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On the formation of thermal caustics in turbulent particle-laden flows

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This study investigates the development of thermal caustics within particle-laden turbulent flows, a concept recently proposed to elucidate the non-smooth behavior of particle temperature during fluid-particle thermal interactions, drawing a parallel to the creation of caustics. The temperature variations observed between closely spaced particles, which are linked to thermal caustics, stem from the history of their different paths. This work delves into the emergence of thermal caustics by analyzing the dynamics of the gradient of particle temperature in the configuration space, highlighting the influence of both particle and thermal inertia. The analysis indicates that thermal caustics arise concurrently with caustics, with the exception of the condition of zero thermal inertia, which represents a singular scenario where particle temperature decouples from velocity.

Turbulent particle-laden flows, ubiquitous in both environmental and engineering contexts, exhibit a complex multi-scale behaviour driven by the chaotic flow field and particle inertia. These factors critically influence both individual and collective particle dynamics. Numerous studies have shown that particles denser than the fluid do not uniformly distribute but instead cluster in high-strain regions due to various mechanisms. These include centrifugal forces, where particles are expelled from rotating fluid regions[1–3]; the "sweep-stick" mechanism, in which particles stick to acceleration stagnation points and are swept following the local fluid velocity[4]; and the path-history effect, a non-local phenomenon where clustering arises from the statistical asymmetry in the paths of converging and diverging particle pairs[5].

Moreover, the relative velocities of particles at small separations increase substantially as the Stokes number (the ratio between particle relaxation time and Kolmogorov timescale) increases, particularly when it exceeds a threshold of order one[6]. Consequently, the relative velocity of inertial particle pairs is significantly larger than the fluid's relative velocity at the same separation. This leads to the formation of the so-called caustics, which arise when the phase-space manifold folds, causing the particle velocity at a given point to become multi-valued, leading to large velocity differences between nearby particles. At the edge of a caustics, the particle velocity gradient becomes singular, with its trace diverging to minus infinity.

The identification of caustics in particle-laden turbulent flows has been extensively studied in recent decades using both Eulerian-Lagrangian (e.g. ref. [7]) and Eulerian-Eulerian simulations (e.g. ref. [8]), normally in the one-way coupling regime, non considering particle feedback, collisions and settling. The compressibility of particle velocity or particle number density in both Eulerian and Lagrangian forms is often analysed by performing an order-of-magnitude analysis of the divergence of the particle velocity. In numerical simulations, caustics are typically identified when the magnitude of this divergence significantly exceeds an assumed threshold. An Eulerian approach was used also by Lee et al.[9] to study the effect of settling. They found that caustics are more likely to form in regions with strong compressive and weak stretching motion. To identify blow-ups, i.e. singularities in finite time, they also studied the dynamics of the particle velocity gradient tensor in terms of its eigenvalues.

Recently, the concept of thermal caustics has been introduced by Carbone et al.[10] and Saito et al.[11] to describe the observed behaviour of fluid-particle thermal interactions. From the analysis of structure functions, it has been noted that the temperature difference between particle pairs is significantly larger than the fluid temperature difference at the same separation, leading to a non-smooth behaviour in particle temperature, even at moderate thermal Stokes numbers. This phenomenon, which is akin to the behaviour of velocity differences between particle pairs, has been attributed to the formation of thermal caustics and to the influence of the path history on temperature differences between particle pairs. It has been used by Li et al.[12] to interpret the role of settling, which changes the way particles sample the fluid, on particle temperature statistics.

In this work, we discuss the formation of thermal caustics on the basis of the dynamics of particle temperature gradient in the configuration space, to underline the leading mechanisms which lead to their formation, and the role of particle inertia and thermal inertia in the process.

The motion of a set of small heavy spherical particles suspended in a flow, much denser than the fluid and much smaller than any relevant flow scale, can be described by a simplified version of the Maxey-Riley equations[13] where only the Stokes drag is retained, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{X}_p(t) = \boldsymbol{V}_p(t), \tag{1}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{V}_p(t) = \frac{1}{\tau_v}\left(\boldsymbol{u}(t,\boldsymbol{X}_p) - \boldsymbol{V}_p(t)\right), \tag{2}$$

where $\boldsymbol{X}_p(t)$ and $\boldsymbol{V}_p(t)$ are the position and velocity of the p-th particle, while $\boldsymbol{u}(t,\boldsymbol{X}_p)$ is the fluid velocity at particle position. The coefficient

