Omega$$

A variant of (61) is obtained by discretizing the end-of-step velocity according to

$$\left(\mathbf{M_u}-\vartheta_3\Delta\bar{t}\,\mathbf{K}\right)\mathbf{u}^{n+1}=\mathbf{M_u}\mathbf{u}^*-\Delta\bar{t}\,\mathbf{D}^T\left(\mathbf{p}^n+\vartheta_2\Delta\mathbf{p}\right)+\frac{\Delta\bar{t}^2}{2}\mathbf{C}^n_{\mathbf{p}}\mathbf{p}^n \tag{62}$$

Temperature Increment

The discrete form of the energy equation in (54) is given by

$$\left(\mathbf{M_T}-\Delta\bar{t}\vartheta_6\mathbf{K_T}\right)\mathbf{T}^{n+1}=\mathbf{M_T}\mathbf{T}^n+\Delta\bar{t}\,\mathbf{R}^n_{\mathbf{T}}+\frac{\Delta\bar{t}^2}{2}\,\hat{\mathbf{R}}^n_{\mathbf{T}} \tag{63}$$

where

$$\mathbf{R}^n_{\mathbf{T}}=-\mathbf{C}^n_{\mathbf{T}}\mathbf{T}^n+(\vartheta_6-1)\mathbf{K_T}\mathbf{T}^n+\mathbf{F}^n_{\mathbf{H}}+\mathbf{F}^n_{\mathbf{Q}}$$
$$\hat{\mathbf{R}}^n_{\mathbf{T}}=-\hat{\mathbf{K}}^n_{\mathbf{T}}\mathbf{T}^n+\hat{\mathbf{F}}^n_{\mathbf{Q}}$$

The discrete matrices in (63) are defined as

$$\mathbf{M_T}=\int_\Omega\mathbf{N}^T_{\mathbf{T}}\mathbf{N_T}\,d\Omega$$

$$\mathbf{C}^n_{\mathbf{T}}=\int_\Omega\mathbf{N}^T_{\mathbf{T}}(\mathbf{u}^n\nabla\mathbf{N_T})\,d\Omega$$

$$\mathbf{F}^n_{\mathbf{H}}=\int_{\Gamma_H}\mathbf{N}^T_{\mathbf{T}}\left(\mathbf{n}^T\mathbf{H}\right)\,d\Gamma$$

$$\mathbf{K_T}=\int_\Omega\nabla\mathbf{N}^T_{\mathbf{T}}\nabla\mathbf{N}_T\,d\Omega$$

$$\hat{\mathbf{K}}^n_{\mathbf{T}}=\int_\Omega\left(\nabla(\mathbf{u}^n\mathbf{N_T})\right)^T(\mathbf{u}^n\nabla\mathbf{N_T})\,d\Omega$$

$$\mathbf{F}^n_{\mathbf{Q}}=\int_\Omega\mathbf{N}^T_{\mathbf{T}}\left(\pi^\beta_N(\theta)\mathbf{Q}^n\right)\,d\Omega$$

$$\hat{\mathbf{F}}^n_{\mathbf{Q}}=\int_\Omega\left(\nabla(\mathbf{u}^n\mathbf{N_T})\right)^T\left(\pi^\beta_N(\theta)\mathbf{Q}^n\right)\,d\Omega$$

where $\mathbf{H}$ denotes the prescribed heat flux on Γ_H.

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8 Optimization Formulation

The general topology optimization formulation for natural convection applications is defined as

