An Extended Moment Method for Crossing Polydisperse Sprays

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Abstract

A moment method for the modelling of polydisperse sprays is developed that captures the polydisperse nature of sprays as well as the bi- (or multi-) modal character of the droplet velocity distribution, for example, when droplets cross each other in a turbulent spray flow. This Eulerian method is a combination of the quadrature-based moment method of Desjardins et al. [1] and the sectional method of Dufour and Villedieu [2]. For the highly unsteady spray behaviour in combustion chambers of car or aeroplane engines, the methodologies of CFD are not matured. In the lean combustion technology in new airplane engines, for example, combustion instabilities are more likely to occur and hence unsteady LES calculations are necessary to predict the behaviour of the reactive, two-phase flow system. The two main approaches used to describe the gas-liquid behaviour in combustion systems are the Euler-Lagrange and the Euler-Euler method. For the spray part, the Lagrangian procedure is widely used, also for unsteady flows but it is limited by the immense computer power which is necessary to obtain results that are not disturbed by statistical noise. In addition, the parallelisation of the Lagrange code leads, for inhomogeneous spray distributions in the computational domain, to an unbalanced workload distribution on the processors. For the Eulerian procedure, on the other hand, the same number of equations has to be solved irrespective of the amount of droplets in the computational domain. The bad news about Eulerian methods is the difficulty to capture droplet size effects like breakage, coalescence, etc. Moreover, the phenomenon of particle trajectory crossing, which is present in turbulent spray flows, was only considered recently by Desjardins et al. [1] for monodisperse sprays.

The combined moment method is tested in three one-dimensional configurations which are organised in such a way that crossing of two spray distributions is always included. In the first test case the polydisperse spray hits a wall, where the droplets break, lose mass and rebound with a certain velocity. In a second test case, two spray distributions are moving towards each other entering the domain with different velocities from $x = 0$ and $x = 1$. During this crossing motion they are evaporating. In the last test case the crossing distributions are affected by a Stokes drag force which results from the velocity difference between the moving droplets and the non-moving gas. For all three test cases parameter studies have been performed for the physical parameters and for the discretisation in real and size space (shown in this paper). In the above test cases, the comparison of the moment method with accurate Lagrangian calculations reveals a convincing agreement even for crude discretisation in size space. This method opens a new way of describing unsteady spray phenomena with Eulerian methods, because it resolves the principle difficulties of classical Eulerian methods, namely the description of polydisperse and crossing sprays.

Introduction

In this work a new method for the prediction of spray phenomena is presented which can be regarded as an alternative to the 'classical' Lagrangian and Eulerian procedures. It will be demonstrated that this method captures the polydisperse nature of sprays as well as the coexistence of two (or more) droplet velocities at one location.

The Lagrangian procedure (cf. [3]), also called particle stochastic method, solves the kinetic spray equation by solving the motion of a large number of numerical particles, called parcels, in phase space. For highly unsteady flows, this method requires a nearly unmanageable amount of parcels to deliver smooth statistics. In addition, the parallelisation technique of dividing the computational domain into equisized sub domains does not ensure the desired linear scaling of the computational time with processors.

Describing the spray behaviour with an Eulerian method, i.e. solving balance equations for various densities of physical droplet quantities at each point of the domain, has the advantage, that irrespective of the amount of droplets in a region, the same number of equations always have to be solved. Consequently, the above problem of parallelisa-

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tion does not arise and the unsteady character of the flow can be treated with higher order time and space discretisations. Nevertheless, the application of an Eulerian description has its limitations. By using a two fluid model, i.e. solving two superposed and coupled sets of Navier-Stokes-like equations to describe the droplet and gas behaviour (cf. [4]), the polydisperse character of the spray can only be captured in a very crude manner. One way to resolve this problem is the sectional method (cf. [5,6,2]), which is able to predict polydisperse effects of the droplets accurately. Still, it does not allow the dispersion of droplet velocities at one location which is necessary, for example, to capture the crossing of two dilute sprays. Recently, in [1] a quadrature-based moment method was proposed that overcomes this drawback by solving balance equations not only for the number, mass and momentum densities but also for higher order moments of the droplet number density function.