$$\tau_v = \frac{2}{9}\frac{\rho_p}{\rho_0}\frac{R^2}{\nu}, \tag{3}$$

where R is the particle radius and ν is the fluid kinematic viscosity, is the particle momentum relaxation time. When the fluid-particle thermal interaction is taken into account, under the same hypotheses the evolution of the particle temperature $\Theta_p(t)$ is described by

$$\frac{\mathrm{d}}{\mathrm{d}t}\Theta_p(t) = \frac{1}{\tau_\vartheta}\left(T(t,\boldsymbol{X}_p) - \Theta_p(t)\right) \tag{4}$$

where $T(t,\boldsymbol{X}_p)$ is the fluid temperature at particle position, and coefficient τ_ϑ is the thermal relaxation time

$$\tau_\vartheta = \frac{1}{3}\frac{\rho_p c_{pp}}{\rho_0 c_{p0}}\frac{R^2}{\kappa}, \tag{5}$$

where c_{pp} and c_{p0} are the particle and fluid specific heat capacities at constant pressure and κ is the fluid thermal diffusivity. In the dilute limit, particles are so far away that they do not interact hydrodynamically, and for very dilute suspension, with a particle volume fraction of no more than around 10^{-6}, particle forces and thermal feedback on the flow can be neglected. In this situation the velocity and temperature of the carrier flow become independent of the presence of suspended particles and equations (1-4) become a linear system of equations with a time dependent external forcing. The dynamics of the particle is determined by the ratio between their momentum and thermal relaxation times and the flow timescale, in particular in a turbulent flow with the Kolmogorov timescale τ_η, so that in dimensionless form by the Stokes and thermal Stokes numbers, $\mathrm{St} = \tau_v/\tau_\eta$ and $\mathrm{St}_\vartheta = \tau_\vartheta/\tau_\eta$ where $\tau_\eta = (\nu/\varepsilon)^{1/2}$.

Gradient dynamics is a convenient tool to describe the small-scale behaviour of turbulence, and as such it has been largely investigated in the literature due to its theoretical and practical importance,[14–16] and particle velocity gradient has been considered to study particle clustering, collisions and the formation of caustics.[17–19] Following a well established formalism[17,20,21], we can consider $\boldsymbol{X}_p$, $\boldsymbol{V}_p$ and Θ_p as state variables for particles, and derive the field representation of the particle phase dynamics in the configuration space, often called a "synthetic" representation. It can be obtained under the assumption that the probability density function of particles can be factored as $\mathscr{P}(t,\boldsymbol{x},\boldsymbol{v},\vartheta) = \delta(\boldsymbol{x}-\boldsymbol{X}_p)\delta(\boldsymbol{v}-\boldsymbol{V}_p)\delta(\vartheta-\Theta_p)$, i.e. that particle velocity and temperature are uniquely determined by the position. By introducing this factorization into the transport equation[22–24] for $\mathscr{P}$, the resulting equations for the particle concentration, mean velocity and temperature fields in the configuration space are

$$\frac{\mathrm{D}_p}{\mathrm{D}t}n(t,\boldsymbol{x}), = -n\nabla\cdot\boldsymbol{v} \tag{6}$$

$$\frac{\mathrm{D}_p}{\mathrm{D}t}\boldsymbol{v}(t,\boldsymbol{x}) = \frac{1}{\tau_v}\left(\boldsymbol{u}(t,\boldsymbol{x}) - \boldsymbol{v}(t,\boldsymbol{x})\right), \tag{7}$$

$$\frac{\mathrm{D}_p}{\mathrm{D}t}\vartheta(t,\boldsymbol{x}) = \frac{1}{\tau_\vartheta}\left(T(t,\boldsymbol{x}) - \vartheta(t,\boldsymbol{x})\right), \tag{8}$$

where $\mathrm{D}_p/\mathrm{D}t = \partial/\partial t + \boldsymbol{v}\cdot\nabla$ is the material derivative along particle paths, defined by

$$\frac{\partial}{\partial t}\boldsymbol{x}(t,\tilde{\boldsymbol{X}}) = \boldsymbol{v}(t,\boldsymbol{x}), \qquad \boldsymbol{x}(0,\tilde{\boldsymbol{X}}) = \tilde{\boldsymbol{X}}.$$

For a generic flow the existence of $\boldsymbol{v}$ and ϑ is not guaranteed a priori, and it breaks when a caustics is formed. However, when these equations generate a smooth single-valued solution $(\boldsymbol{v},\vartheta)$, then the underlying assumption is valid and self-consistent. Moreover, caustics are concentrated in small regions in space and have a lifetime of order τ_v[19,25], so that these equations keep their validity before (and after) their formation. The formation of finite-time singularities in $\boldsymbol{v}$ and ϑ marks the formation of caustics and thermal caustics. Therefore, the problem of the generation of caustics and thermal caustics leads to the determination of the conditions under which the gradient of $\boldsymbol{v}$ or the gradient of ϑ have a finite time blow-up, so that equations (7) and (8) can still be used as a tool to analyze the path to caustics.