$$
\begin{aligned}
\underset{\boldsymbol{\Theta}\in\mathbb{R}^{N_\theta}}{\text{minimize}}: \quad & J(\boldsymbol{\Theta}, \mathbf{u}^n, \mathbf{p}^n, \mathbf{T}^n) \\
\text{subject to:} \quad & G(\boldsymbol{\Theta}, \mathbf{u}^n, \mathbf{p}^n, \mathbf{T}^n)_{i_c} \leq 0, \qquad i_c = 1, \ldots, N_c \\
& \mathbf{R}_{\mathbf{u}^*}(\boldsymbol{\Theta}, \mathbf{u}^{n-1}, \mathbf{p}^{n-1}, \mathbf{T}^{n-1}, \mathbf{u}^*)_{i_u} = 0, \qquad i_u = 1, \ldots, N_u \\
& \mathbf{R}_{\mathbf{p}}(\boldsymbol{\Theta}, \mathbf{u}^{n-1}, \mathbf{p}^n, \mathbf{p}^{n-1}, \mathbf{u}^*)_{i_p} = 0, \qquad i_p = 1, \ldots, N_p \\
& \mathbf{R}_{\mathbf{u}}(\boldsymbol{\Theta}, \mathbf{u}^n, \mathbf{u}^{n-1}, \mathbf{p}^n, \mathbf{p}^{n-1}, \mathbf{u}^*)_{i_u} = 0, \qquad i_u = 1, \ldots, N_u \\
& \mathbf{R}_{\mathbf{T}}(\boldsymbol{\Theta}, \mathbf{u}^{n-1}, \mathbf{T}^n, \mathbf{T}^{n-1})_{i_T} = 0, \qquad i_T = 1, \ldots, N_T \\
& 0 \leq \boldsymbol{\Theta} \leq 1 \quad \forall \quad \mathbf{x} \in \Omega
\end{aligned}
\tag{64}
$$

where $\boldsymbol{\Theta}$ is the vector of design variables, J is the design objective (objective function), G_{i_c} is the i_c-th design constraint (inequality constraint), $\mathbf{R}_{\mathbf{u}^*}$ is the momentum predictor residual at a fluid velocity degree of freedom i_u, $\mathbf{R}_{\mathbf{p}}$ is the pressure increment residual at a pressure degree of freedom i_p, $\mathbf{R}_{\mathbf{u}}$ is the momentum corrector residual at a fluid velocity degree of freedom i_u, and $\mathbf{R}_{\mathbf{T}}$ is the temperature increment residual at a temperature degree of freedom i_T. The parameter N_c denotes the total number of design constraints. Likewise, the parameters N_θ, N_u, N_p, and N_T denote the total number of design variables, fluid velocity, pressure, and temperature degrees of freedom.

Adjoint Formulation

The total derivative of the objective and constraints with respect to the design variables are derived by applying the adjoint method to the optimization formulation introduced in (64). For the sake of brevity, the adjoint formulation will be derived only for the objective function. The derivation for the constraints can be developed analogously.

A Lagrangian functional is defined to derived the set of adjoint equations needed to calculate the Lagrange multipliers used to compute the total derivative of the objective function with respect to the design variables Θ. The Lagrangian functional for the opti-

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mization problem introduced in (64) is defined as

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{\Theta}, \mathbf{u}^n, \mathbf{u}^{n-1}, \mathbf{p}^n, \mathbf{p}^{n-1}, \mathbf{T}^n, \mathbf{T}^{n-1}, \mathbf{u}^*; \lambda_{\mathbf{u}}^n, \lambda_{\mathbf{p}}^n, \lambda_{\mathbf{T}}^n, \lambda_{\mathbf{u}^*}) = \\
J(\boldsymbol{\Theta}, \mathbf{u}^n, \mathbf{p}^n, \mathbf{T}^n) + \sum_{n=1}^{N_t} (\lambda_{\mathbf{u}^*}^n)^T \, \mathbf{R}_{\mathbf{u}^*}(\boldsymbol{\Theta}, \mathbf{u}^{n-1}, \mathbf{p}^{n-1}, \mathbf{T}^{n-1}, \mathbf{u}^*) \\
+ \sum_{n=1}^{N_t} (\lambda_{\mathbf{p}}^n)^T \, \mathbf{R}_{\mathbf{p}}(\boldsymbol{\Theta}, \mathbf{u}^{n-1}, \mathbf{p}^n, \mathbf{p}^{n-1}, \mathbf{u}^*) \\
+ \sum_{n=1}^{N_t} (\lambda_{\mathbf{u}}^n)^T \, \mathbf{R}_{\mathbf{u}}(\boldsymbol{\Theta}, \mathbf{u}^n, \mathbf{u}^{n-1}, \mathbf{p}^n, \mathbf{p}^{n-1}, \mathbf{u}^*) \\
+ \sum_{n=1}^{N_t} (\lambda_{\mathbf{T}}^n)^T \, \mathbf{R}_{\mathbf{T}}(\boldsymbol{\Theta}, \mathbf{u}^{n-1}, \mathbf{T}^n, \mathbf{T}^{n-1})
\end{aligned}
\tag{65}
$$

