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# AN EVALUATION OF SELECTED NUMERICAL METHODS FOR SOLVING THE POPULATION BALANCE EQUATION

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## ABSTRACT

The capability of high order methods to solve the population balance equation is studied in this work. The Least Square Method, the Nyström Method and a low order version of the Nyström method, called the Discrete Method, are applied to a general population balance equation containing breakage terms only.
In order to perform a rigorous error analysis, analytical solutions are used. In general the Least Square Method shows a good agreement with the test cases proposed, and a better performance than the other two methods.

## INTRODUCTION

The behaviour of dispersed systems such as gas-liquid or liquid-liquid systems is strongly dependent on the hydrodynamic properties of the dispersed phase. The flow pattern in such systems is also sensitive to changes in the dispersed phase size and shape distributions. Typical two fluid models are not able to handle these complex phenomena because only one characteristic size of the dispersed phase is used. For that reason considerable efforts have been made in order to develop polydispersed multi-fluid models with an inherent population balance equation, PBE.
By using PBE, the dispersed phase is commonly treated using a probability density function, PDF, which gives for example the probability that a bubble of a given size is presented in some point in the domain. The characteristics of the PDF and its evolution are governed by different processes such as breakage, coalescence, growth and convective transport of the particles.
On the other hand, the use of PBE increases the complexity of the problem, due to the fact that a nonlinear partial integro-differential equation, PIDE, needs to be solved. Although analytical approximations can sometimes be derived for some particular cases, in most practical situations it is necessary to use a suitable numerical method.

The method of moments represents an efficient method to solve the PBE, but it is applicable for some particular cases. For example, Frenklach (1985) shows that the application of the method of moments to coagulation process where the coagulation rate is constant works well, since the problem is closed. This means that the value of a given moment of the distribution is only related to the value of the lower order moments of the distribution.

For the general case, McGraw (1997) proposes to close the problem by using numerical quadrature, calling this approach the quadrature method of moments, QMOM. This eliminates the problem of the coupling between a given moment with high order moments by replacing integral expressions with a quadrature rule computed based on the Product-Difference algorithm, Gordon (1968). However, this approach is limited to particular problems due to the ill--conditioned behaviour of the method. This ill--conditioned behaviour is inherited as a consequence of using moments to compute the quadrature rules (e.g. Gautshi (1968) and Press (2002) ).

The sectional methods denote a well established group of solution techniques in population balance modelling. These types of methods require the use of some ad-hoc constrains in order to satisfy the conservation of certain properties of the distribution, such as mass conservation, but with the cost of altering the original problem, Ramkrishna (2000). These low order methods present the disadvantage of high computational cost, due to the fact that in general more than 20 -30 points, pivots, groups, classes, etc. are required to obtain reasonable results. It is important to note that, although it is common to use constraint in order to improve the conservation of the pertinent properties, the convergence rate is not modified.

An alternative strategy is to employ projection methods, such as finite element methods, FEM, in which the solution is approximated as a linear combination of the basis functions over a finite number of sub-domains. For example, Niemanis and Hounslow (1998) apply FEM to the steady state PBE, finding more accurate solutions than using the sectional methods and at the same time using less computational power. The low order nature of the FEM approach demands also high computational costs which could be reduced if a higher order version is applied.

Due to the fact that for some applications such as chemical reactor simulations the computational costs of the solver of the PBE have to be reduced, higher order polynomial approximation methods could be an option. The global approximation of the solution, compared with the local one of FEM or sectional methods, permits us to reduce the final computational cost since less points are required for achieving the same accuracy.

Higher order methods, such as the Nyström, the Least Square and spectral Galerkin methods, are commonly used for solving integral equations like the Fredholm equation, (Hackbush, 1995), but they are not normally applied to PBEs. One of the few existing examples of this

approach applied to PBEs can be found in Mantzaris(2001) who discussed a Galerkin, Tau and pseudo-spectral methods as a tool for solving multi-variable cell population balance models which contains growth and breakage processes.

In this work, the capability of high order methods to solve the population balance equation is studied. The Least Square Method (Dorao and Jakobsen, 2004a), the Nyström Method (Dorao and Jakobsen, 2004b) and a low order version of the Nyström method, which we refers to as the Discrete Method in the rest the work, are applied to a general population balance equation containing breakage terms only. In order to perform a rigorous error analysis, analytical solutions are used, although they have no counter part in any physical process.

## THE POPULATION BALANCE EQUATION

The Population Balance Equation describes the evolution of the Probability Density Function, PDF, representing the behaviour of a population of particles such as bubbles, droplets or solid particles. The evolution of this PDF must take into account the different processes that control the population such as breakage, coalescence, growth and convective transport of the particles. In this work, we focus on numerical methods for the solution of the pure breakage population balance equation.

The breakage operator can be defined as

$$L_b\{f(\xi)\} = -b(\xi)f(\xi) + \int_0^1 k(\xi,\eta)f(\xi)d\xi \quad (1)$$

where

$$k(\xi,\eta) = b(\eta)h(\xi,\eta)$$

$f(\xi)$ is the unknown PDF which for instance can represent the number of particles per unit volume with the property $\xi + d\xi$. The chosen property $\xi$ depends on the particular problem, for example $\xi$ can represent the mass of a population of bubbles or the diameter of a population of droplets.

The breakage operator $L_b\{f(\xi)\}$ represents the rate of change of the individuals with property $\xi$ in the population, i.e. in the PDF $f(\xi)$. The first term on the RHS represents the change in the population due to loss of the individuals in the population, for example due to a breakage process; in this case $b(\xi)$ is the breakage rate of the particles of type $\xi$. The second term in the RHS gives us the change in the population due to the arrivals of new individuals with property $\xi$. The breakage of particles of type $\eta$ will produce particles of type $\xi$ according to the breakage yield function $h(\xi,\eta)$.