Therefore, we define the Eulerian particle velocity gradient tensor $\boldsymbol{\sigma} = \nabla\boldsymbol{v}$ and particle temperature gradient vector $\boldsymbol{\xi} = \nabla\vartheta$, whose components are

$$\sigma_{ij} = \frac{\partial v_i(t,\boldsymbol{x})}{\partial x_j}, \qquad \xi_j = \frac{\partial\vartheta(t,\boldsymbol{x})}{\partial x_j}.$$

An equation for the gradient of particle temperature and velocity can be derived by taking the gradient of equations (7) and (8). The gradient of (8) leads to

$$\frac{\partial\xi_k}{\partial t} + v_j\frac{\partial\xi_k}{\partial x_j} + \sigma_{jk}\xi_j = \frac{G_k - \xi_k}{\tau_\vartheta}$$

where $\boldsymbol{G} = \nabla T$ is the Eulerian fluid temperature gradient, or, in vectorial notation,

$$\frac{\mathrm{D}_p}{\mathrm{D}t}\boldsymbol{\xi} = \frac{\boldsymbol{G}-\boldsymbol{\xi}}{\tau_\vartheta} - \boldsymbol{\sigma}^T\boldsymbol{\xi}. \tag{9}$$

Analogously, the gradient of equation (7) gives the particle velocity gradient tensor evolution equation,[6,26]

$$\frac{\mathrm{D}_p}{\mathrm{D}t}\boldsymbol{\sigma}(t) = \frac{\boldsymbol{A}-\boldsymbol{\sigma}}{\tau_v} - \boldsymbol{\sigma}^2, \tag{10}$$

where $\boldsymbol{A} = \nabla\boldsymbol{u}$ is the fluid velocity gradient. The dynamics of $\boldsymbol{A}$ and $\boldsymbol{G}$ can be obtained from the gradient of Navier-Stokes equations (e.g. Zhang et al.[27]),

$$\frac{\mathrm{D}}{\mathrm{D}t}\boldsymbol{A} = -\frac{1}{\rho_0}\boldsymbol{H} + \nu\nabla^2\boldsymbol{A} - \boldsymbol{A}^2, \tag{11}$$

$$\frac{\mathrm{D}}{\mathrm{D}t}\boldsymbol{G} = \kappa\nabla^2\boldsymbol{G} - \boldsymbol{A}^T\boldsymbol{G}, \tag{12}$$

where $\mathrm{D}/\mathrm{D}t = \partial/\partial t + \boldsymbol{u}\cdot\nabla$ is the fluid material derivative, and $H_{ij} = \partial^2 p/\partial x_i\partial x_j$ denotes the pressure Hessian. The velocity gradient is enhanced by the non-linear and local term $-\boldsymbol{A}^2$ stretching-tilting term in (11) and is damped by both diffusion and the non-local pressure Hessian term, which acts in a way to reorientate the fluid velocity gradient tensor[14,28,29], while, on the contrary, the temperature gradient is only driven by the stretching due to the velocity gradient and the diffusion (e.g. Xhang et al.[27]). Both equations are not closed from a Lagrangian point of view, because all the spatial derivatives are unknown, and both the diffusive terms and the pressure

Hessian require modelling. Still they are they key for the understanding of small-scale phenomena, and the basis for stochastic models, which have been able to reproduce some important features, like the onset of a non Gaussian probability density function, intermittency, the average alignments of vorticity and strain-rate.