where $\lambda_{\mathbf{u}^*} \in \mathbb{R}^{N_u}$ is the vector of Lagrange multipliers associated with the momentum predictor residual, $\lambda_{\mathbf{p}}^n \in \mathbb{R}^{N_p}$ is the vector of Lagrange multipliers associated with the pressure increment residual, $\lambda_{\mathbf{u}} \in \mathbb{R}^{N_u}$ is the vector of Lagrange multipliers associated with the momentum corrector residual, and $\lambda_{\mathbf{T}}^n \in \mathbb{R}^{N_T}$ is the vector of Lagrange multipliers associated with the temperature increment residual.

The stationary point of the Lagrangian functional introduced in (65) with respect to the design variables is given as

$$
\begin{aligned}
\frac{d\mathcal{L}}{d\boldsymbol{\Theta}} = \frac{\partial J^n}{\partial \boldsymbol{\Theta}} + \sum_{n=1}^{N_t} \left(\frac{\partial \mathbf{J}^n}{\partial \mathbf{u}^n} \frac{\partial \mathbf{u}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{J}^n}{\partial \mathbf{p}^n} \frac{\partial \mathbf{p}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{J}^n}{\partial \mathbf{T}^n} \frac{\partial \mathbf{T}^n}{\partial \boldsymbol{\Theta}} \right) \\
+ \sum_{n=1}^{N_t} (\lambda_{\mathbf{u}^*}^n)^T \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{u}^n} \frac{\partial \mathbf{u}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{u}^{n-1}} \frac{\partial \mathbf{u}^{n-1}}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{p}^n} \frac{\partial \mathbf{p}^n}{\partial \boldsymbol{\Theta}} \right. \\
\left. + \frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n-1}}{\partial \mathbf{p}^{n-1}} \frac{\partial \mathbf{p}^{n-1}}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{T}^n} \frac{\partial \mathbf{T}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n-1}}{\partial \mathbf{T}^{n-1}} \frac{\partial \mathbf{T}^{n-1}}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{u}_*^n} \frac{\partial \mathbf{u}_*^n}{\partial \boldsymbol{\Theta}} \right) \\
+ \sum_{n=1}^{N_t} (\lambda_{\mathbf{p}}^n)^T \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{u}^n} \frac{\partial \mathbf{u}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{p}}^{n-1}}{\partial \mathbf{u}^{n-1}} \frac{\partial \mathbf{u}^{n-1}}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{p}^n} \frac{\partial \mathbf{p}^n}{\partial \boldsymbol{\Theta}} \right. \\
\left. + \frac{\partial \mathbf{R}_{\mathbf{p}}^{n-1}}{\partial \mathbf{p}^{n-1}} \frac{\partial \mathbf{p}^{n-1}}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{T}^n} \frac{\partial \mathbf{T}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{p}}^{n-1}}{\partial \mathbf{T}^{n-1}} \frac{\partial \mathbf{T}^{n-1}}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{u}_*^n} \frac{\partial \mathbf{u}_*^n}{\partial \boldsymbol{\Theta}} \right) \\
+ \sum_{n=1}^{N_t} (\lambda_{\mathbf{u}}^n)^T \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{u}^n} \frac{\partial \mathbf{u}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{u}^{n-1}} \frac{\partial \mathbf{u}^{n-1}}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{p}^n} \frac{\partial \mathbf{p}^n}{\partial \boldsymbol{\Theta}} \right. \\
\left. + \frac{\partial \mathbf{R}_{\mathbf{u}}^{n-1}}{\partial \mathbf{p}^{n-1}} \frac{\partial \mathbf{p}^{n-1}}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{T}^n} \frac{\partial \mathbf{T}^n}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}}^{n-1}}{\partial \mathbf{T}^{n-1}} \frac{\partial \mathbf{T}^{n-1}}{\partial \boldsymbol{\Theta}} + \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{u}_*^n} \frac{\partial \mathbf{u}_*^n}{\partial \boldsymbol{\Theta}} \right)
\end{aligned}
$$

