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A Lagrangian formalism for thermal analysis of laminar convective heat transfer

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Abstract. Heat transfer in essence is the transport of thermal energy along certain paths in a similar way as fluid motion is the transport of fluid parcels along fluid paths. This similarity admits Lagrangian heat-transfer analyses by the geometry of such "thermal paths" analogous to well-known Lagrangian mixing analyses. Essential to Lagrangian heat-transfer formalisms is the reference state for the convective flux. Existing approaches admit only uniform references. However, for convective heat transfer, a case of great practical relevance, the conductive state that sets in for vanishing fluid motion is the more natural reference. This typically is an inhomogeneous state and thus beyond the existing formalism. The present study closes this gap by its generalisation to non-uniform references and thus substantially strengthens Lagrangian methods for thermal analyses. This ansatz is demonstrated by way of a 2D case study and offers new fundamental insight into thermal transport that is complementary to the Eulerian picture based on temperature and heat-transfer coefficients.

1. Introduction
Convective heat transfer in laminar flows is essential to a wide range of emerging technologies: compact systems for process intensification [1, 2]; micro-fluidics [3, 4]; electronics cooling [5, 6]. This mode of heat transfer is traditionally characterised by the proven method of Nusselt relations [1]. However, such relations offer limited insight into the actual heat-transfer mechanisms – and then in particular in the flow interior. Such insight becomes increasingly important for further technological development, though. This motivates the present study.

Heat transfer fundamentally is the combined thermal transport by fluid motion (convection) and molecular motion (conduction). This effective heat flux, similar to fluid transport along fluid paths, delineates “thermal paths” by which heat is transferred. Thus a Lagrangian description of heat transfer can be formulated analogous to that of fluid motion [7, 8, 9]. To date such representations describe thermal fluxes and paths relative to a – in principle arbitrary – uniform reference temperature [9, 10]. However, in the present context, the conductive state for stagnant fluid – expanding on the concept of Nusselt relations – is the more natural reference. This usually is an inhomogeneous state and thus beyond existing Lagrangian heat-transfer formalisms. The present study closes this gap by their generalisation to non-uniform references.

The discussion is organised as follows. Section 2 introduces the generalised Lagrangian formalism for heat transfer. The generic geometrical composition of the thermal paths and its connection with heat transfer is elaborated in Section 3. The concepts are demonstrated in Section 4 by way of an illustrative 2D example. Conclusions and outlook are in Section 5.
2. Convective heat transfer: Lagrangian representation

2.1. Temperature field: conductive and convective contributions

Heat transfer inside a domain $D$ with boundary $\Gamma = \partial D$ and outward normal $\mathbf{n}$ is for solenoidal flow ($\nabla \cdot \mathbf{u} = 0$) governed by the non-dimensional energy equation

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{Pe} \nabla^2 T, \quad T|_{\Gamma} = h(x|\Gamma), \quad T(x, 0) = T_0(x), \quad (1)$$

with $Pe$ the well-known Péclet number and $h$ a generic Dirichlet boundary condition. The temperature admits decomposition into conductive ($\bar{T}$) and convective ($T'$) contributions, $T = \bar{T} + T'$, governed by

$$\frac{\partial \bar{T}}{\partial t} = \frac{1}{Pe} \nabla^2 \bar{T}, \quad \frac{\partial T'}{\partial t} + \nabla \cdot (u T' - Pe^{-1} \nabla T') = -\mathbf{u} \cdot \nabla \tilde{T}, \quad (2)$$

with boundary conditions $\bar{T}|_{\Gamma} = h(x|\Gamma, t)$ and $T'|_{\Gamma} = 0$ and initial conditions $\bar{T}(x, 0) = T_0(x)$ and $T'(x, 0) = 0$ [11]. Contribution $T'$ meets $\lim_{Pe \to 0} T' = 0$ and thus represents the effect of fluid motion – and thereby of convective heat transfer – upon the temperature distribution.