The general pure breakage equation can be expressed as

$$L_b\{f(\xi)\} + g(\xi) = 0 \qquad \xi \in (0,1) \quad (2)$$

where $g(\xi)$ is the source term, which represents a sink or source of individuals with property $\xi$.

## NUMERICAL METHODS

A simple way to classify numerical methods for the solution of PBEs constitutes the methods based on **quadrature rules** and methods based on **a projection strategy**. The former approximates the integral expressions using quadrature rules, while the latter consists in approximating the solution which lay in a large space, using a smaller, more manageable one.

### Methods based on quadrature rules

Quadrature rule is the generic name given to any numerical method approximating an integral, for example

$$\int_0^1 g(\xi)d\xi \approx \sum_{q=1}^{N} g(\xi_q)w_q$$

where the set $\{\xi_q, w_q\}_{q=1}^{N}$ is referred to as the points and weight of the quadrature rule. The quadrature rule can be classified as low order methods such as the Trapezoid or Simpson's rules or high order methods such as the Gauss quadrature rule. Although, the Trapezoid and Simpson's rules are familiar and/or trivial quadrature rules to program, efficiency is more important in the context of computational codes in which we want to solve PBEs. Thus, these methods should not be considered in general, but rather be replaced by high order quadrature rules. In spite of the high computation cost, low order methods are normally used for solving PBEs, (e.g. Ramkrishna, 2000). For that reason we include the low order quadrature approach in this work.

The Nyström method belongs to the high order quadrature methods, while the Discrete method belongs to the low order quadrature methods.

#### *The Nyström Method*

The Nyström method consists in approximating the integral term by using a quadrature rule. This method is discussed in detail for population balance problems by Dorao and Jakobsen (2004b).
The second term in equation (1) can be approximated like

$$\int_0^1 k(\xi,\eta)f(\xi)d\xi \approx \sum_{j=1}^{N} k(\xi,\xi_j)f(\xi_j)w_j \quad (3)$$

Thus, the pure breakage equation can be expressed like

$$-b(\xi)f(\xi) + \sum_{j=1}^{N} k(\xi,\xi_j)f(\xi_j)w_j + g(\xi) = 0 \quad (4)$$

In order to close the problem, we can choose $\xi = \xi_i$ with $i = 1,\ldots,N$. Thus, we get

$$-b(\xi_i)f(\xi_i) + \sum_{j=1}^{N} k(\xi_i,\xi_j)f(\xi_j)w_j + g(\xi_i) = 0 \quad (5)$$

Finally, defining

$$A_{ij} = -b(\xi_i)\delta_{ij} + k(\xi_i, \xi_j)w_j$$
$$F_i = g(\xi_i)$$
$$x_i = f(\xi_i)$$

where $\delta_{ij} = 1$ if $i = j$ or $\delta_{ij} = 0$ if $i \neq j$. We can write

$$\sum_{j=1}^{N} A_{ij} x_j = F_i \qquad (6)$$

or in matrix form

$$Ax = F$$

When the solution is obtained, the moment of the PDF can computed like

$$Q_k = \int_0^1 \xi^k f(\xi) d\xi \approx \sum_{j=1}^{N} \xi_j^k f(\xi_j) w_j \qquad (7)$$

An important characteristic of this method is that it presents a high convergence rate due to the fact that a high order quadrature rule is used. In general, and if the kernels functions are analytic functions, the expected convergence rate is $O(e^{-\mu N})$, i.e. spectral convergence, where $\mu$ depend on the problem.

The computational cost of this approach is determined by the cost used to ensemble the system, i.e. to write the matrix $A$ and vector $F$. This task has an approximated cost of

$$A \rightarrow O(N^2)$$
$$F \rightarrow O(N)$$

In addition to the previous assembling cost, the computational cost for solving it must be added. In the general case, the cost for solving it can be approximated as $O(N^3)$ if Gauss elimination is used. In consequence the dominant computational cost is $O(N^3)$.

#### *The Discrete Method*

This method corresponds to the low order quadrature approximation of the Nyström method. In this case the quadrature rule is chosen to be the rectangular or Trapezoid quadrature rule.

The computational cost involved is the same for as the Nyström method. On the other hand, the convergence rate is $O(N^{-p})$, i.e. algebraic convergence, where $p$ represent the order of the approximation. For example, if the Trapezoid rules is used $p = 2$. In consequence, this method presents no advantage compared to the Nyström method for a general case.

The Discrite method can be seen as the starting point for the low order methods such as the Classes Method or Course Grid Method, (e.g. Ramkrishna, 2000), which introduce additional constraint rules in order to fulfil the conservation of certain moments of the distribution. These rules do not improve the convergence rate in general. On the other hand, high order methods such as the Nyström method do not require any additional rules to be conservative. Increasing the number of points, the conservation properties are satisfied as part of the convergence process.

### Methods based on projection strategies

These methods consist in approximating the solution which lay in a large space, using a smaller, more manageable one. Finite element methods, FEM, are an example of projection methods, in which the solution is approximated as a linear combination of the basis functions over a finite number of sub-domains.
In this work, we focus on the Least Square Method, LSQ, which is a particular projection method which is commonly applied to integral equations such as the Freadholm equation. In this case, we discuss a higher order version of the Least Square Finite Element Method, (Jiang, 1998). This method is discussed in detail for a general population balance problem in Dorao and Jakobsen (2004a).