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$$
\begin{aligned}
&+\sum_{n=1}^{N_t}(\lambda_{\mathbf{T}}^{n})^{T}\left(\frac{\partial \mathbf{R}_{\mathbf{T}}^{n}}{\partial \boldsymbol{\Theta}}+\frac{\partial \mathbf{R}_{\mathbf{T}}^{n}}{\partial \mathbf{u}^{n}}\frac{\partial \mathbf{u}^{n}}{\partial \boldsymbol{\Theta}}+\frac{\partial \mathbf{R}_{\mathbf{T}}^{n-1}}{\partial \mathbf{u}^{n-1}}\frac{\partial \mathbf{u}^{n-1}}{\partial \boldsymbol{\Theta}}+\frac{\partial \mathbf{R}_{\mathbf{T}}^{n}}{\partial \mathbf{p}^{n}}\frac{\partial \mathbf{p}^{n}}{\partial \boldsymbol{\Theta}}\right.\\
&\left.+\frac{\partial \mathbf{R}_{\mathbf{T}}^{n-1}}{\partial \mathbf{p}^{n-1}}\frac{\partial \mathbf{p}^{n-1}}{\partial \boldsymbol{\Theta}}+\frac{\partial \mathbf{R}_{\mathbf{T}}^{n}}{\partial \mathbf{T}^{n}}\frac{\partial \mathbf{T}^{n}}{\partial \boldsymbol{\Theta}}+\frac{\partial \mathbf{R}_{\mathbf{T}}^{n-1}}{\partial \mathbf{T}^{n-1}}\frac{\partial \mathbf{T}^{n-1}}{\partial \boldsymbol{\Theta}}+\frac{\partial \mathbf{R}_{\mathbf{T}}^{n}}{\partial \mathbf{u}_{*}^{n}}\frac{\partial \mathbf{u}_{*}^{n}}{\partial \boldsymbol{\Theta}}\right)
\end{aligned}
\tag{66}
$$

Rearranging the partial derivatives in (66) leads to the following set of adjoint equations

Final Time Step

$$
\begin{aligned}
&\frac{\partial J^{N}}{\partial \mathbf{u}_{*}^{N}}+(\lambda_{\mathbf{u}^{*}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}^{*}}^{N}}{\partial \mathbf{u}_{*}^{N}}+\left(\lambda_{\mathbf{p}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{p}}^{N}}{\partial \mathbf{u}_{*}^{N}}+(\lambda_{\mathbf{u}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{N}}{\partial \mathbf{u}_{*}^{N}}+\left(\lambda_{\mathbf{T}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{T}}^{N}}{\partial \mathbf{u}_{*}^{N}}+\left(\lambda_{\mathbf{u}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{N}}{\partial \mathbf{u}_{*}^{N}}=0\\
&\frac{\partial J^{N}}{\partial \mathbf{p}^{N}}+(\lambda_{\mathbf{u}^{*}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}^{*}}^{N}}{\partial \mathbf{p}^{N}}+\left(\lambda_{\mathbf{p}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{p}}^{N}}{\partial \mathbf{p}^{N}}+(\lambda_{\mathbf{u}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{N}}{\partial \mathbf{p}^{N}}+\left(\lambda_{\mathbf{T}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{T}}^{N}}{\partial \mathbf{p}^{N}}+\left(\lambda_{\mathbf{u}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{N}}{\partial \mathbf{p}^{N}}=0\\
&\frac{\partial J^{N}}{\partial \mathbf{u}^{N}}+(\lambda_{\mathbf{u}^{*}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}^{*}}^{N}}{\partial \mathbf{u}^{N}}+\left(\lambda_{\mathbf{p}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{p}}^{N}}{\partial \mathbf{u}^{N}}+(\lambda_{\mathbf{u}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{N}}{\partial \mathbf{u}^{N}}+\left(\lambda_{\mathbf{T}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{T}}^{N}}{\partial \mathbf{u}^{N}}+\left(\lambda_{\mathbf{u}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{N}}{\partial \mathbf{u}^{N}}=0\\
&\frac{\partial J^{N}}{\partial \mathbf{T}^{N}}+(\lambda_{\mathbf{u}^{*}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}^{*}}^{N}}{\partial \mathbf{T}^{N}}+\left(\lambda_{\mathbf{p}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{p}}^{N}}{\partial \mathbf{T}^{N}}+(\lambda_{\mathbf{u}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{N}}{\partial \mathbf{T}^{N}}+\left(\lambda_{\mathbf{T}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{T}}^{N}}{\partial \mathbf{T}^{N}}+\left(\lambda_{\mathbf{u}}^{N}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{N}}{\partial \mathbf{T}^{N}}=0
\end{aligned}
\tag{67}
$$