The above decomposition exposes contribution $F = -\mathbf{u} \cdot \nabla T$ to the convective term $\mathbf{u} \cdot \nabla T$ effectively acting as source for the convective temperature contribution $T'$ – and thus as “driving force” behind convective heat transfer. This notion implies a physical separation of said convective term (using $\nabla \cdot \mathbf{u} = 0$) according to $\mathbf{u} \cdot \nabla T = \mathbf{u} \cdot \nabla T' + \mathbf{u} \cdot \nabla \bar{T} = \nabla \cdot \mathbf{q}_c - F$, with $F$ as before and $\mathbf{q}_c = u T'$ the convective heat flux solely by the transport of fluid parcels into regions at different temperature (“direct convective flux”). Essential is that $F$ is globally-conservative, i.e. $\int_D F dv = 0$, and thus leaves the net energy content of the system unaffected; it merely “drives” convective heat transfer through non-zero $T'$. Transport of warmer fluid into a colder region ($T' > 0$) causes a convective heat flux in the flow direction (direct convective heating). Conversely, transport of colder fluid into a warmer region ($T' < 0$) effectively sets up a convective heat flux against the flow direction (direct convective cooling).

The convective heat flux $\mathbf{q}_c$ is of fundamental importance to Lagrangian heat-transfer analyses in that the thermal transport routes depend essentially on its definition. Such analyses hitherto identified this flux with the enthalpy flux: $\mathbf{q}_c = \mathbf{u} T'$ [7, 8, 9]. However, the enthalpy flux depends on a – in principle arbitrary – global reference temperature $T_R$, which, though conceptually entirely correct, hampers physical interpretation of the associated thermal transport routes [9, 10]. The current representation of $\mathbf{q}_c$, on the other hand, adopts the conductive state $\bar{T}$ as reference for the convective flux, which is intuitively more accessible in that, first, non-zero $\mathbf{q}_c$ occurs only for non-zero convective departures $T'$ from $\bar{T}$ and, second, $\mathbf{q}_c$ is independent of the reference $T_R$ for $T$. Hence, $\mathbf{q}_c$ represents the “true” convective heat flux.

Decomposition (2) admits expression in the transport form

$$\frac{\partial \bar{T}}{\partial t} + \nabla \cdot \mathbf{\tilde{q}} = 0, \quad \frac{\partial T'}{\partial t} + \nabla \cdot \mathbf{Q}' = F, \quad \mathbf{\tilde{q}} = -\frac{1}{Pe} \nabla \bar{T}, \quad \mathbf{q}' = -\frac{1}{Pe} \nabla T', \quad \mathbf{Q}' = \mathbf{q}_c + \mathbf{q}', \quad (3)$$

with $F$ and $\mathbf{q}_c$ as before. Fluxes $\mathbf{\tilde{q}}$ and $\mathbf{q}'$ are the conductive and convective contributions, respectively, to the total conduction. Flux $\mathbf{Q}'$ represents the net heat transfer induced by the fluid motion (“net convective flux”) relative to the conductive background $\bar{T}$ and comprises the direct convective flux $\mathbf{q}_c$ and the additional conductive contribution $\mathbf{q}'$ by non-zero $T'$. This renders $\mathbf{Q}'$ the key quantity in analyses on heat-transfer enhancement by convection. Distinction can again be made between net convective heating ($T' > 0$) and net convective cooling ($T' < 0$).
2.2. Thermal transport routes

