Application of the Stochastic Field Method to Cavitating Flows in an Injection Nozzle

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Abstract

In this paper a fully Eulerian Monte Carlo method called 'Stochastic Field Method' (SFM) is applied on cavitating flows in an injection nozzle from the automotive industry. After the successful application to the field of combustion [1], the Stochastic Field Method is now applied to two phase flow. In the presence of numerous bubbles the method provides advantages in computational speed and statistical convergence compared to the classical Lagrangian-particle Monte Carlo methods. Modeling random processes which are omnipresent in combustion and cavitation requires careful treatment: Unphysical results are obtained, if in a nonlinear process a randomly distributed variable is merely approximated by its average. Thus the whole distribution must be considered. A probability density function (PDF) is used to describe the probabilistic behavior. The corresponding evolution and transport in space is governed by the PDF transport equation. Instead of solving the high dimensional PDF transport equation directly it is less complex to discretely approximate the PDF by random samples. In contrast to other stochastic methods that usually consider these samples as Lagrangian particles, the Stochastic Field Method describes them as fluctuating Eulerian fields. This point of view allows PDF description in a fully Eulerian framework, thus omitting the cumbersome coupling of Eulerian and Lagrangian solvers. The very first application of the Stochastic Field Method to a multi-phase flow was published by our working group [2]. Here, stochastic partial differential equations (SPDEs) describe samples of the disperse phase volume fraction as Eulerian fields. The collective of all samples approximates the probability density function at a considered location. Within the present paper the implementation to a commercial code is discussed. Application to an industrial case namely a cavitating flow within an injection nozzle is presented. Collecting samples of several time steps allows the SFM to visualize the volume fraction's or bubble size's distribution within individual computational cells. When applying the Stochastic Field Method to multiphase problems a number of physical aspects have to be considered which require careful analysis. These difficulties are pointed out and discussed.

Keywords: stochastic, multi-phase, stochastic field method, cavitation, nozzle, Monte Carlo, Eulerian

Introduction

Random behavior can be observed experimentally in both, combustion and cavitation problems. When including this behavior in numerical simulations the consideration of rare events is advantageous in the presence of nonlinear processes. Stochastic models yield an attractive possibility to observe these fluctuations in numerical investigations. The direct calculation of the PDF is associated with exhaustive numerical costs. Instead of considering the PDF, it is usually approximated by samples with a Monte Carlo method to reduce effort. Methods that treat these samples as Lagrangian particles are well known, where virtual particles are added to the flow and observed in a Lagrangian point of view. The flow itself is investigated in a Eulerian frame.

Basics of the Stochastic Field Method

The Stochastic Field Method regards samples approximating the PDF in a fully Eulerian description. Instead of Lagrangian particles Eulerian fields of concentrations are considered. Several Lagrangian particles and their corresponding stochastic field are presented in Figure 1 for an exemplary peculiarity. Here, the stochastic field delivers for every computational cell one concentration which is interpreted as a sample to approximate the PDF. Note that Figure 1 only represents one peculiarity. Note that, in the presence of fluctuations (e.g. in a turbulent flow) the Lagrangian particles are not located at deterministic positions. Analogously, the corresponding stochastic field exhibits statistical fluctuations. To include several peculiarities into the numerical investigation, several stochastic fields are calculated. Several possibilities are shown in Figure 2. To approximate the PDF within a specific cell, the concentrations from the stochastic fields are exploited. For illustration, the concentrations from eight stochastic fields are marked green in Figure 3 ('samples'). Building the histogram of these samples clearly approximates the corresponding PDF. Considering samples using stochastic fields offers several advantages: The fully Eulerian description makes the computationally expensive coupling of two solver architectures obsolete, which is the case for

Lagrangian particles. For a statistically reliable description of the PDF a sufficient number of samples is necessary. When using Lagrangian particles regions of dilute sample concentration or high sample concentration can occur. To overcome this, the methods of "clustering" and "cloning" were developed, see e.g. [3], but require additional computational time. The Stochastic Field Method delivers within every computational cell the same number of samples which avoids the need for methods like "clustering" and "cloning": It automatically delivers a predefined number of stochastic fields. In general the usage of 8, 16 [4] or 12 and 18 [5] fields is a good compromise between accuracy and computational effort.