N-th Time Step

$$
\begin{aligned}
&\frac{\partial J^{n}}{\partial \mathbf{u}_{*}^{n}}+(\lambda_{\mathbf{u}^{*}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}^{*}}^{n}}{\partial \mathbf{u}_{*}^{n}}+\left(\lambda_{\mathbf{p}}^{n}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{p}}^{n}}{\partial \mathbf{u}_{*}^{n}}+(\lambda_{\mathbf{u}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{n}}{\partial \mathbf{u}_{*}^{n}}+(\lambda_{\mathbf{T}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{T}}^{n}}{\partial \mathbf{u}_{*}^{n}}\\
&+(\lambda_{\mathbf{u}}^{n})^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{n}}{\partial \mathbf{u}_{*}^{n}}+\left(\lambda_{\mathbf{u}^{*}}^{n+1}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{u}^{*}}^{n+1}}{\partial \mathbf{u}_{*}^{n}}+\left(\lambda_{\mathbf{p}}^{n+1}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{u}_{*}^{n}}\\
&+\left(\lambda_{\mathbf{T}}^{n+1}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{u}_{*}^{n}}+\left(\lambda_{\mathbf{u}}^{n+1}\right)^{T}\frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{u}_{*}^{n}}=0
\end{aligned}
$$

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$$
\begin{aligned}
&\frac{\partial J^n}{\partial \mathbf{p}^n} + (\lambda_{\mathbf{u}^*}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{p}^n} + \left(\lambda_{\mathbf{p}}^n\right)^T \frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{p}^n} + (\lambda_{\mathbf{u}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{p}^n} + (\lambda_{\mathbf{T}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{T}}^n}{\partial \mathbf{p}^n} \\
&+ (\lambda_{\mathbf{u}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{p}^n} + \left(\lambda_{\mathbf{u}^*}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n+1}}{\partial \mathbf{p}^n} + \left(\lambda_{\mathbf{p}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{p}^n} \\
&+ \left(\lambda_{\mathbf{T}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{p}^n} + \left(\lambda_{\mathbf{u}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{p}^n} = 0
\end{aligned}
$$

$$
\begin{aligned}
&\frac{\partial J^n}{\partial \mathbf{T}^n} + (\lambda_{\mathbf{u}^*}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{T}^n} + \left(\lambda_{\mathbf{p}}^n\right)^T \frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{T}^n} + (\lambda_{\mathbf{u}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{T}^n} + (\lambda_{\mathbf{T}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{T}}^n}{\partial \mathbf{T}^n} \\
&+ (\lambda_{\mathbf{u}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{T}^n} + \left(\lambda_{\mathbf{u}^*}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n+1}}{\partial \mathbf{T}^n} + \left(\lambda_{\mathbf{p}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{T}^n} + \left(\lambda_{\mathbf{u}_{**}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{T}^n} \\
&+ \left(\lambda_{\mathbf{T}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{T}^n} + \left(\lambda_{\mathbf{u}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{T}^n} = 0
\end{aligned}
$$