Equations (11-12) and equations (9-10) show a fundamental difference, due to the lack of stabilizing terms in the particle gradient equations (9-10), like the diffusion and pressure Hessian, which can prevent a finite time blow-up in the fluid equations. The properties of equations (10) have been studied in many papers[6,20,30], which have highlighted the role of the quadratic term on the right-hand side, which leads to singularities, called also sling effect[25], in which the trace of $\boldsymbol{\sigma}$ diverges to $-\infty$, producing also a singularity in particle concentration through (6). Gustavsson et al.[20] discussed how the dynamics of σ_{ij} can explain the formation of velocity caustics through the sling effect when particle Stokes number exceeds the unity and becomes very large ($\mathrm{St} \to \infty$), a situation which allows to use the hypothesis of random uncorrelated motion. Ravichandran et al.[31] related caustics with enhanced collision rates of droplets in clouds, and Esmaily and Ali Mani[32] derived an asymptotic solution for the rate of contraction of a cloud of inertial particles in regimes relevant to turbulent flows, predicting a maximum rate of contraction when the Stokes number is $\mathscr{O}(1)$. Recently, by using they employed optimal fluctuation, Meibohm et al.[33] found that caustics can be formed even at the very low inertia range, when $\mathrm{St} \ll 1$, by a spatial instability in particles neighbourhoods. Finally, Bätge et al.[19] gave a quantitative prediction of the rate of sling events based on the velocity gradient history along particle paths.

On the contrary, equation (9), which can be used to characterize the formation of thermal caustics for heavy particles, has never been considered. Along each particle Lagrangian path, the linearity of (9) makes that no singularity can arise in finite time unless the coefficients, $\boldsymbol{G}$ and $\boldsymbol{\sigma}$ become singular. But we already know that $\boldsymbol{G}$ cannot become singular due to the presence of the diffusive term in the fluid temperature gradient equation, so that the only source of singularity is $\boldsymbol{\sigma}$. In case of slowly varying $\boldsymbol{G}$ and $\boldsymbol{\sigma}$, particle temperature gradient tends to relax to an equilibrium gradient given by

$$\boldsymbol{\xi}_e = \left[\boldsymbol{I} + \tau_\vartheta \boldsymbol{\sigma}^T\right]^{-1} \boldsymbol{G}. \tag{13}$$

A unique equilibrium state exists, for any given temperature gradient $\boldsymbol{G}$, only if the operator

$$\boldsymbol{M} = \boldsymbol{I} + \tau_\vartheta \boldsymbol{\sigma}^T \tag{14}$$

can be inverted, i.e. if $-\tau_\vartheta$ is not an eigenvalue of $\boldsymbol{\sigma}$, which is verified if the flow timescales are much larger than the particle thermal relaxation time. Formally, equation (9) has an analytical solution provided that $\boldsymbol{G}$ and $\boldsymbol{\sigma}$ are known functions along particle Lagrangian paths: the general solution of (9) can be expressed as[34]

$$\boldsymbol{\xi}(t,\tilde{\boldsymbol{X}}) = \boldsymbol{\Phi}(t;t_0,\tilde{\boldsymbol{X}})\boldsymbol{\xi}(t_0) + \frac{1}{\tau_\vartheta}\int_{t_0}^{t} \boldsymbol{\Phi}(t;s,\tilde{\boldsymbol{X}})\boldsymbol{G}(s,\tilde{\boldsymbol{X}})\mathrm{d}s, \tag{15}$$

where $\boldsymbol{\Phi}(t,t_0)$ is the transfer operator, given by the solution of

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Phi}(t;t_0,\tilde{\boldsymbol{X}}) = -\frac{1}{\tau_\vartheta}\boldsymbol{M}(t,\tilde{\boldsymbol{X}})\boldsymbol{\Phi}(t;t_0,\tilde{\boldsymbol{X}}), \tag{16}$$

$$\boldsymbol{\Phi}(t_0;t_0,\tilde{\boldsymbol{X}}) = \boldsymbol{I}. \tag{17}$$

This formal solution explicitly shows that the evolution of $\boldsymbol{\xi}$ is driven by the fluid temperature gradient $\boldsymbol{G}$, modulated by the $\boldsymbol{M}$ along particle paths. Thus, the properties of the operator $\boldsymbol{M} = \boldsymbol{I} + \tau_\vartheta \boldsymbol{\sigma}$ govern the dynamics of the particle temperature gradient. Since $\boldsymbol{G}$ is a smooth field, albeit possibly strongly intermittent, $\boldsymbol{M}$ determines the possibility for the formation of thermal caustics. Therefore, the evolution of $\boldsymbol{\xi}$ is dictated by the interplay between the thermal relaxation time and the particle velocity gradient which, unless buoyancy forces are significant, is independent from the particle temperature. A low but non-zero thermal inertia can mitigate the effect of an increase in $||\boldsymbol{\sigma}||$ but cannot entirely suppress a singularity of the particle velocity gradient.To identify thermal caustics, it is more straightforward to consider the only scalar invariant of $\boldsymbol{\xi}$, its norm. The scalar product of equation (9) by $\boldsymbol{\xi}$ gives

$$\frac{\tau_\vartheta}{2}\frac{\mathrm{D}_p}{\mathrm{D}t}||\boldsymbol{\xi}||^2 = -\boldsymbol{\xi}\cdot\left[\boldsymbol{I} + \tau_\vartheta \boldsymbol{\sigma}_S\right]\boldsymbol{\xi} + \boldsymbol{\xi}\cdot\boldsymbol{G}, \tag{18}$$

where $\boldsymbol{\sigma}_S = (\boldsymbol{\sigma} + \boldsymbol{\sigma}^T)/2$ is the symmetric part of the particle velocity gradient, i.e. the strain experienced by particles.