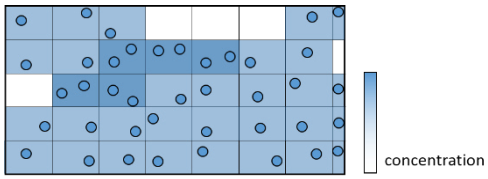

Figure 1: Lagrangian particles and corresponding Stochastic Field.

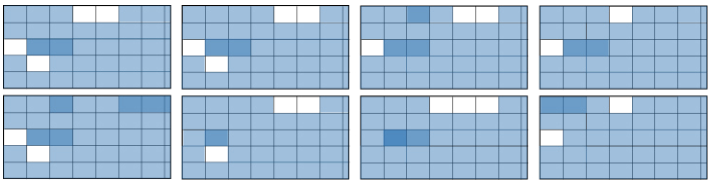

Figure 2: Several Stochastic Fields each representing one peculiarity and differing by the influence of the random term.

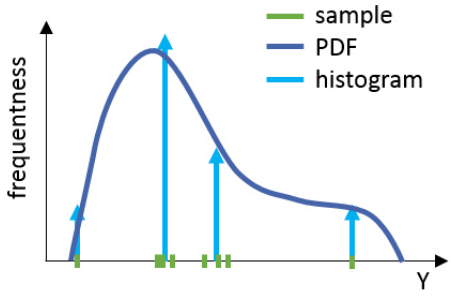

Figure 3: the histogram of the samples approximates the PDF.

Stochastic Field Method in the field of combustion

The stochastic partial differential equation describing a stochastic field was derived by Valiño [1] and Sabel'nikov and Soulard [6] in the field of combustion. It goes back to the joint probability density function (JPDF) of a scalar c and a velocity U derived by Pope [7]. This derivation builds on the conservation equation of a scalar c which reads

$$\rho \frac{\partial c}{\partial t} + \rho U_i \frac{\partial c}{\partial x_i} = -\frac{\partial J}{\partial x_i} + \rho S \qquad (1)$$

where J represents the diffusive mass flux. With Fick's first law this can be expressed

$$J = -D \frac{\partial c}{\partial x_i}$$

with the molecular diffusion coefficient D, the fluid density ρ and the source term S. The mean scalar transport equation reads [8]

$$\frac{\partial \bar{c}}{\partial t} + \bar{U} \frac{\partial \bar{c}}{\partial x_j} = \frac{\partial}{\partial x_i}\left[(D + D_t)\frac{\partial \bar{c}}{\partial x_i}\right] + \bar{S} \qquad (2)$$

with the turbulent diffusion coefficient D_t. Valiño [1] derived the transport equation of the stochastic fields (eq. (3)). Sabel'nikov's and Soulard's work [6] presents a less restrictive derivation, which results in the same equation, but with vanishing molecular diffusivity D. In many practical examples the molecular diffusivity is small compared to the turbulent diffusivity D_t. Consequently, both results are considered to be equivalent.

$$\frac{\partial Y}{\partial t} + \widetilde{U}_j \frac{\partial Y}{\partial x_j} + \sqrt{2D_t}\dot{W}_j \frac{\partial Y}{\partial x_j} - \frac{1}{\langle\rho\rangle}\frac{\partial}{\partial x_j}\left(\langle\rho\rangle(D + D_t)\frac{\partial Y}{\partial x_j}\right) = M(Y; x, t) + S(Y) \qquad (3)$$

In equation (3) Y is one sample of the concentration of a species and W is a Wiener Process where the Ito interpretation was used. M represents the micromixing term which can be modeled, e.g. by the Interaction by Exchange

with the Mean (IEM) model [9]. In the PDF transport equation of the species concentration the turbulent advection is modelled by the gradient diffusion assumption, which creates the 'diffusion-like' term (second derivative) in the transport equation of the corresponding stochastic field equation (see [6] for details). Several Stochastic fields are calculated differing by the influence of the Wiener process term approximating the PDF; depending on the influence of the Wiener process, the individual samples may have bigger or smaller values. For the calculation of the PDF's expectation Pope's [7] definition of the ensemble average of a random variable $\phi = \phi(\underline{x_0}, t_0)$ is used

$$\langle \phi \rangle_N \equiv \frac{1}{N} \sum_{n=1}^{N} \phi^{(n)}. \quad (4)$$