After introducing a kinetic model for polydisperse sprays in Section 2, the idea of Desjardins et al. [1] is followed and combined with the propositions of Dufour & Villedieu [2] in Section 3. This combination allows for the description of changes in the droplet size distribution and at the same time considers the droplet velocity dispersion at one location. In Section 4 the new moment method is compared to reference Lagrangian calculations, in a one-dimensional setting, where droplets are reflected on a wall but break and lose mass and momentum (hereafter called splashing). In a second and third configuration two crossing spray distributions are, first, decelerated by a Stokes drag force, and then evaporated according a d^2-law. Conclusions are drawn in Section 5.

Mathematical Model for Polydisperse Sprays

Similar to the description of molecules in the kinetic gas theory, Williams [7] proposed a general type of equation to model the behaviour of spray systems. Here, the reduced version

$$\frac{\partial f}{\partial t}+\frac{\partial (vf)}{\partial x}+\frac{\partial (\mathrm{F}\, f)}{\partial v}+\frac{\partial (\mathrm{K}\, f)}{\partial s}=0 \qquad (1)$$

of the general spray model is used which, for simplicity, does not include the thermodynamic and interaction behaviour of droplets. In equation (1), f is a function of time t, space x, droplet velocity v and a scalar that characterises the droplet size s (here, the droplet surface). It is physically interpreted as number of droplets per infinitesimal volume $[x,\ x+dx]\times[v,\ v+dv]\times[s,\ s+ds]$ and is therefore called number density function (NDF). The forces on the droplets of the type $\mathrm{F}=(U_g(t,x)-v)/\tau_\mathrm{d}(s,v)$, which excludes gravity, buoyancy and other, more subtle forces are considered. The above drag force model includes the velocity difference between a droplet and the gas, and the relaxation time of the droplets in the surrounding gas, τ_d. In the remainder of this note the one-dimensional version of equation (1) is dealt with,

$$\frac{\partial f}{\partial t}+\frac{\partial (vf)}{\partial x}+\frac{\partial}{\partial v}\left(\frac{U_g-v}{\mathrm{St}(s,v)}\,f\right)-\frac{\partial (\mathrm{Ev}\, f)}{\partial s}=0\,, \qquad (2)$$

in which all quantities are disposed of their units. For the definition of the Stokes number, $\mathrm{St}=\tau_\mathrm{d}/\tau_\mathrm{g}$, and the evaporation number, $\mathrm{Ev}=\tau_\mathrm{g}/\tau_\mathrm{ev}$, the characteristic time scales for the gas flow, τ_g and for the evaporation, $\tau_\mathrm{ev}:=-S^*/\mathrm{K}$, are introduced. S^* represents a characteristic surface (here, the maximum surface).

Moment Closure

The moment transform in s- and v space is performed by using the set of moments (cf. [1,2])

$$V_k=\left\{\mathrm{M}^{(k)}_{0,0},\mathrm{M}^{(k)}_{3/2,0},\mathrm{M}^{(k)}_{3/2,1},\mathrm{M}^{(k)}_{3/2,2},\mathrm{M}^{(k)}_{3/2,3}\right\},\qquad \text{with} \qquad (3)$$

$$\mathrm{M}^{(k)}_{K,L}=\int_{s_k}^{s_{k+1}} s^K \int_{-\infty}^{\infty} v^L\, f(t,x,s,v)\,dv\,ds\,, \qquad (4)$$

in each of the *N* fixed intervals $I_k = [s_k, s_{k+1}] \subset [0,1]$, called sections. The balance equations for the above moments are derived by multiplying the reduced spray equation (2) with the appropriate powers of the phase-space variables and integrating the emerging equations over the whole velocity space and each section I_k. This set of 5*N* moment equations is not closed, because in the equation for $\mathrm{M}^{(k)}_{3/2,3}$ the unspecified moment $\mathrm{M}^{(k)}_{3/2,4}$ arises. In addition, the integrals $\left(\int_{s_k}^{s_{k+1}} s^K \int_{-\infty}^{\infty} v^L \frac{\partial}{\partial v}\left(\frac{U_g - v}{\mathrm{St}} \right) f \; dvds \right)$ and $\left(\int_{s_k}^{s_{k+1}} s^K \int_{-\infty}^{\infty} v^L \frac{\partial}{\partial s}\left(\mathrm{Ev}\, f \right) \; dvds \right)$ which are part of each of these equations can not be evaluated unless the generality of *f* has been reduced. Here, U_g is given by some analytical or numerical solution of the gas flow and St is modelled by the Stokes law.