#### *The Least Square Method*

The Least Square Method (LSQ) is based on expressing the approximate solution, in a similar way as for the Method of Weighted Residuals

$$f(\xi) = \sum_{j=0}^{\infty} a_j \varphi_j(\xi) \qquad (8)$$

If the approximate solution is substituted into the original equation, the left hand side of the equation (2) will not generally be identically zero. Therefore, we can write the residual equation as

$$R(f(\xi)) = L_b f(\xi) + g(\xi) \qquad (9)$$

The basic idea of the LSQ is to determine the coefficients $a_j$ by minimizing the integral of the square of the residual over the computational domain. Thus, it is possible to construct the quadratic functional

$$I(f) = \|R(f)\|^2 = \int_0^1 [L_b f(\xi) + g(\xi)]^2 d\xi \qquad (10)$$

for all $f \in V$, where $V$ is a functional space.

The necessary condition for $f \in V$ to be a minimizer of the functional $I(f)$ is that its first variation vanishes at $f$ for all admissible function $v \in V$. Thus, we get

$$\lim_{t\to 0}\frac{d}{dt}I(f+tv)=0\Rightarrow$$

$$2\int_0^1 [L_b f(\xi)-g(\xi)]L_b v(\xi)d\xi=0$$

Restricting the functional space to $V_N \subset V$, and with a little of algebra we get

$$\sum_{j=1}^{N} a_j \left\langle L_b\varphi_j(\xi), L_b\varphi_i(\xi)\right\rangle + \left\langle g(\xi), L_b\varphi_i(\xi)\right\rangle = 0$$

for $i, j = 1,2,\cdots,N$

where $\langle\cdot,\cdot\rangle$ represents the inner product defined like

$$\left\langle f(\xi), g(\xi)\right\rangle = \int_0^1 f(\xi)g(\xi)d\xi$$

Defining

$$A_{ij} = \left\langle L_b\varphi_j(\xi), L_b\varphi_i(\xi)\right\rangle$$

$$F_i = \left\langle g(\xi), L_b\varphi_i(\xi)\right\rangle$$

$$x_i = a_i$$

we can obtain the matrix form like

$$Ax = F$$

When the solution is obtained, the moment of the PDF can computed like

$$Q_k = \int_0^1 \xi^k f(\xi)d\xi = \sum_{j=1}^{N} a_j \int_0^1 \xi^k \varphi_j(\xi)d\xi$$

$$\approx \sum_{j=1}^{N} a_j \sum_{q=1}^{N} \xi_q^k \varphi_j(\xi_q)w_q$$

In order to reduce the computational cost the coefficient of the matrix $A$ and $F$ can be computed using a Gauss quadrature rule like:

$$A_{ij} = \left\langle L_b\varphi_j(\xi), L_b\varphi_i(\xi)\right\rangle$$

$$\approx \sum_{q=1}^{N} L_b\varphi_j(\xi_q)L_b\varphi_i(\xi_q)w_q$$

$$F_i = \left\langle g(\xi), L_b\varphi_i(\xi)\right\rangle$$

$$\approx \sum_{q=1}^{N} g(\xi_q)L_b\varphi_i(\xi_q)w_q$$

The computational cost of this approach is determined by the cost used to ensemble the system,

$$A \to \mathrm{O}(N^3)$$

$$F \to \mathrm{O}(N^2)$$

plus the computational cost involved in solving it. In the general case, the cost for solving it is $\mathrm{O}(N^3)$ if Gauss elimination is used. In consequence the dominant computational cost is still $\mathrm{O}(N^3)$. The number of points used in the approximation of the integral, $N$, should be increased by adding a factor $M$ depending of the functional property of the kernels functions $b(\xi)$ and $h(\xi,\eta)$. Therefore, the number of quadrature points used should be $N+M$, and the previous cost should be modified to

$$A \to \mathrm{O}(N^3 + N^2 M)$$

$$F \to \mathrm{O}(N^2 + NM)$$

In consequence, the original cost is not affected significantly though.

This method presents a higher convergence rate due to the fact that a higher order expansion is used. In general, and if the kernels functions are analytical functions, the expected convergence rate is $\mathrm{O}(e^{-\mu N})$, i.e. spectral convergence, where $\mu$ depend on the problem. The spectral convergence rate can be severely reduced if no proper orthogonal polynomials are used. In particular by using the Legendre or Chebyshev orthogonal polynomials we obtain spectral convergence rates for this problem.

## RESULT AND DISCUSIONS

Five test problems are proposed for assessing the ability of the different methods to solve the pure breakage equation. Each case depends on at most 4 parameters which determine the characteristics of the yield function, $h(\eta,\xi)$, and the source function, $g(\xi)$, see definitions in appendix A.

Case 1, 2 and 3 are used to evaluate the behaviour of the solvers with a strong peak in the yield function, while case 4 and 5 are used to evaluate the effects in the accuracy of the solution for different source functions.

In order to obtain the average behaviour of the solvers, a numerical experiment is performed to obtain the average error and percentual moment error. For each case, 50 experiments are performed keeping the same order of expansion fixed for the cases of the LSQ, and the number of discrete points fixed for the cases of the NM and DM. The parameters which determine the characteristics of the functions in each experiment (see appendix A) are chosen randomly from a uniform distribution.

The error with respect to the analytical solution is defined like

$$error = \frac{1}{N}\sqrt{\sum_{k=1}^{N}\left[f(\xi_k) - f_N(\xi_k)\right]^2}$$

where $\xi_k$ are the points where the numerical and analytical solution are compared, and $N$ is the expansion order.

The Percentual moment error in the first moments is defined like

$$error\% = 100\frac{\left|Q_k^N - Q_k\right|}{Q_k}$$

where $Q_k^N$ is the numerical approximation of the moment $Q_k$.