$$
\begin{aligned}
&\frac{\partial J^n}{\partial \mathbf{u}^n} + (\lambda_{\mathbf{u}^*}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{u}^n} + \left(\lambda_{\mathbf{p}}^n\right)^T \frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{u}^n} + (\lambda_{\mathbf{u}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{u}^n} + (\lambda_{\mathbf{T}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{T}}^n}{\partial \mathbf{u}^n} \\
&+ (\lambda_{\mathbf{u}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{u}^n} + \left(\lambda_{\mathbf{u}^*}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n+1}}{\partial \mathbf{u}^n} + \left(\lambda_{\mathbf{p}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{u}^n} \\
&+ \left(\lambda_{\mathbf{T}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{u}^n} + \left(\lambda_{\mathbf{u}}^{n+1}\right)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{u}^n} = 0
\end{aligned}
\tag{68}
$$

The adjoint system of equations solved to calculate the Lagrange multipliers are derived from Equations (67) and (68), which results in the following set of equations

Final Time Step

$$
\begin{aligned}
\lambda_{\mathbf{u}^*}^N &= -\left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^N}{\partial \mathbf{u}_*^N}\right)^{-T} \left[\frac{\partial J^N}{\partial \mathbf{u}_*^N} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^N}{\partial \mathbf{u}_*^N}\right)^T \lambda_{\mathbf{u}}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^N}{\partial \mathbf{u}_*^N}\right)^T \lambda_{\mathbf{p}}^N + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^N}{\partial \mathbf{u}_*^N}\right)^T \lambda_{\mathbf{T}}^N\right] \\
\lambda_{\mathbf{p}}^N &= -\left(\frac{\partial \mathbf{R}_{\mathbf{p}}^N}{\partial \mathbf{p}^N}\right)^{-T} \left[\frac{\partial J^N}{\partial \mathbf{p}^N} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^N}{\partial \mathbf{p}^N}\right)^T \lambda_{\mathbf{u}^*}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^N}{\partial \mathbf{p}^N}\right)^T \lambda_{\mathbf{T}}^N + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^N}{\partial \mathbf{p}^N}\right)^T \lambda_{\mathbf{u}}^n\right] \\
\lambda_{\mathbf{T}}^N &= -\left(\frac{\partial \mathbf{R}_{\mathbf{T}}^N}{\partial \mathbf{T}^N}\right)^{-T} \left[\frac{\partial J^N}{\partial \mathbf{T}^N} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^N}{\partial \mathbf{T}^N}\right)^T \lambda_{\mathbf{u}^*}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^N}{\partial \mathbf{T}^N}\right)^T \lambda_{\mathbf{p}}^N + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^N}{\partial \mathbf{T}^N}\right)^T \lambda_{\mathbf{u}}^n\right] \\
\lambda_{\mathbf{u}}^N &= -\left(\frac{\partial \mathbf{R}_{\mathbf{u}}^N}{\partial \mathbf{u}^N}\right)^{-T} \left[\frac{\partial J^N}{\partial \mathbf{u}^N} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^N}{\partial \mathbf{u}^N}\right)^T \lambda_{\mathbf{u}^*}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^N}{\partial \mathbf{u}^N}\right)^T \lambda_{\mathbf{p}}^N + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^N}{\partial \mathbf{u}^N}\right)^T \lambda_{\mathbf{T}}^N\right]
\end{aligned}
\tag{69}
$$