Mass conservation for fluid is governed by the continuity constraint

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{M} = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = F_\rho, \quad (4)$$

with $\mathbf{M}$ the mass flux of fluid parcels with density $\rho$ and velocity $\mathbf{u}$. The volumetric fluid source $F_\rho$ is a generalisation of the usual case $F_\rho = 0$ and, consistent with $F$, restricted by constraint $\int_D F_\rho dV = 0$. Hence, fluid motion in a Lagrangian framework concerns the transport of quantity $\rho$ by the flow field $\mathbf{u}$. Mathematical similarity with (3) admits this notion to carry over to convective heat transfer, upon reformulation of (3) resulting in

$$\frac{\partial T'}{\partial t} + \nabla \cdot Q' = \frac{\partial T'}{\partial t} + \nabla \cdot (T' \mathbf{v}) = F, \quad \mathbf{v} \equiv \frac{Q'}{T'} = \mathbf{u} - \frac{1}{Pc} \nabla (\log |T'|), \quad (5)$$

meaning that this mode of heat transfer in essence involves the Lagrangian transport of quantity $T'$ by the “flow field” $\mathbf{v}$. This exposes the fundamental analogy $(T', \mathbf{v}, Q', F) \leftrightarrow (\rho, \mathbf{u}, \mathbf{M}, F_\rho)$ between fluid motion and convective heat transfer. The latter in Lagrangian sense thus is the transport of virtual fluid parcels (“heat parcels”) with “density” $T'$ by the “velocity” $\mathbf{v}$.

Key to Lagrangian transport analysis is the notion that transport of relevant quantities occurs along particular paths or “transport routes.” The latter coincide with the Lagrangian fluid trajectories $\mathbf{x}(t)$ in case of fluid flow. The above representation of convective heat transfer as the “motion” of a “fluid” naturally leads to “thermal trajectories” $\mathbf{x}'(t)$ as transport routes for heat. Fluid and thermal trajectories are described by the analogous kinematic equations

$$\frac{dx}{dt} = \mathbf{u} \, \Rightarrow \, \mathbf{x}(t) = \Phi(\mathbf{x}(0)) \quad \Leftrightarrow \quad \frac{dx'}{dt} = \mathbf{v} \, \Rightarrow \, \mathbf{x}'(t) = \Phi'(\mathbf{x}'(0)), \quad (6)$$

with the corresponding fluid and thermal flows subject to the equivalent continuity constraints (4) and (5), respectively. These constraints play a fundamental role by “organising” the trajectories into coherent structures that geometrically determine the transport (Section 3).

3. Generic composition of the thermal topology in 2D steady systems

The trajectories described by kinematic equations of the form (6) are organised into coherent structures that geometrically determine the transport [12]. This facilitates topological transport analyses by well-established methods from classical mechanics and has proven its worth in studies on (chaotic) mixing [4]. Recently, first generalisations of this ansatz to heat transfer have been undertaken [13, 14, 9]. Said studies concern locally-conservative mass and heat fluxes, i.e. $F_\rho = 0$ and $F = 0$ in (4) and (5), respectively, which are in essence special instances of the generic globally-conservative cases $\int_D F_\rho dV = 0$ and $\int_D F dV = 0$ introduced in Section 2.2 [11].

Key coherent structures in non-conservative systems are attractors and repellors, that is, entities upon which trajectories asymptotically converge or from which they emanate, respectively, in the course of time. In 2D steady flows, they emerge as stagnation points or closed trajectories [12]. Two kinds of point attractors exist: node and focus. The former attracts along two principal transport directions (“stable manifolds” $W_I^s$ and $W_{II}^s$) (Fig. 1a); the latter attracts along spiralling trajectories (Fig. 1b). Attracting trajectories (“limit cycles”) are characterised by converging trajectories from both inside and outside the region they enclose (Fig. 1c). Repellors are identical yet with reversed transport. Saddles (or “hyperbolic points”) complete the set and also have two principal transport directions yet, in contrast with the node, one towards (“stable manifold” $W^s$) and one away from (“unstable manifold” $W^u$) said point (Fig. 1d). Hence, they are neither attracting nor repelling entities. In 2D steady flows, manifolds
merge into streamlines connecting nodes or saddles, denoted homoclinic and heteroclinic orbits upon linking one isolated or two different points, respectively.