Since $\boldsymbol{\sigma}_S$ and $\boldsymbol{I}$ commute, the eigenvectors of the symmetric part of $\boldsymbol{M}$ coincide with the eigenvectors of the particle strain rate tensor, and its eigenvalues are given by $1 + \tau_\vartheta \lambda_i$, where λ_i are the eigenvalues of the symmetric part of particle velocity gradient tensor $\boldsymbol{\sigma}_S$. Let us call $\lambda_1 \geq \lambda_2 \geq \lambda_3$ the three real eigenvalues of $\boldsymbol{\sigma}_S$. Their sum is the divergence of the particle velocity field, which tends to be negative because particles heavier than the fluid tend to sample regions with high strain and low vorticity — as, for small inertia, $\nabla\cdot\boldsymbol{\sigma} \simeq -\tau_v(||\boldsymbol{S}||^2 - ||\boldsymbol{\Omega}||^2)$ — and tends to vanish for $\tau_v \to 0^+$, when particles sample uniformly the fluid. Thus, we may assume that almost everywhere the first eigenvalue is positive, the last one is negative and the second one can be either positive or negative.[19]

In the equation (18) the alignment of $\boldsymbol{\xi}$ with $\boldsymbol{\sigma_S}$ and $\boldsymbol{G}$ plays a crucial term in the evolution of $\boldsymbol{\xi}$. The alignment with $\boldsymbol{\sigma_S}$ can be computed by mustering the angel between $\boldsymbol{\xi}$ and the principal eigenvectors of $\boldsymbol{\sigma_S}$, similar the approach is used in order to capture the alignment between the fluid vorticity and the eigenvectors of fluid strain-rate tensor. Therefore, we can assume that for three eigenvalues λ_1, λ_2 and λ_3 which are ordered such that $\lambda_1 \geq \lambda_2 \geq \lambda_3$, $\boldsymbol{p}_1$ $\boldsymbol{p}_2$, and $\boldsymbol{p}_3$ denote the corresponding eigenvectors. Now, we are able to see the stretching or compressing of $||\boldsymbol{\xi}||$ in the directions of the eigenvectors of $\boldsymbol{\sigma_S}$. In the principal frame of $\boldsymbol{\sigma_S}$ first term in right-hand side of (18) is expresses as

$$-\left[\left(\frac{1}{\tau_\vartheta} + \lambda_1\right)\xi_1^2 + \left(\frac{1}{\tau_\vartheta} + \lambda_2\right)\xi_2^2 + \left(\frac{1}{\tau_\vartheta} + \lambda_3\right)\xi_3^2\right]. \tag{19}$$

Since $\lambda_i \geq \lambda_3\ \forall i$, we obtain the following estimate for the solution of the magnitude of $\boldsymbol{\xi}$ from the equation (18),

$$-(1+\tau_\vartheta\lambda_1)\,||\boldsymbol{\xi}||^2 \lesssim \frac{\tau_\vartheta}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,||\boldsymbol{\xi}||^2 - \boldsymbol{G}\cdot\boldsymbol{\xi} \lesssim -(1+\tau_\vartheta\lambda_3)\,||\boldsymbol{\xi}||^2\,. \tag{20}$$

The norm decays when $\lambda_3 > -1/\tau_\vartheta$, and a growth, bounded by $\exp(-(1+\tau_\vartheta \inf\{\lambda_3\})(t-t_0))$ is possible only when $\lambda_3 > -1/\tau_\vartheta$. Consequently, we can say that when $\boldsymbol{\sigma}$ remains bounded, then a smooth solution of the equation (18) exists, implying that no thermal caustics occur.

If the case a thermal caustics occurs, both $||\boldsymbol{\xi}||$ and its time derivative diverge to $+\infty$. Since $\boldsymbol{G}$ is a smooth, even if intermittent, field, the bounds to the growth of $||\xi||$ are determined only by λ_3.