The moment equations are closed by assuming the NDF to have the form

$$\tilde{f}(t,x,s,v) = \sum_{k=1}^{N} \exp(-b_k(t,x)s) \sum_{i=1}^{I} \mathbf{1}_{s_k \le s < s_{k+1}} a_k^i(t,x) \delta(v - U_k^i(t,x)) \tag{5}$$

with $I = 2$. This closure allows the emerging moment equations to be solved with the available numerical methods and, more importantly, it does not contradict the velocity dispersion and the polydisperse nature of sprays (see Section 4). Furthermore, it is to remark that, as indicated in (5), any value of *I* is admissible to describe the velocity dispersion at one location. If the NDF in the moment equations derived from (2) is replaced with its approximation $\tilde{f}$ the following closed system of equations for the set of moments V_k is obtained,

$$\begin{aligned}
&\frac{\partial}{\partial t}(\mathrm{M}^{(k)}_{0,0}) + \frac{\partial}{\partial x}(\mathrm{M}^{(k)}_{0,1}) = -\mathrm{Ev}\left(E^{(k,k)1}_{0,0} + E^{(k)2}_{0,0} \right) + \mathrm{Ev}\, E^{(k,k+1)1}_{0,0}, \\
&\frac{\partial}{\partial t}(\mathrm{M}^{(k)}_{3/2,0}) + \frac{\partial}{\partial x}(\mathrm{M}^{(k)}_{3/2,1}) = -\mathrm{Ev}\left(E^{(k,k)1}_{3/2,0} + E^{(k)2}_{3/2,0} \right) + \mathrm{Ev}\, E^{(k,k+1)1}_{3/2,0}, \\
&\qquad\qquad \vdots \\
&\frac{\partial}{\partial t}(\mathrm{M}^{(k)}_{3/2,3}) + \frac{\partial}{\partial x}(\mathrm{M}^{(k)}_{3/2,4}) = -\mathrm{Ev}\left(E^{(k,k)1}_{3/2,3} + E^{(k)2}_{3/2,3} \right) + \mathrm{Ev}\, E^{(k,k+1)1}_{3/2,3} \\
&\quad + 3 \int_{s_k}^{s_{k+1}} s^{3/2} \exp(-b_k s) \left[a_k^1 (U_k^1)^2 \frac{U_g - U_k^1}{\mathrm{St}(U_k^1, s)} + a_k^2 (U_k^2)^2 \frac{U_g - U_k^2}{\mathrm{St}(U_k^2, s)} \right] ds,
\end{aligned} \tag{6}$$

where $\mathrm{E}^{(\mathrm{k,m})1}_{\mathrm{K,L}}$ is an evaporation flux from section I_k to section I_{k-1} of moment $\mathrm{M}^{(k)}_{K,L}$ and $\mathrm{E}^{(\mathrm{k})2}_{\mathrm{K,L}}$ is a flux from section I_k to the gas. They are defined as

$$E^{(k,m)1}_{K,L} = s_m^K \exp(-b_k s_m) \sum_{i=1}^{2} a_k^i (U_k^i)^L, \qquad E^{(k)2}_{K,L} = K \int_{s_k}^{s_{k+1}} \int_{\mathbb{R}} s^{K-1} v^L \tilde{f} \, dvds \,. \tag{7}$$

In each section, $\tilde{f}$ is defined by five parameters that are linked to the moments in (3). It is straight forward to compute the moments in set V_k from the set of parameters,

$$W_k = \left[b_k, \left(a_k^1, U_k^1 \right), \left(a_k^2, U_k^2 \right) \right], \tag{8}$$

by simply inserting $\tilde{f}$ into definition (4) of the moments. The inverse problem of uniquely determining the parameters W_k from the moments V_k is the subject of following proposition. It constitutes the main part of the numerical algorithm and allows the treatment of the moment equations (6).