Attractors/repellors are accompanied by so-called “basin of attraction/repulsion” that in thermal sense act as heat sinks/sources due to heat infusion/extraction by source $F$ and the non-adiabatic walls. Their manifolds delineate the principal heat-transfer directions within these regions. Continuity dictates that (thermal) trajectories must start/end on a non-adiabatic wall or in a repellor/attractor. This implies four basic interactions:

(i) **wall-attractor** basin of attraction is sink for heat supplied via wall segment;
(ii) **wall-repellor** basin of repulsion is source for heat rejected via wall segment;
(iii) **attractor-repellor** basins of attraction and repulsion merge;
(iv) **wall-wall** channels setting up heat exchange between wall segments.

These basic configurations constitute the elementary topological building blocks of generic thermal topologies and are shown schematically in Fig. 2. Thus the generalised Lagrangian formalism admits a richer thermal topology – and may therefore distinguish a wider (and more subtle) array of heat-transfer phenomena – compared to the existing approach.

Local conservation suppresses attraction and repulsion and thus restricts coherent structures to (i) saddles and associated manifolds and (ii) centres (or “elliptic points”), i.e. the degenerate state separating an attracting and repelling focus, encircled by concentric closed orbits [12]. The latter define so-called “islands” [4], which are isolated regions devoid of (thermal) exchange with their environment, and basically are limit cases of attractor-repellor interactions (Fig. 2c). This more restrictive geometric organisation holds for solenoidal (thermal) flux.

4. **An illustrative case study: convective heat transfer in 2D steady vortex flow**

4.1. **Introduction**

Lagrangian thermal analysis by the above concepts is demonstrated for the non-dimensional configuration introduced in [14]. It concerns the 2D domain $(x, y) = [0, 1] \times [0, 1/2]$ with
spatially-periodic inlet \((x = 0)\) and outlet \((x = 1)\) and solid bottom \((y = 0)\) and top \((y = 1/2)\) walls. Heat transfer is induced via a “hot” bottom wall \((T(x, 0) = T_H)\) and a “cold” top wall \((T(x, 1/2) = T_C < T_H)\) and governed by the steady simplification of (1). Fluid motion is according to the double-gyre flow \(u = [\sin(2\pi x) \cos(2\pi y), -\cos(2\pi x) \sin(2\pi y)]\) and the sole system parameter is the Péclet number. Numerical methods are detailed in [14, 9].

The flow topology coincides with the streamline portrait shown in Fig. 3a and consists of two “islands” formed by closed streamlines, arranged concentrically around centre-type stagnation points. The islands are encapsulated by the heteroclinically-merged manifolds of two saddles (crosses) on the bounding walls that coincide with the domain boundary and the separatrix \(x = 1/2\). Thus the flow topology comprises of coherent structures according to the generic geometrical organisation of locally-conservative systems (Section 3).

Case-specific symmetries result in further topological organisation. Symmetry analysis by methods following [15, 16] yields the time-reversal reflectional symmetry

\[
\Phi = S_1 \Phi^{-1} S_1, \tag{7}
\]

with \(S_1 : (x, y) \rightarrow (1 - x, 1/2 - y)\), in the flow (4). This causes a symmetric arrangement of coherent structures about the axis of reflection (diagonal \(y = x/2)\), advancing \(x_H^{(1)} = S_1(x_H^{(2)})\) and \(W_t^{(1)} = S_1(W_t^{(2)})\) as symmetries between saddles and their manifolds [16] (Fig. 3). The thermal topology, though locally non-conservative, has a similar composition. This is elaborated below.

4.2. Heat transfer and thermal topology

The total temperature \(T\) and corresponding total heat flux \(Q = q_c + \bar{q} + q'\) for \(Pe = 100\) are given in Fig. 3b. (Red and blue indicate highest and lowest temperatures, respectively.) Both clearly reveal the heat transfer from hot bottom to cold top wall. Figs 4a and b show the associated direct convective flux \(q_c\) and total convective flux \(Q'\), respectively, together with the convective temperature contribution \(T'\). The latter exposes the convective heating \((T' > 0; \text{red})\) and cooling \((T' < 0; \text{blue})\) zones. Location of former and latter in the proximity of cold top and hot bottom wall, respectively, reflects the upward transport of warmer fluid in the centre and downward transport of colder fluid near the adiabatic side walls by the vortical flow.