Therefore, the only way a thermal caustics can form is when $\boldsymbol{\sigma}$ is not smooth and has a finite time singularity. As discussed in Ref. [19], the dynamics of the trace of $\boldsymbol{\sigma}$ is dictated by the smallest eigenvalues of $\boldsymbol{A}$, which in turn determines the behaviour of the smallest eigenvalue of $\boldsymbol{\sigma}$, making it diverge. In such a case, it is possible to reduce the problem into a one-dimensional problem, corresponding to a projection on the smallest eigenvalue eigenvector of $\boldsymbol{A}$. Analogously to the onset of caustics in particle velocity field,[9,19] two stages of evolution can be individuated: until $|\sigma| \ll 1/\tau_v$ the nonlinear terms in the equation for $\boldsymbol{\sigma}$ can be neglected and its growth can be approximated by the solution of the linearized equation. By assuming that the timescale of variation of $\boldsymbol{A}$ and $\boldsymbol{G}$ is larger than the timescale of the variation of the particle gradients, dictated by the Stokes relaxation time, so that it is possible to consider a sort of "frozen" flow approximation, it gives an exponential growth

$$\sigma \simeq \int_0^t A(t')\exp(-(t-t')/\tau_v)\mathrm{d}t'. \tag{21}$$

When $|\sigma| \sim 1/\tau_v$ nonlinear terms become significant and when $|\sigma| \gg 1/\tau_v$ they are the dominant term so that $\dot{\sigma} \simeq -\sigma^2$, which leads to finite-time blowup

$$\sigma \simeq C_0(t-t_*)^{-1}. \tag{22}$$

If $\sigma(0)$ is given, we can determine C_0, i.e. the scaling factor related to the initial value of σ and the time of blowup t_*, by evaluating equation (22) at $t=0$. Therefore, we can have $\sigma(0) \simeq -C_0/t_*$. If we impose the initial value as $\sigma(0) = -1/\tau_v$, we can have $C_0 = t_*/\tau_v$. Note that in the equation (22) we assumed that the sufficient condition for caustics is met by considering $C_0 > 0$ leading to exponential growth of σ. This implies that t_* being positive ensuring the blowup occurs at a positive time. This indicates that as t approaches t_*, σ increases rapidly and diverges to $-\infty$, leading to a blowup.

The same analysis, indeed for the first time, is performed here for the particle temperature gradient to characterize the thermal caustics. Accordingly, the one-dimensional version of the temperature gradient equation is

$$\dot{\xi} = -\left[\frac{1}{\tau_\vartheta} + \sigma\right]\xi + \frac{G}{\tau_\vartheta}, \tag{23}$$

which could be obtained by projection onto the eigenvector of the smallest eigenvalue of σ_S. In the second stage of the caustics formation we have

$$\dot{\xi} \simeq -\left[\frac{1}{\tau_\vartheta} + \frac{C_0}{t_*-t}\right]\xi + \frac{G}{\tau_\vartheta}, \tag{24}$$

so that from eq. (15), since $|\sigma\xi| \gg |G|/\tau_\vartheta$ when a caustics is approached, the particle temperature gradient is given by

$$\xi(t) \simeq \xi_0 \exp(-t/\tau_\vartheta)\,|1-t/t_*|^{-t_*/\tau_v}\,. \tag{25}$$

Therefore any thermal inertia (whatever small) cannot prevent the formation of a thermal caustic. However, in the limit $\tau_\vartheta \to 0^+$ there is no caustic, as the solution is $\xi = G$ and G is a smooth, even if intermittent, field. The condition for a growth of ξ is that $\sigma < -1/\tau_\vartheta$, so that a small thermal inertia can delay the begin of the growth dominated by σ which brings to the blowup.

In Carbone et al.[10] a lower intermittency at small St_ϑ has been observed from the probability density function of the particle temperature and in the exponents of the structure functions, which can be seen as a signature of the fact that thermal caustics have a lower impact on the statistics in this range of thermal inertia. Note that the $\exp(-t/\tau_\vartheta)$ factor in eq. eq. (25), even if it cannot suppress the formation of thermal caustics, can reduce the duration of the caustics event, i.e. the time during which $||\xi||$ has a high value (e.g. above a predetermined threshold in numerical simulations), thus reducing the intermittency observed in simulations. Thus a low but non zero thermal inertia reduces the impact of caustics on the statistics of particle temperature by reducing the life of thermal caustics. However, the thermal caustics formation rate remains the same, because it is equal to the caustics formation rate, which depends only on the Stokes and Reynolds numbers[19].