Proposition: *Let V_k be the set of moments defined in (3) and (4) such that*

$$(i)\ \mathrm{M}_{0,0}^{(k)} > 0\ ,\quad (ii)\ \mathrm{M}_{3/2,0}^{(k)} > 0\ ,\quad (iii)\ \mathrm{M}_{3/2,2}^{(k)} > \frac{\left(\mathrm{M}_{3/2,1}^{(k)}\right)^2}{\mathrm{M}_{3/2,0}^{(k)}} \quad \text{and} \quad (iv)\ \frac{\mathrm{M}_{3/2,0}^{(k)}}{\mathrm{M}_{0,0}^{(k)}} \in \left]s_k, s_{k+1}\right[, \tag{9}$$

then, up to a permutation between superscripts 1 and 2, there exists only one set moments W_k (see (8)) of parameters that solves the inverse problem. This solution is given by the inverse function

$$b_k = g_k^{-1}\left(\frac{\mathrm{M}_{3/2,0}^{(k)}}{\mathrm{M}_{0,0}^{(k)}}\right) \quad \text{with} \quad g_k(b) = \begin{cases} \dfrac{2}{5}\dfrac{\left(s_{k+1}^{5/2} - s_k^{5/2}\right)}{\left|I_k\right|}, & b = 0 \\ \dfrac{\int_{s_{k+1}}^{s_k} s^{3/2}\exp(-b_k s)ds}{\int_{s_{k+1}}^{s_k} e\exp(-b_k s)ds}, & b \neq 0 \end{cases} \tag{10}$$

and the relations

$$a_k^1 = (\tfrac{1}{2} + x_k)(\bar{\mathrm{M}}_{3/2,0}^{(k)}), \qquad a_k^2 = (\tfrac{1}{2} - x_k)(\bar{\mathrm{M}}_{3/2,0}^{(k)}),$$
$$U_k^1 = U_k^p - \left(\frac{a_k^2}{a_k^1}\right)^{1/2}\sigma_k^p, \quad U_k^2 = U_k^p + \left(\frac{a_k^1}{a_k^2}\right)^{1/2}\sigma_k^p, \quad x_k = \frac{q_k^p/2}{\left(\left(q_k^p\right)^2 + 4\left(\sigma_k^p\right)^6\right)^{1/2}}. \tag{11}$$

The quantities $\bar{\mathrm{M}}_{3/2,0}^{(k)}$, U_k^p, σ_k^p and q_k^p are defined by

$$\bar{\mathrm{M}}_{K,L}^{(k)} = \frac{\mathrm{M}_{K,L}^{(k)}}{\int_{s_k}^{s_{k+1}} s^{3/2}\exp(-b_k s)ds}, \quad U_k^p = \frac{\bar{\mathrm{M}}_{3/2,1}^{(k)}}{\bar{\mathrm{M}}_{3/2,0}^{(k)}}, \quad \sigma_k^p = \left(\frac{\bar{\mathrm{M}}_{3/2,0}^{(k)}\bar{\mathrm{M}}_{3/2,2}^{(k)} - \left(\bar{\mathrm{M}}_{3/2,1}^{(k)}\right)^2}{\left(\bar{\mathrm{M}}_{3/2,0}^{(k)}\right)^2}\right)^{1/2},$$
$$q_k^p = \frac{1}{\bar{\mathrm{M}}_{3/2,0}^{(k)}}\left(\bar{\mathrm{M}}_{3/2,3}^{(k)} - \bar{\mathrm{M}}_{3/2,0}^{(k)}\left(U_k^p\right)^3 - 3\left(\bar{\mathrm{M}}_{3/2,0}^{(k)}\right)\left(\sigma_k^p\right)^2 U_k^p\right). \tag{12}$$

Equations (10) to (12) constitute the mapping $V_k \to W_k$.

The proof of this proposition as well as the numerical algorithm of the new method that follow from closure (5) are not shown due to the limited space. They will be presented in a future publication [8].

Results and Discussion

The method outlined above was applied to three test cases that change the distribution of droplets in surface space, first, through splashing, second, through a size-dependent drag force, and third through evaporation. All test cases were organised in such a way that crossing of two different droplet distributions was included. Solutions to the same test cases were also computed using a Lagrangian method. They are regarded as accurate reference solutions. The numerical algorithms for the Lagrangian solver are explained in [3].