The direct convective flux \(q_c\) (vectors in Fig. 4a) visualises the corresponding heat circulation set up purely by the fluid motion. Its running counter to the flow \((u \cdot q_c < 0)\) in the convective-cooling zone (blue) signifies transport of colder fluid from the upper region towards the warmer bottom wall. This effectuates heating of the colder fluid and, inherently, results in an effective
thermal transport against the flow direction. The associated convective flux $Q'$ is given in Fig. 4b (vectors) and represents the total heat flux emanating from the fluid motion. Flux $Q'$, contrary to $q_c$, is non-zero everywhere, save at isolated positions, meaning that convective heat transfer manifests itself throughout the entire domain. Its predominantly inward and outward orientation on bottom and top walls, respectively, in fact signifies augmented fluid-wall heat exchange and thus directly represents heat-transfer enhancement by convection.

![a) $T'$ and $q_c$](image1)

![b) $T'$ and $Q'$](image2)

Figure 4. Thermal decomposition for $Pe = 100$: convective ($T'$) temperature vs. direct convective ($q_c$) and net convective ($Q'$) heat flux. Vectors indicate heat flux; blue/red indicate minimum/maximum convective temperature ($\min T' = - \max T'$).

The thermal streamlines $x'$ (net convective flux $Q'$) according to (6) are given in Fig. 5 in combination with total ($T$) and convective ($T'$) temperatures. (Colours again indicate $T$ and $T'$ with the same colour-coding as before.) The portrait clearly visualises a heat transfer from hot bottom to cold top wall and exposes a significant effect by the fluid circulation in the flow interior. Symmetry analysis of the thermal field, similar to the flow topology, yields

$$\Phi' = S_2 \Phi'^{-1} S_2, \quad \Phi' = S_3 \Phi' S_3,$$

with $S_2 : (x, y) \rightarrow (x + 1/2, 1/2 - y)$ and $S_3 : (x, y) \rightarrow (1 - x, y)$, as relevant case-specific symmetries in the net convective heat flux $\Phi'$. Both symmetries are evident in Fig. 5. The convective thermal topology $x'$ accommodates two stagnation points, one on $x = 0, 1$ and one on $x = 1/2$, and is examined hereafter by the concepts outlined in Section 3.

The present system is subject to thermal Dirichlet conditions. This implies global conservation of $Q'$ and thus coupled emergence of attracting and repelling entities in the thermal topology [11]. Here this causes the node-type attractor $x_A$ on line $x = 0, 1$ (gray circle) to be accompanied by the node-type repellor $x_R$ on line $x = 1/2$ (black cross), as shown in Fig. 6a. Former and latter lines define the associated stable manifold $W_{A,1}^s$ (heavy gray line) and unstable manifold $W_{R,1}^u$ (heavy black line), respectively; the companion manifolds $W_{A,2}^s$ and $W_{R,2}^u$ merge into a heteroclinic orbit $W := W_{A,2}^s = W_{R,2}^u$ connecting $x_A$ and $x_R$ (heavy gray/black curve). These entities relate through the symmetries

$$x_A = S_2(x_R), \quad W_{A,1}^s = S_2(W_{R,1}^u), \quad W_{A,2}^s = S_2(W_{R,2}^u), \quad W = S_2(W),$$

and imply the time-reversal symmetry $S_2$ in (8). Symmetries (8) impose strong geometrical restrictions upon the thermal topology and thus play an essential role in its composition.