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N-th Time Step

$$\lambda_{\mathbf{u}^*}^n = -\left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{u}_*^n}\right)^{-T}\left[\frac{\partial J^n}{\partial \mathbf{u}_*^n} + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^n}{\partial \mathbf{u}_*^n}\right)^T \lambda_{\mathbf{T}}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{u}_*^n}\right)^T \lambda_{\mathbf{p}}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{u}_*^n}\right)^T \lambda_{\mathbf{u}}^n \right.$$
$$+ \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n+1}}{\partial \mathbf{u}_*^n}\right)^T \lambda_{\mathbf{u}^*}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{u}_*^n}\right)^T \lambda_{\mathbf{p}}^{n+1}$$
$$\left. + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{u}_*^n}\right)^T \lambda_{\mathbf{T}}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{u}_*^n}\right)^T \lambda_{\mathbf{u}}^{n+1}\right]$$
$$\lambda_{\mathbf{p}}^n = -\left(\frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{p}^n}\right)^{-T}\left[\frac{\partial J^n}{\partial \mathbf{p}^n} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{u}^*}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^n}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{T}}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{u}}^n \right.$$
$$+ \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n+1}}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{u}^*}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{p}}^{n+1}$$
$$\left. + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{T}}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{u}}^{n+1}\right]$$

$$\lambda_{\mathbf{T}}^n = -\left(\frac{\partial \mathbf{R}_{\mathbf{T}}^n}{\partial \mathbf{T}^n}\right)^{-T}\left[\frac{\partial J^n}{\partial \mathbf{T}^n} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{T}^n}\right)^T \lambda_{\mathbf{u}^*}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{T}^n}\right)^T \lambda_{\mathbf{p}}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{T}^n}\right)^T \lambda_{\mathbf{u}}^n \right.$$
$$+ \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n+1}}{\partial \mathbf{T}^n}\right)^T \lambda_{\mathbf{u}^*}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{T}^n}\right)^T \lambda_{\mathbf{p}}^{n+1}$$
$$\left. + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{T}^n}\right)^T \lambda_{\mathbf{T}}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{T}^n}\right)^T \lambda_{\mathbf{u}}^{n+1}\right]$$
$$\lambda_{\mathbf{u}}^n = -\left(\frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{u}^n}\right)^{-T}\left[\frac{\partial J^n}{\partial \mathbf{u}^n} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{u}^n}\right)^T \lambda_{\mathbf{u}^*}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{u}^n}\right)^T \lambda_{\mathbf{p}}^n \right.$$
$$+ \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n+1}}{\partial \mathbf{u}^n}\right)^T \lambda_{\mathbf{u}^*}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{u}^n}\right)^T \lambda_{\mathbf{p}}^{n+1} \tag{70}$$
$$\left. + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{u}^n}\right)^T \lambda_{\mathbf{T}}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{u}^n}\right)^T \lambda_{\mathbf{u}}^{n+1}\right]$$

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Equations (69) and (70) denote the general set of adjoint equations used to calculate the Lagrange multipliers. The Lagrange multipliers are then used to calculate the total derivative of the objective with respect to the design variables, which is given as

$$\frac{dJ}{d\boldsymbol{\Theta}} = \sum_{n=1}^{N_t} \left(\frac{\partial J^n}{\partial \boldsymbol{\Theta}} + (\lambda_{\mathbf{u}^*}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \boldsymbol{\Theta}} + \left(\lambda_{\mathbf{p}}^n\right)^T \frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \boldsymbol{\Theta}} + (\lambda_{\mathbf{u}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \boldsymbol{\Theta}} + (\lambda_{\mathbf{T}}^n)^T \frac{\partial \mathbf{R}_{\mathbf{T}}^n}{\partial \boldsymbol{\Theta}} \right) \tag{71}$$

A simplified set of adjoint equations can be derived by removing redundant terms, i.e. zero terms, from Equations (69) and (70) and rearranging non-zero terms, which gives