The LSQ method was based on the Legendre polynomials and the evaluation of the integral terms were performed by Gauss-Legendre quadrature rules. Due to the fact that from this method we obtain a continuous solution, the error is evaluated using $N$ points distributed according to Gauss-Legendre points, shown as dots in the figures 1 to 5, where $N$ correspond to the expansion order used.

The Nyström method is based on Gauss-Legendre quadrature rule, while the Discrete method is based on an uniform rectangular quadrature rule.

#### Error in the Probability Density Function

In figure 1 to 5 the solution for cases 1 to 5 with the LSQ, Nyström and Discrete Method are presented. These figures represent one run of the 50 experiments used to compute the average behaviour. In general, the LSQ shows a better agreement with the analytical solution than the NM and DM. In order to get a better understanding of the performance of the different methods, the effects in the error depending on the number of points or expansions are analysed in the next section.

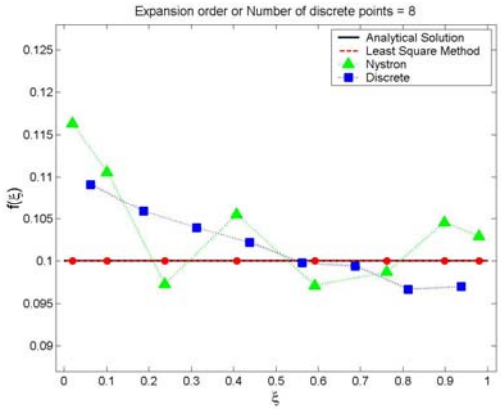


**Figure 1:** Solution Example Case 1

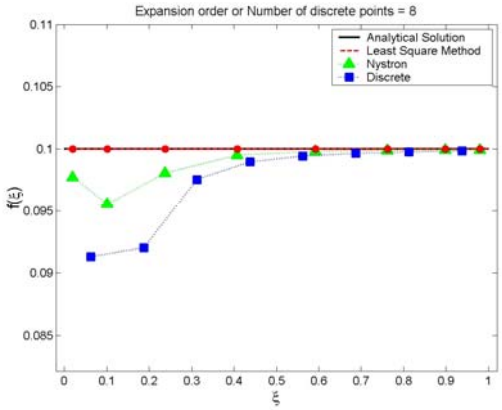


**Figure 2**: Solution Example Case 2

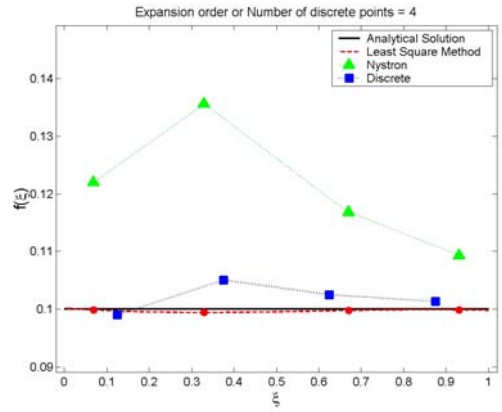


**Figure 3**: Solution Example Case 3

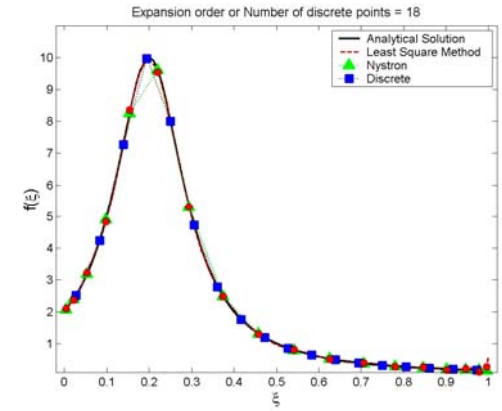


**Figure 4**: Solution Example Case 4

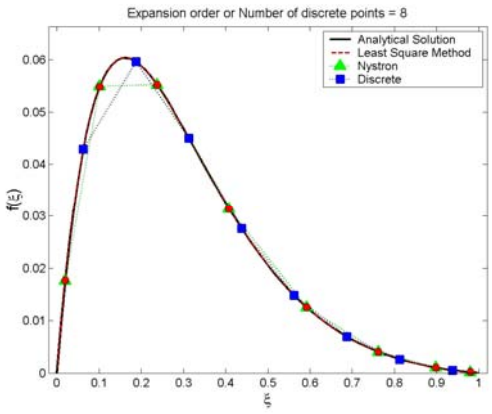


**Figure 5**: Solution Example Case 5

### Average Error

The average errors of performing 50 numerical runs per case are shown in figure 6 to 8 corresponding to case 1 to 5.

The average error corresponding to use the Discrete method is presented in figure 6, as expected algebraic convergence is observed. In figure 7, the spectral convergence of the Nyström method is presented. Spectral convergence is also observed for the LSQ method, figure 8.

For few points, i.e. $N$ around $4$ to $12$ the Nyström and Discrete methods behave in a similar way. On the other hand, if $N$ is increased due to the spectral convergence, the Nyström method performs better than the Discrete Method.

Due to the fact that the computational cost of the Discrete and Nyström methods are practically the same, and the DM has algebraic convergence while the NM has spectral one, there is no apparent reason to use the DM. In consequence the NM could be replacing the commonly used low order schemes for the solution of the population balance equations containing pure breakage only.

On the other hand, the LSQ method shows a better behaviour compared with the Nyström method, except for the case 4 for which the behaviour is quite similar. This effect can be attributed to the complex source term, which requires a high order polynomial representation.

The computational cost of the assembling process for the LSQ method is around $\mathrm{O}\left(N^3\right)$, while for the Nyström method it is around $\mathrm{O}\left(N^2\right)$. In spite of this, in general we can recommend the use of the LSQ method over the Nyström method. Apparently an expansion order N=12 for the LSQ method is equivalent to about 30 points for the Nyström method.