In the splashing test case a truncated Gaussian distribution of droplets in surface space, with mean value 0.5, standard deviation 0.1 and initial velocity 1.0 (for all sections), enters the domain of size $x \in [0,1]$ from the left and is freely transported through it. At the right boundary the spray is reflected, but speed reduces by a factor of α, diameter by a factor of β and a fraction γ of its mass is lost. Figure 1 depicts the steady state solutions of the number of droplets, $\mathrm{M}_{0,0}^{(k)}(s)$, in a section I_k obtained for 5, 10 and 20 sections. They are compared with the Lagrangian cal-

culations for the parameter set $(\alpha,\beta,\gamma)=(0.9,0.7,0.1)$. The number of cells is not varied because the spray is freely transported in the computational domain. Only at the boundary is the spray distribution changed.

The high peak on the left side represents the splashed spray and is moving away form the wall, whereas the smaller peak on the right, agreeing with the inlet distribution (dashed line), is moving towards the wall. It is observed that for this test case the Lagrangian and Eulerian solutions for 10 and 20 sections are very close to each other. Reduction of the number of sections to 5 results in some discrepancies, but the qualitative behaviour of the moment method persists. The sensitivity of the method was studied for the changes of parameters (α,β,γ), but due to the limited space the results can not be presented here.

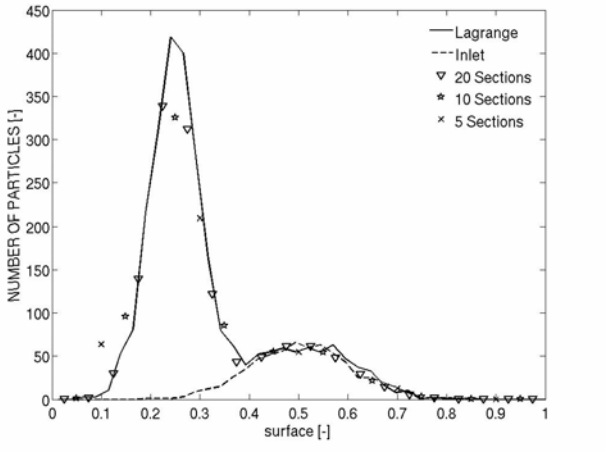

Figure 1: Splashing; α = 0.9, β = 0.7, γ = 0.1, at x = 0.9.

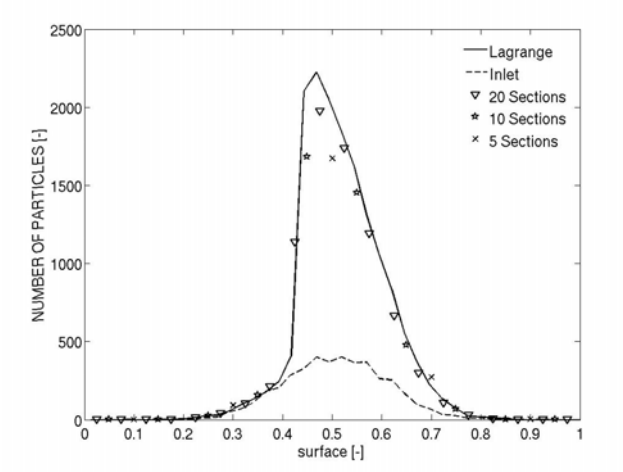

Figure 2: Crossing sprays and Drag, St = 2.43, x = 0.9.

In the drag test case two truncated Gaussian distributions of droplets in surface space, with the same mean value, variance and initial velocity (see splashing test case), are moving towards each other. Both distributions are affected by the Stokes drag that results from the velocity difference between the non-moving air and the water-droplets. The size and initial velocities of the droplets are chosen such that the two distributions cross each other. This drag test case can never reach a steady state, because those droplets that are stopped by the gas before leaving the computational domain accumulate at a certain position until the computation stops. Smaller droplets decelerate faster and stop closer to where they come from. In Figure 2 the Eulerian results of the drag test case at $x=0.9$ are depicted and compared to the calculations using the 'reference' Lagrangian method. Again, the number of sections is changed according to $\{5,10,20\}$ but the number of cells remains constant at 200. It is observed that the droplet distributions are much higher than the initial distribution. The reason for this behaviour is, first, the deceleration of droplets which leads to an accumulation and secondly, the overlap of the crossing distributions. It is also observed that the graphs in Figure 2 exhibit an asymmetry in the distribution. This effect is due to the drag force. Small droplets on the left side of the graph experience a strong deceleration and even stop before they reach $x=0.9$. The steep gradient marks the border between stopped droplets (left side of the steep gradient) and moving droplets (right side of the steep gradient). The small leftover on the right of the gradient agrees with the droplet distribution of the inlet distribution. Those droplets belong to the distribution coming from the right of the computational domain.