The attractor-repellor pair organises the thermal topology $x'$ into an arrangement of the basic building blocks identified in Section 3. The basin of attraction of $x_A$ comprises sections
attached to the bottom \((B_{A,B})\) and top \((B_{A,T})\) walls; the basin of repulsion of \(x_R\), similarly, also comprises sections attached to the bottom \((B_{R,B})\) and top \((B_{R,T})\) walls. The remaining sections of both basins merge into a shared region \(B_{RA}\). These regions amalgamate into the thermal topology in the way shown in Fig. 6a and adopt the above symmetry properties, i.e.

\[
B_{A,B} = S_2(B_{R,T}), \quad B_{A,T} = S_2(B_{R,B}), \quad B_{RA} = S_2(B_{RA}), \quad B_i = S_3(B_i),
\]

with \(B_i\) representing any of said regions. The manifolds of the attractor-repellor pair delineate the principal transport directions within these regions: heat influx from the non-adiabatic walls in \(B_{A,B}\) and \(B_{A,T}\) along \(W_{A1}\); heat outflux into these walls in \(B_{R,T}\) and \(B_{R,T}\) along \(W_{R1}\); internal heat redistribution in \(B_{RA}\) along \(W\). This is investigated further below.

The above regions play distinct roles in the thermal transport. Consider to this end the areas with net convective cooling \(C_C\ (T' < 0)\) and net convective heating \(C_H\ (T' > 0)\) (Fig. 6b). Region \(B_{A,B} \in C_C\) accommodates convective heat influx from the hot bottom wall by supply of relatively colder fluid \((T' < 0)\); region \(B_{R,T} \in C_H\), conversely, accommodates convective heat outflux into the cold top wall by supply of relatively warmer fluid \((T' > 0)\). These fluxes signify a higher heat exchange from hot to cold walls compared to the conductive state and thus represent (local) heat-transfer enhancement by convection. Thermal streamlines in region \(B_{RA}\) invariably cross separatrix \(T' = 0\) (heavy gray curve in Fig. 6b), meaning that convective heat transfer switches from heating to cooling. This reflects the internal heat redistribution from the upward stream of warmer fluid in the centre to the downward stream of colder fluid along the periodic inlet-outlet. The remaining regions \(B_{A,T} \in C_C\) and \(B_{R,B} \in C_H\) deteriorate the overall convective heat-transfer enhancement via heat influx from the cold top wall and heat outflux into the hot bottom wall, respectively. However, adverse effects are weak, since they (i) are very localised and (ii) local heat-transfer coefficients are extremely small due to nearly-uniform \(T'\).

5. Conclusions
The present study generalises existing Lagrangian heat-transfer formalisms to non-uniform reference temperatures and thus enables investigation of convective heat transfer relative to its natural reference, the conductive state corresponding with stagnant fluid. This facilitates accessible physical interpretation of thermal fluxes and thermal paths and eliminates the ambiguity involved with the (in principle arbitrary) uniform reference state of the original formalism. Hence, the generalised ansatz may elevate Lagrangian heat-transfer analyses to the level of maturity required for universal and unambiguous application.
The generalised formalism affords important new insight into convective heat transfer by disclosing attracting/repelling entities in its underlying thermal topology that form virtual heat sinks/sources and act as its “driving mechanisms.” This results in convective-cooling and convective-heating zones. Thus the thermal topology and corresponding fluxes directly visualise convective heat transfer and its role in (local) heat-transfer enhancement. This insight is beyond conventional methods based on temperature and heat-transfer coefficients.

The proposed generalisation admits extension to unsteady 3D systems and generic scalar quantities (additives, chemical species, reactants) [11]. Its application to convective scalar transport may enable unravelling the – hitherto ill-understood – role of (chaotic) fluid motion in two primary practical objectives: transfer-rate enhancement and homogenisation. A further fundamental issue may concern the role of the scalar transport topology and corresponding fluxes in the structure and interplay of (dominant) eigenmodes that underly the evolution of temperature and concentration fields [17]. Finally, the Lagrangian formalism may contribute to realisation of novel aims such as creation of specific gradient fields and targeted delivery of heat and mass in designated flow regions, which may benefit versatility and multi-functionality of e.g. lab-on-a-chip systems [18]. Efforts to address such issues are underway.

References