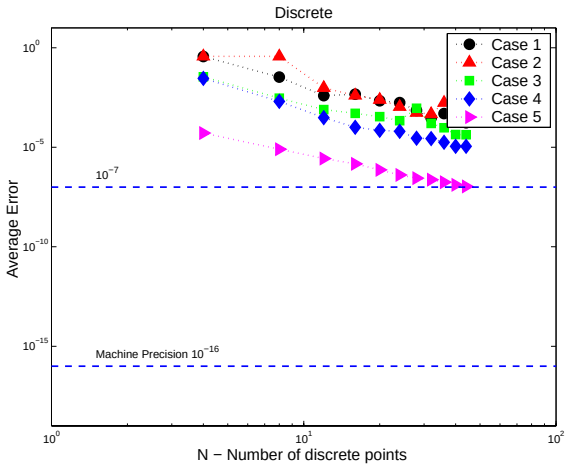


**Figure 6**: Average error for the Discrete Method.

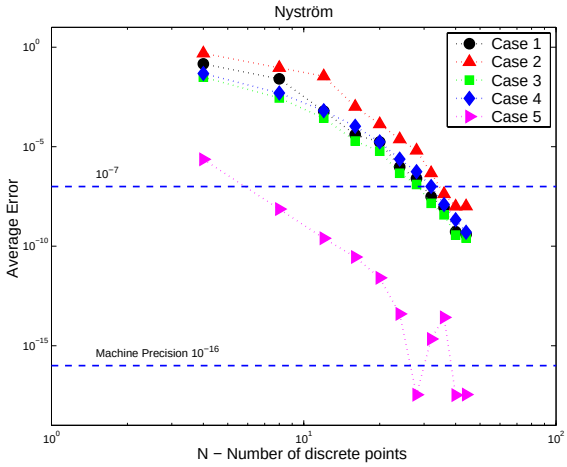


**Figure 7**: Average error for the Nyström Method.

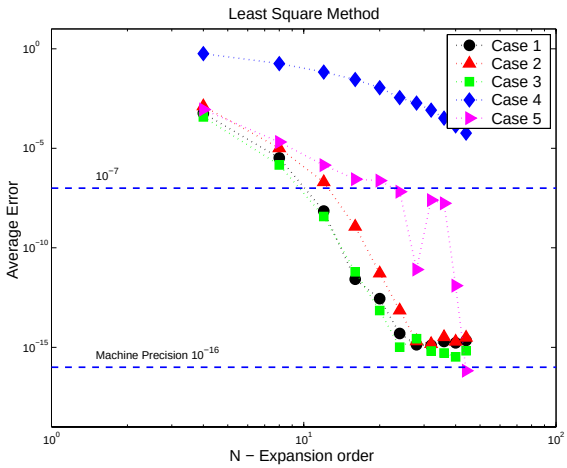


**Figure 8**: Average error for the Least Square Method.

### Percentual Moment Average Error

In the previous section, the error in the computation of the PDF was presented. In this part, the effects of the computation of the moments of the distribution are discussed. In particular, only case 1 (figure 9 to 11) and case 4 (figure 12 to 14) are shown. Case 1 shows a representative behaviour, while case 4 is considered

because the convergence rate of LSQ is reduced for this case.
As expected for the case 1, the Discrete method presents a poor behaviour, see figure 9, compared with the spectral convergence of the Nyström method, figure 10. On the other hand, the LSQ method shows an excellent behaviour, figure 11. With an expansion order of N=8 the percentual error in the computation of the moments is around 0.001%. For the same percentual error the Nyström requires around 20 points, while for the Discrete case, if possible, around 500 points.

On the other hand, for a small number of points, i.e. N around 8, for the case 4 the Discrete method, figure 12, shows a similar or better behaviour than the Nyström, figure 13, and LSQ method, figure 14.
Increasing the number of points the Nyström and LSQ method become superior to the Discrete method again.
In particular, for this case the Nyström method shows better behaviour than the LSQ method.
Summing up, the LSQ methods presents a good behaviour for handling pure breakage problems compared with the Nyström and Discrete methods. The LSQ method allows us to obtain the first moments with accuracy lower then 0.001% with an order of expansion N=8 for the general case. In the less favourable case 4, LSQ can demands at most N=20 in order to obtain the moments with accuracy around 1%. It is important to note that case 4, containing a source term with a high order polynomial behaviour, do not appear normally in the PBEs.

If the source term, case 4, presents a high order polynomial behaviour the performance of the LSQ can be reduced, but still LSQ will perform in a competitive way with the Nyström method.
The LSQ method presents the disadvantage that it can be more complex to understand, although the complexity of the implementation is about the same as for the Nyström or Discrete Method.
On the other hand, if we compare the Nyström and Discrete Methods in terms of the computational cost (which is the same) and error convergence (algebraic vs spectral convergence), the Nyström method is strongly recommended compared to the Discrete method.