In his example $\phi^{(n)}$ is the *n*th 'experiment' from *N* nominally identical 'apparatus' and $\langle \phi \rangle_N$ estimates $\langle \phi \rangle$ since

$$\mathbf{E}(\langle \phi \rangle_N) = \langle \phi \rangle \quad (5)$$

for any N. Further Pope states that 'for large N, the Central Limit Theorem reveals the relationship between $\langle \phi \rangle_N$ and $\langle \phi \rangle$' [7]. Analogously this definition (eq. (4)) can be used to calculate the expected value $\langle Y \rangle_N$ from the samples $Y^{(n)}$ approximating the PDF

$$\langle Y \rangle_N \equiv \frac{1}{N} \sum_{n=1}^{N} Y^{(n)}. \quad (6)$$

Ensemble averaging stochastic fields in the corresponding transport equation (eq. (3)) yields the transport equation of the expected value. With vanishing Wiener process [10] and vanishing micromixing term it matches the mean concentration from the averaged scalar transport equation (cmp. eq. (2)).

Application to the field of two phase flow

Two phase flows are often described by using the two fluid model [11], [12]. The authors present the average balance equation of mass of phase *k*, the so called volume fraction equation. In both descriptions the volume fraction equation reads

$$\frac{\partial \alpha_k \overline{\overline{\rho_k}}}{\partial t} + \nabla \cdot \left(\alpha_k \overline{\overline{\rho_k}} \widehat{\boldsymbol{U}_k} \right) = S_k, \quad (7)$$

with the volume fraction[1] of phase *k* defined as

$$\alpha_k = \overline{X_k}, \quad (8)$$

with the component indicator function of a realization *r* [12]

$$X_k(\boldsymbol{x}, t; r) = \begin{cases} 1, \text{if } x \in k \text{ in realization } r \\ 0, \text{otherwise} \end{cases} \quad (9)$$

and the average defined for a function F_k [11]

$$\overline{F_k}(\boldsymbol{x}_0; t_0) = \lim_{\delta \to 0} \frac{1}{\Delta t} \int_{[\Delta t]_T} F_k(x_0; t) dt, \quad (10)$$

where δ depicts the interface thickness. The phase average of a function F_k, in equation (7) applied e.g. on the density, is defined as [11]

$$\overline{\overline{F_k}} = \frac{\overline{F_k}}{\alpha_k}. \quad (11)$$

The density weighted average of a function F_k, in equation (7) applied e.g. on the velocity, is defined as [11]

$$\widehat{F_k} = \frac{\overline{\rho_k F_k}}{\overline{\rho_k}}. \quad (12)$$

Applying the Stochastic Field Method to two phase flows where the stochastic fields are formulated for the scalar volume fraction α reads

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[1] Mostly α_k is referred to as the volume fraction of phase *k*. In fact, it is the probability of phase *k* occurring at location $\boldsymbol{x}$ at time *t* [13].

$$\frac{\partial \alpha}{\partial t} + \widehat{U}_j \frac{\partial \alpha}{\partial x_j} + R = S(\alpha). \qquad (13)$$

Here, R represents a stochastic term in Ito interpretation. Note that even though we distinguish several fields we use the common average velocity field from the two fluid model. This equation requires some comments:

1. For a stationary and incompressible flow ($\nabla \widehat{\boldsymbol{U}_k} = 0$) the average balance equation (eq. (7)) can be divided by $\overline{\overline{\rho_k}}$ and simplified:
$$\frac{\partial \alpha_k}{\partial t} + \widehat{\boldsymbol{U}_k}\, \nabla \alpha_k = \frac{S_k}{\overline{\overline{\rho_k}}} = \widetilde{S_k} \qquad (14)$$
It is evident that the PDF's expectation should be identical to the average volume fraction from eq. (14). Analogously, the transport equation of the PDF's expectation should be identical to the average balance equation (eq. (14)).
Applying Pope's definition (4) to calculate the expected volume fraction $\langle \alpha \rangle_N$ from the samples $\alpha^{(n)}$ approximating the PDF yields
$$\langle \alpha \rangle_N \equiv \frac{1}{N} \sum_{n=1}^{N} \alpha^{(n)}. \qquad (15)$$
The transport equation of the expected volume fraction can be derived by averaging the equation of the stochastic field (eq. (13)) over an ensemble of N stochastic fields with the operator $\langle \cdot \rangle_N$
$$\langle \frac{\partial \alpha}{\partial t} \rangle_N + \langle \widehat{U}_j \frac{\partial \alpha}{\partial x_j} \rangle_N + \langle R \rangle_N = \langle S(\alpha) \rangle_N. \qquad (16)$$
The averages of the first two and the last term yield (cmp. [7])
$$\langle \frac{\partial \alpha}{\partial t} \rangle_N = \frac{\partial \langle \alpha \rangle_N}{\partial t} \qquad \langle \widehat{U}_j \frac{\partial \alpha}{\partial x_j} \rangle_N = \widehat{U}_j \frac{\partial \langle \alpha \rangle_N}{\partial x_j} \qquad \langle S(\alpha) \rangle_N = \overline{S(\alpha)}. \qquad (17)$$
Since R represents a stochastic term in Ito interpretation its average vanishes (see [13] for details). Consequently the transport equation of the expected volume fraction corresponds to the average balance equation (14). An essential difference between the original stochastic field formulation taken from the field of combustion (eq. (3)) and the proposed formulation for the two fluid model is the exclusion of a 'diffusion-like' term. If the 'diffusion-like' term was retained it would appear in the transport equation of the expected volume fraction rendering equation (16) and equation (14) inconsistent.
2. The micro-mixing term M in equation (3) represents the molecular mixing on the smallest scales (cmp. eq. (1)). Since no small-scale mixing is included in the local instant formulation of the continuity equation for each phase [11], there is no reason for including micro-mixing into the stochastic partial differential equation. This was also confirmed by the group of Oevermann [14].
3. In analogy to the average balance equation (eq. (7)) the convection term in equation (13) contains the density averaged velocity $\widehat{U}_j$.
4. The formulation of the stochastic term R should be formulated problem dependent. The formulation which applies the analogy to the Stochastic Field Method in combustion (eq. (3)) is conceivable. However, the Ito interpretation should be used to retain the equality of the ensemble average over stochastic fields (eq. (16)) and the average balance equation (eq. (14)).

The stochastic fields represent samples approximating the PDF of volume fractions. Since the two fluid model needs for further calculations an average volume fraction, samples are averaged after each iteration step. Nevertheless, nonlinear processes depending on the volume fraction can use the PDF approximated by samples, and this avoids the modelling error which is evident in models based on one average value.

Application to a cavitation example from automotive industry

The Stochastic Field Method is implemented into the commercial CFD Code AVL FIRE™ and applied to a 2D as well as a 3D flow in an injection nozzle where cavitation occurs. The resulting average volume fraction of the disperse phase is shown in Figure 4. For a specific cell the average volume fraction and the volume fractions from the stochastic fields can be plotted over the time.

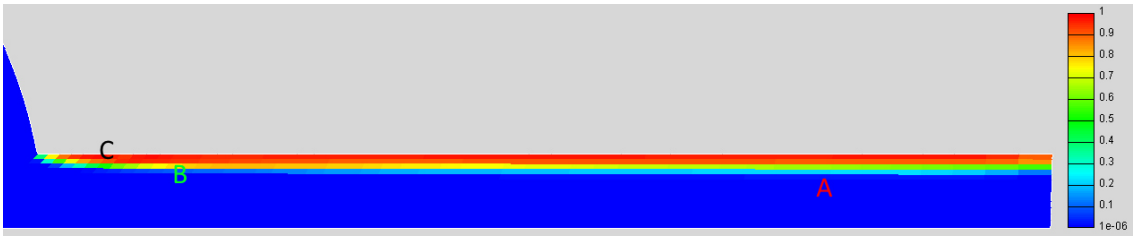

Figure 4: average volume fraction of the disperse phase in a 2D injection nozzle. The positions for the distributions in Figure 7 are marked with A, B and C.

Figure 5 compares the development of the stochastic fields for a cell within the cavitation area. The stochastic fields representing the possible peculiarities are clearly influenced by the random term. They are perturbed around the averaged field. Using the Stochastic Field Method allows a consideration of peculiarities that greatly differ from the averaged value (big difference between stochastic field and averaged field in Figure 5). This might have strong influence on the simulation result when strong nonlinear processes are present. This influence is ignored in methods dealing only with one average value.