To verify the validity of our conclusions we have analyzed the data from direct numerical simulations of homogeneous and isotropic turbulence, in the same flow configuration as Ref. [10], i.e. with a Taylor-microscale Reynolds number around 90 and unit Prandtl number. The flow is solved with the same code, which uses a pseudo-spectral method with a second order exponential Runge-Kutta time integration and fourth order B-spline interpolations[35,36]. A double spatial and temporal resolution has been used to improve the numerical accuracy of the solution of the small-scales of the flow. Although only the solution of the equations (9) and (10) for particle gradients along particle paths would give a complete picture of the statistical behaviour of $\boldsymbol{\xi}$, and show that a thermal caustics occurs whenever a caustics occurs if $\tau_\vartheta > 0$, but cannot occur when $\tau_\vartheta = 0$, some conclusions can be drawn just looking at the temperature difference between colliding particles. Indeed, since a collision is a caustic, collisions can be used as indicators of the occurrence of caustics, without the need to track $\boldsymbol{\xi}$ along particle trajectories. If there would be no thermal caustics when a caustics occurs, then the particle temperature field would be smooth and the temperature difference between colliding particles would approach zero.

Figure 1 shows the probability density function of the temperature difference at various Stokes and thermal Stokes num-

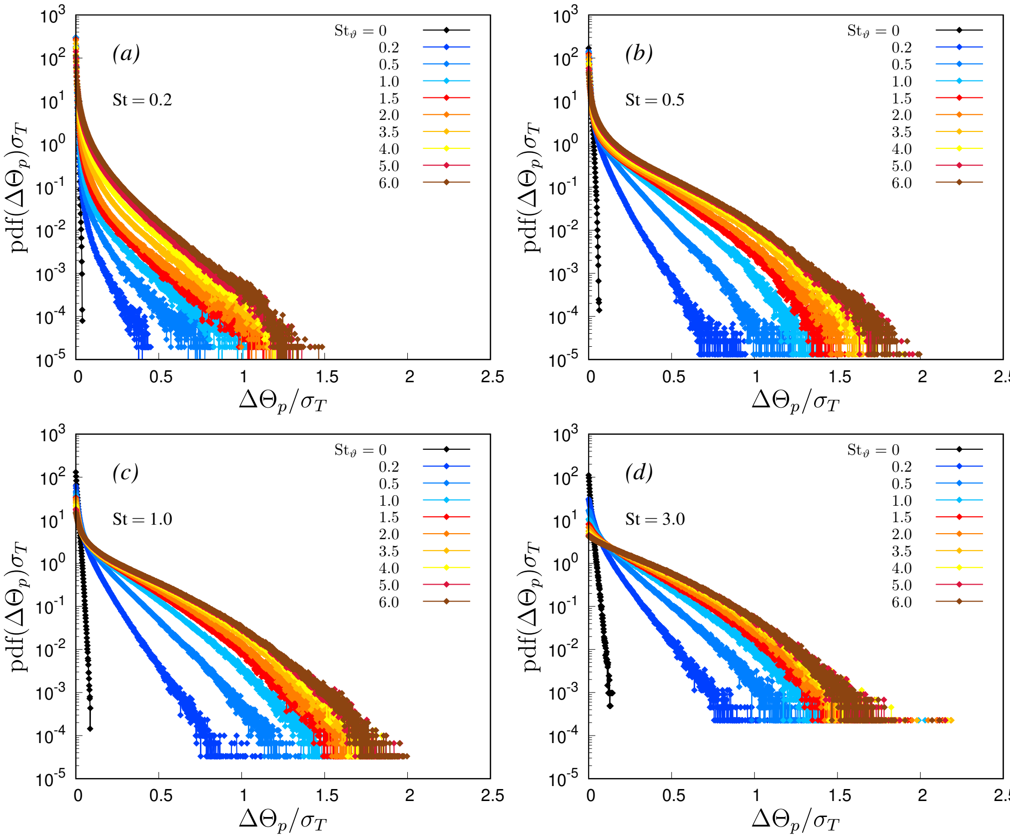

FIG. 1. Probability density function of particle temperature difference $\Delta\Theta_p$ between colliding particles at different Stokes numbers and thermal Stokes numbers, normalized with the carrier fluid temperature standard deviation σ_T: (a) St $= 0.2$, (b) St $= 0.5$, (c) St $= 1$, (d) St $= 3$. The black lines correspond to thermal tracers, $\tau_\vartheta = 0$.