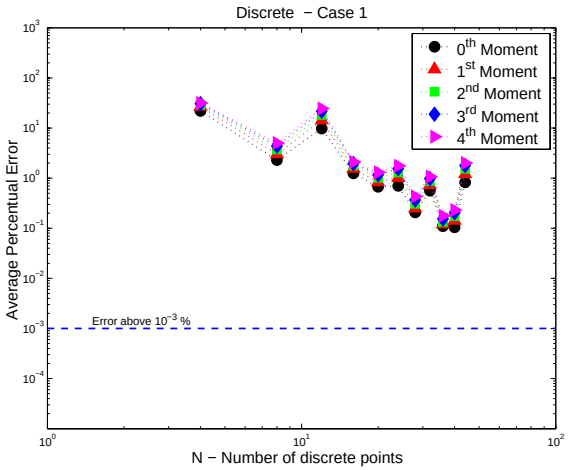


**Figure 9**: Average Percentual Error for the Discrete Method.

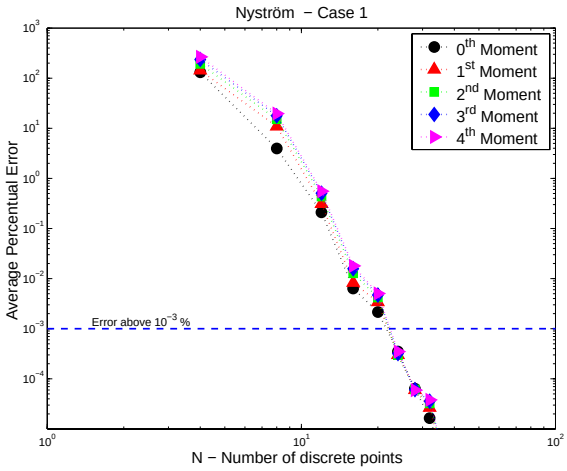


**Figure 10**: Average Percentual Error for the Nyström Method.

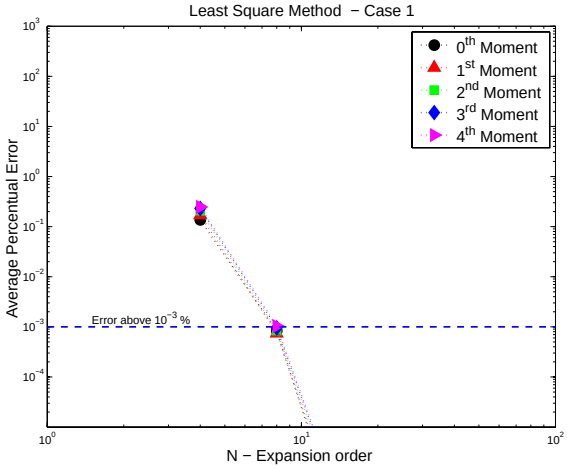


**Figure 11**: Average Percentual Error for the Least Square Method.

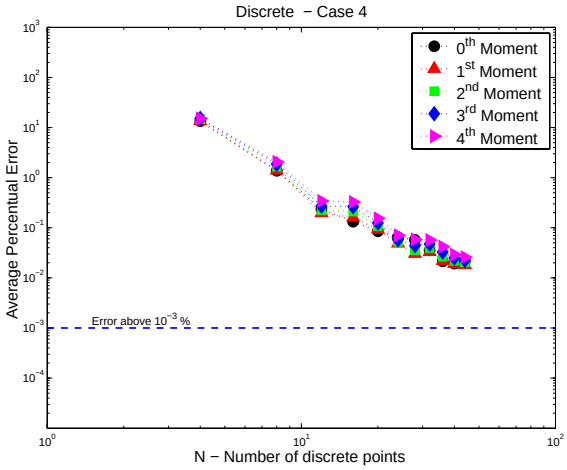


**Figure 12**: Average Percentual Error for the Discrete Method.

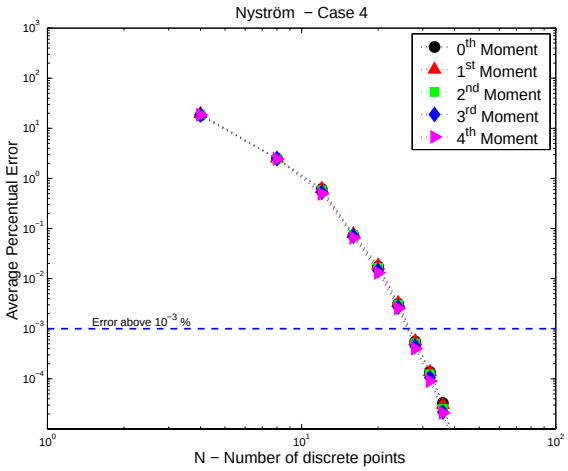


**Figure 13**: Average Percentual Error for the Nyström Method.

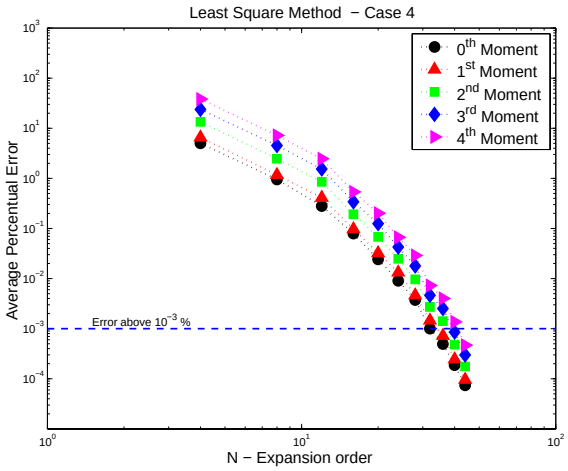


**Figure 14**: Average Percentual Error for the Least Square Method.

## CONCLUSION

In this work, the capability of higher order methods to solve the population balance equation was studied. The Least Square Method, the Nyström Method and a low order version of the Nyström method, called the Discrete Method, were applied to a general population balance equation containing breakage terms only. In order to perform a rigorous error analysis, analytical solutions were used.

The Discrete method shows algebraic convergence behaviour while the Nyström method shows a spectral one. Considering that the computational costs for both methods are practically the same, the NM seems to be advantageous compared to the commonly used low order schemes for the treatment of population balance equations containing breakage only.