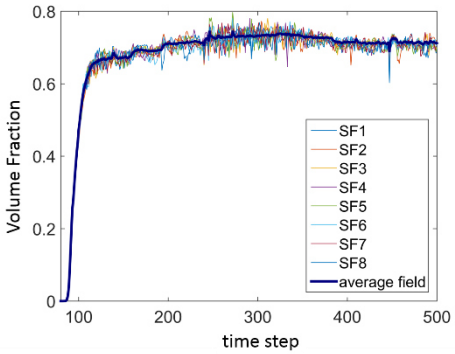

Figure 5: volume fraction of the stochastic fields and the average field for a cell within the cavitation zone.

Figure 6 shows simulation results for a 3D injection nozzle with moving needle. Due to cavitation effects the disperse vapor phase is generated at the nozzle entrance on the left-hand side. Its average volume fraction is plotted in Figure 6 (top). In addition two stochastic fields are plotted (bottom). Taking a closer look, the stochastic differences can be observed.

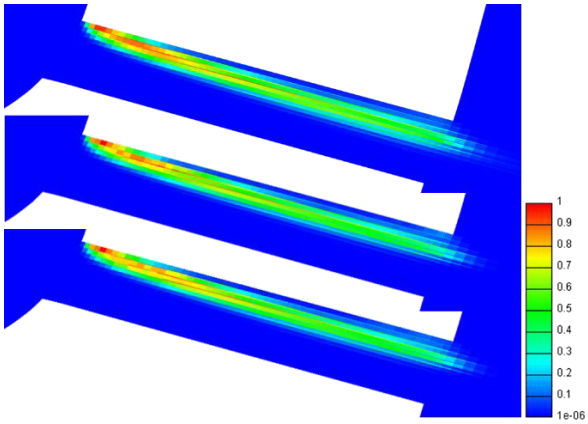

Figure 6: volume fraction of the dispersed phase; top: mean, bottom: two stochastic fields

Collecting values occurring in the stochastic fields over several time steps allows the construction of a histogram. It gives access to distributions of volume fraction within different regions. The distribution of the volume fraction of the disperse phase is given in Figure 7 for a cell outside, at the edge or within the cavitation sheet, respectively. Starting from a region outside the cavitation sheet (Figure 7a) the distribution is shifted towards higher volume fractions on

the way to the center of the cavitation sheet. The distribution of the volume fraction can be used for the derivation of other distributions, such as the distribution of bubble size.

Conclusion

Originating from the field of combustion the Stochastic Field Method was applied to cavitating multi-phase flow. It was pointed out that the SPDE describing the stochastic fields cannot contain a 'diffusion-like' term nor a micro-mixing term to be consistent with the two fluid model. The Stochastic Field Method was applied to a cavitating flow within an injection nozzle. Distributions of volume fractions were shown.

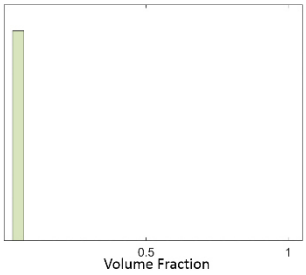

Figure 7a: Distribution of volume fraction for a cell outside the cavitation sheet (marked in Figure 4 with A). The stochastic fields only contain low volume fractions

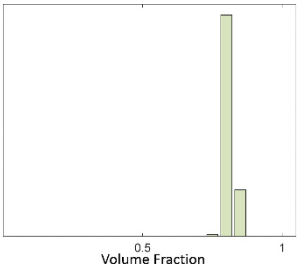

Figure 7b: Distribution of volume fraction for a cell at the edge of the cavitation sheet (marked in Figure 4 with B).

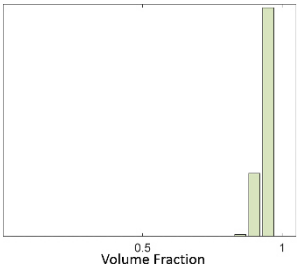

Figure 7c: Distribution of volume fraction for a cell within the cavitation sheet (marked in Figure 4 with C). The stochastic fields contain volume fractions with values close to 1.

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