ber in the one-way coupling regime, normalized with the standard deviation of fluid temperature fluctuations. According to the previous discussion, for any positive thermal Stokes number a caustics is always associated to a thermal caustic. Therefore, as expected, all the pdf shows a wide tail, which widens for increasing St and St_ϑ, indicating the relatively high probability of large temperature differences during collision. To remove any bias due to numerical approximations in the trajectories and temperatures of colliding particles, we have considered also the case of thermal tracers, i.e. of particles with no thermal inertia ($\tau_\vartheta \to 0$ and $\mathrm{St}_\vartheta \to 0$) but finite non-zero inertia ($\tau_v > 0$ and $\mathrm{St} > 0$) (black curves). Since a collision occurs when the particles are at a distance equal to their diameter, in case of thermal tracers, whose temperature is equal to the fluid temperature, the temperature difference $\Delta\Theta_p = |\Theta_1 - \Theta_2|$ between two colliding particles without thermal inertia is $\Delta\Theta_p \simeq |\nabla T \cdot (\boldsymbol{X}_1 - \boldsymbol{X}_2)| \leq 2R||\nabla T||$, so that is at most of order $2R||\nabla T||$, and thus its should follow closely the statistics of the fluid temperature gradient. In fact, the pdf of the thermal tracer is much narrower than the one at any St_ϑ for the same St. They closely resemble the ones of the fluid temperature derivatives (see Ref. [10]), and widen with St as, all the other parameters being equal, $R \propto \mathrm{St}^{1/2}$.

A simple quantitative evaluation of the qualitatively different behaviour at $\mathrm{St}_\vartheta = 0$ and $\mathrm{St}_\vartheta > 0$ can be obtained from the non centered moments of the temperature difference at collision. Figure 2 shows the variance $\langle \Delta\Theta_p^2 \rangle$ as a function of St_ϑ for different values of St. The horizontal lines indicate the maximum possible value of this variance for a thermal tracer for the different Stokes numbers, $4R^2\langle||\nabla T||^2\rangle = 12R^2\langle(\partial T/\partial x_1)^2\rangle$, which is the reference threshold for identifying caustics from collisions. While the simulated thermal

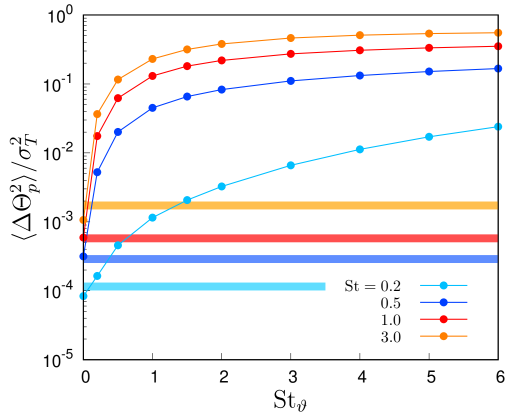

FIG. 2. Second order moment of the temperature difference at collision, normalized with the carrier fluid temperature standard deviation σ_T. The thick horizontal lines correspond to the limit finite size thermal tracers for each Stokes number.

tracers remain all below this threshold (within numerical uncertainty), all simulations with a finite thermal inertia show a higher variance. At $\mathrm{St} = 0.5$ and above, it appears as a sort of discontinuous behaviour, whereas a smoother transition appears only at the lowest simulated St. However in this case the caustics frequency is much lower[19] and, consequently, caustics contribute less to the variance, which, anyway, still always remains above the threshold for any $\tau_\vartheta > 0$, indicating the presence of multivalued regions.

In conclusion, we have shown that caustics inherently lead to the formation of thermal caustics, except in the limit case of zero thermal inertia, because in such a case particle temperature becomes independent of particle velocity. This is a sort of singular limit in the sense of asymptotic perturbation. This is in agreement with the attribution of the formation of thermal caustics to the influence of the path history on the temperature difference between particles,[10] particularly pronounced at higher thermal Stokes numbers. In fact, particle temperature is determined by its interaction with the carrier fluid, and particles keep memory of the fluid temperature they encountered along their path up to times $\mathscr{O}(\tau_\vartheta)$ in the past. As a result, necessary condition to have a thermal caustics is that a caustics occurs and that $\tau_\vartheta > 0$, so that the two colliding particles have experienced different fluid temperatures in a $\mathscr{O}(\tau_\vartheta)$ time before the collision, making the particle temperature multivalued in correspondence of the caustics.

Data availability — The data that support the findings of this study are available from the authors upon reasonable request.

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