The LSQ method shows good behaviour compared with the Nyström method, except for the case 4 for which the behaviour is quite similar. This effect can be attributed to the complex source term, which requires a higher order polynomial representation.

Although, the computational costs of the assembling process of the LSQ method are higher than for the Nyström method, the LSQ method can be recommended due to the better convergence rate for most cases.

The use of high order methods allows us to reduce the number of points or equivalently the expansion order considered for a given accuracy. In particular, the LSQ method allows us to obtain the first moments with accuracy lower then 0.001% with an order of expansion N=8 in the general case. In the less favourable case 4, the LSQ method can require at most N=20 in order to obtain the moments with accuracy around 1%. It is important to note that case 4, containing a source term with a higher order polynomial behaviour, does not appear in a typical PBE case.

## ACKNOWLEDGEMENTS

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## APPENDIX A

In this section the definitions of the analytical expressions used to define the problem cases are presented.

The parameters $p_1, p_2, p_3$ and $p_4$ are chosen randomly from a uniform distribution in the interval $[0,1]$, for each run. In figure 16 to 25, the breakage yield and source functions for the different cases are shown.

### Case 1

$$f(\xi) = p_1 \xi$$

$$k(\xi,\eta) = \frac{c}{\left((1-p_4)(\xi-p_2)-p_4(\eta-p_3)\right)^2 + c^2}$$

$$b(\xi) = 1$$

$$g(\xi) = p_1 + \frac{p_1}{p_4}\tan^{-1}\frac{(1-p_4)(\eta-p_2)-p_4(b-p_3)}{c} - \frac{p_1}{p_4}\tan^{-1}\frac{(1-p_4)(\eta-p_2)-p_4(a-p_3)}{c}$$

where $c = 0.1$, $b = 1$ and $a = 0$

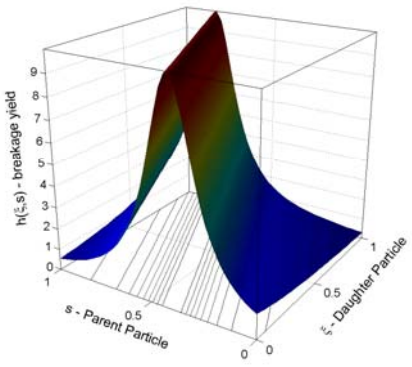


**Figure 15**: Breakage yield Case 1

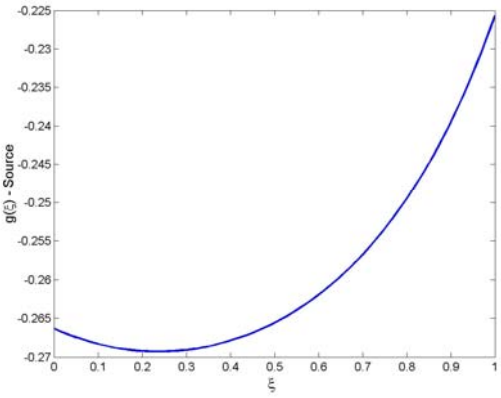


**Figure 16**: Source Case 1

### Case 2

$$f(\xi) = p_1 \xi$$

$$k(\xi,\eta) = \frac{c^2}{\left((\xi-p_2)^2 + c^2\right)\left((\eta-p_3)^2 + c^2\right)}$$

$$b(\xi) = 1$$

$$g(\xi) = p_1 - p_1 c \frac{\tan^{-1}\frac{(b-p_3)}{c} - \tan^{-1}\frac{(a-p_3)}{c}}{(\eta-p_2)^2 + c^2}$$

where $c = 0.1$, $b = 1$ and $a = 0$

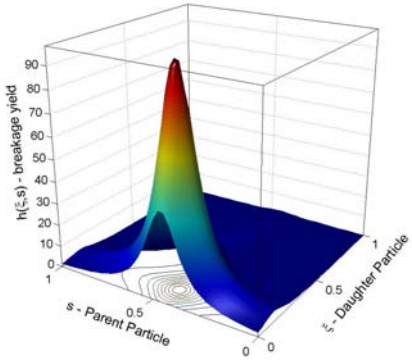


**Figure 17**: Breakage yield Case 2

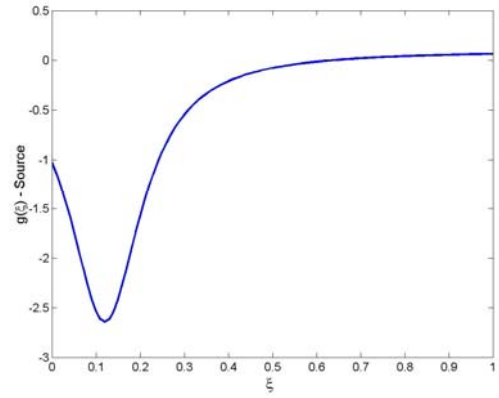


**Figure 18**: Source Case 2

**Case 3**

$$f(\xi) = p_1 \xi$$

$$k(\xi,\eta) = \frac{c}{(1-p_4)(\xi-p_2)^2 + p_4(\eta-p_3)^2 + c^2}$$

$$b(\xi) = 1$$

$$g(\xi) = p_1 + \frac{p_1 c}{\sqrt{p_4}\, d} \tan^{-1} \frac{(-b+p_3)\sqrt{p_4}}{d} -$$