Final Time Step

$$\begin{aligned}
\lambda_{\mathbf{u}^*}^N &= -\left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^N}{\partial \mathbf{u}_*^N}\right)^{-T} \left[\left(\frac{\partial \mathbf{R}_{\mathbf{u}}^N}{\partial \mathbf{u}_*^N}\right)^T \lambda_{\mathbf{u}}^N + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^N}{\partial \mathbf{u}_*^N}\right)^T \lambda_{\mathbf{p}}^N \right] \\
\lambda_{\mathbf{p}}^N &= -\left(\frac{\partial \mathbf{R}_{\mathbf{p}}^N}{\partial \mathbf{p}^N}\right)^{-T} \left[\frac{\partial J^N}{\partial \mathbf{p}^N} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^N}{\partial \mathbf{p}^N}\right)^T \lambda_{\mathbf{u}}^N \right] \\
\lambda_{\mathbf{T}}^N &= -\left(\frac{\partial \mathbf{R}_{\mathbf{T}}^N}{\partial \mathbf{T}^N}\right)^{-T} \left[\frac{\partial J^N}{\partial \mathbf{T}^N} \right] \\
\lambda_{\mathbf{u}}^N &= -\left(\frac{\partial \mathbf{R}_{\mathbf{u}}^N}{\partial \mathbf{u}^N}\right)^{-T} \left[\frac{\partial J^N}{\partial \mathbf{u}^N} \right]
\end{aligned} \tag{72}$$

N-th Time Step

$$\begin{aligned}
\lambda_{\mathbf{u}^*}^n &= -\left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^n}{\partial \mathbf{u}_*^n}\right)^{-T} \left[\left(\frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{u}_*^n}\right)^T \lambda_{\mathbf{u}}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{u}_*^n}\right)^T \lambda_{\mathbf{p}}^n \right] \\
\lambda_{\mathbf{p}}^n &= -\left(\frac{\partial \mathbf{R}_{\mathbf{p}}^n}{\partial \mathbf{p}^n}\right)^{-T} \Bigg[\frac{\partial J^n}{\partial \mathbf{p}^n} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^n}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{u}}^n + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{p}}^{n+1} \\
&\qquad + \left(\frac{\partial \mathbf{R}_{\mathbf{u}^*}^{n+1}}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{u}^*}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{p}^n}\right)^T \lambda_{\mathbf{u}}^{n+1} \Bigg] \\
\lambda_{\mathbf{T}}^n &= -\left(\frac{\partial \mathbf{R}_{\mathbf{T}}^n}{\partial \mathbf{T}^n}\right)^{-T} \left[\frac{\partial J^n}{\partial \mathbf{T}^n} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}_*}^{n+1}}{\partial \mathbf{T}^n}\right)^T \lambda_{\mathbf{u}_*}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{T}^n}\right)^T \lambda_{\mathbf{T}}^{n+1} \right]
\end{aligned}$$

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$$\lambda_{\mathbf{u}}^{n} = -\left(\frac{\partial \mathbf{R}_{\mathbf{u}}^{n}}{\partial \mathbf{u}^{n}}\right)^{-T} \left[\frac{\partial J^{n}}{\partial \mathbf{u}^{n}} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}_*}^{n+1}}{\partial \mathbf{u}^{n}}\right)^{T} \lambda_{\mathbf{u}_*}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{p}}^{n+1}}{\partial \mathbf{u}^{n}}\right)^{T} \lambda_{\mathbf{p}}^{n+1} \right.$$
$$\left. + \left(\frac{\partial \mathbf{R}_{\mathbf{T}}^{n+1}}{\partial \mathbf{u}^{n}}\right)^{T} \lambda_{\mathbf{T}}^{n+1} + \left(\frac{\partial \mathbf{R}_{\mathbf{u}}^{n+1}}{\partial \mathbf{u}^{n}}\right)^{T} \lambda_{\mathbf{u}}^{n+1}\right] \tag{73}$$

Equations (72) and (73) are the set of adjoint equations used in this work to calculate the Lagrange multipliers.

The following steps are carry out in sequence to compute the total total derivative of the objective function with respect to the design variables at every optimization iteration

1. Solve the conservation equations to calculate the state, i.e. primal, variables;

2. Solve Equations (72) and (73) to calculate the Lagrange multipliers, i.e. dual variables; and

3. Calculate the total derivative of the objective function with respect to the design variables using Equation (71)

Recall, the total derivative of the constraints with respect to the design variables can be computed analogously to how the total derivative is computed for the objective function.

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