The new moment method is also tested in a configuration in which two truncated Gaussian spray distributions (see inlet in Figure 3) with different initial velocities ($v_{\text{left}}=1$, $v_{right}=2/3$) at $x=0$ and $x=1$ are transported in real space, $x\in[0,1]$, towards each other. The two initial spray distributions evaporate according to the d^2-law, i.e. in surface space they are solely shifted towards $s=0$. In Figure 3 the droplet distribution $\mathrm{M}_{0,0}^{(k)}(s)$ is shown for steady calculations of the moment method with 5, 10 and 20 sections and 200 cells at position $x=0.9$. In addition, the inlet distribution (dashed line) at $x=0$ (and $x=1$) are depicted as well as the Lagrangian solution (solid lines). In

Figure 3 the two distributions have evaporated and overlap. This behaviour indicates that the distributions are crossing each other. If the method could not predict this behaviour, a delta shock would have formed at the point where the distributions first cross ($x = 0.6$).This shock would have moved according to the relation between the momenta of droplets in each section. All droplets that arrive at the delta shock would have concentrated there. Figure 3 is the proof that no delta shock has been created, because droplets from the left ($x = 0$) are present at $x = 0.9$. Calculations with 5 sections are very crude but can still capture the evaporation and crossing effect of the spray. Using a larger number of sections improves the results considerably but still, as shown in Figure 3, there is a discrepancy between the Lagrangian and Eulerian calculations. This defect of the moment method may originate from either numerical diffusion in surface space or follow from small numerical interactions between the two distributions crossing each other in the middle of the computational domain. The analysis of this behaviour and the improvement of the numerical procedures will be carried out in future study.

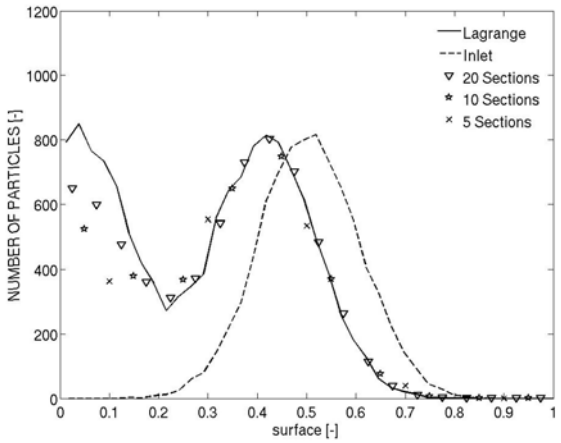

Figure 3: Crossing and Evaporation, Ev = 0.52 , $x = 0.9$

Conclusion

It is demonstrated in a one-dimensional setting that the new moment method can describe polydisperse sprays that splash on a wall and that cross each other while they are evaporating or experiencing a Stokes drag force. So far, Eulerian methods (cf. [5,6,2]) were only able to describe the dispersion with respect to the size variable, then being able to capture accurately evaporation, coalescence and drag of polydisperse sprays. On the other hand, [1] took into account the dispersion with respect to the velocity variable, allowing the description of crossing and splashing monodisperse sprays. The moment method derived and tested here considers both variables and is therefore able to predict all combinations of polydisperse and crossing effects of sprays. In the cases of splashing and drag, the comparison of the new moment method with accurate Lagrangian calculations reveals a convincing agreement even for small numbers of sections. The results indicate that 5 to 10 sections are enough to describe polydisperse effects. Using more sections, the application of the new method becomes computationally too expensive, particularly when it is extended to higher dimensions in real space. Obviously, the new moment method still awaits the extension to higher dimensions in real space and finer discretisation of the velocity space (see parameter I in (5)). Its ability to capture the polydisperse nature of sprays as well as the coexistence of two droplet velocities at one location is clearly demonstrated. Despite the strong assumptions made in this work, it opens a new way of describing unsteady spray phenomena with Eulerian methods.

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