$$\frac{p_1 c}{\sqrt{p_4}\, d} \tan^{-1} \frac{(a+p_3)\sqrt{p_4}}{d}$$

where $c = 0.1,\ b = 1, a = 0$ and

$$d = \sqrt{c^2 - (p_4 - 1)(p_2 - \eta)^2}$$

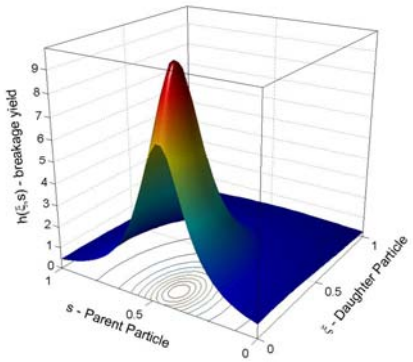


**Figure 19**: Breakage yield Case 3

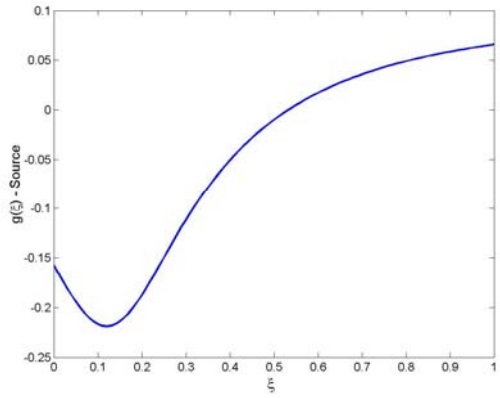


**Figure 20**: Source Case 3

**Case 4**

$$f(\xi) = \frac{c}{(\xi - p_1)^2 + c^2}$$

$$k(\xi,\eta) = (\xi - p_2)(\eta - p_3)$$

$$b(\xi) = 1$$

$$g(\xi) = \frac{c}{(\xi - p_1)^2 + c^2} -$$

$$\frac{c(\xi - p_2)}{2} \log \frac{\left((b-p_1)^2 + c^2\right)}{(a-p_1)^2 + c^2} +$$

$$\frac{(p_1 - p_3)(\xi - p_2)}{2}\left(\tan^{-1}\frac{(b-p_1)}{c} - \tan^{-1}\frac{(a-p_1)}{c}\right)$$

where $c = 0.1,\ b = 1$ and $a = 0$

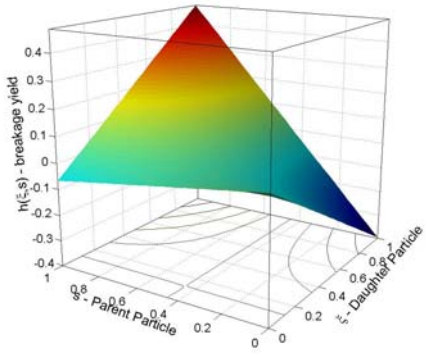


**Figure 21**: Breakage yield Case 4

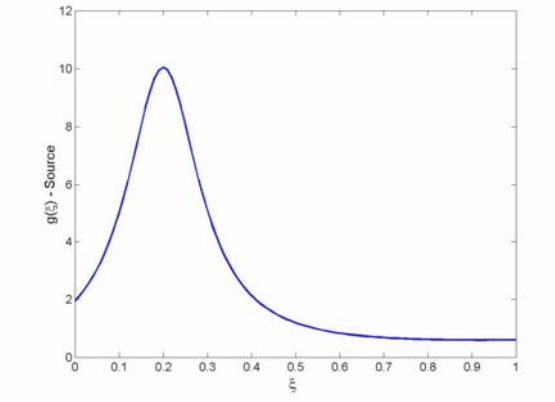


**Figure 22**: Source Case 4

**Case 5**

$$f(\xi) = \left(\xi - \xi^2\right)\exp(a\xi)$$

$$k(\xi,\eta) = \xi - \xi^{\eta+1}$$

$$b(\xi) = 1$$

$$g(\xi) = \frac{-1}{a^3\left(a + \log(\xi)\right)^3}(\xi(a^3(-(-2 + a)\exp(a) +$$

$$a^3 \exp(a\xi))*(-1+ \xi) +$$

$$a^2(6 - 6\exp(a) + a(2 - \exp(a)*(-3+ \xi)) +$$

$$3a^3 \exp(a\xi)(-1+\xi))\log(\xi) +$$

$$3a(2 - 2\exp(a) + a(1 + \exp(a)) +$$

$$a^3 \exp(a\xi)(-1+\xi))\log(\xi)^2 +$$

$$(2 - 2\exp(a) + a(1 + \exp(a)) +$$

$$a^3 \exp(a\xi)(-1+\xi))\log(\xi)^3))$$

where $a = -1/\ p_1$

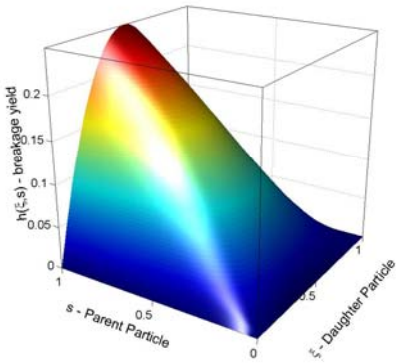


**Figure 23**: Breakage yield Case 5

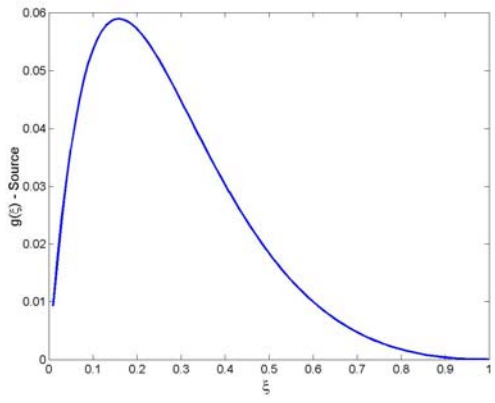


**Figure 24**: Case 5