Fast Algorithm for the Continuous Solution of the Population Balance Equation

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Abstract

Population balance models are used because of different system heterogeneities due to complex prevailing phenomena governed by particle fusion, splitting and growth. We present a Minimum Relative Entropy Population Density Estimator (MREPDE) based on the fast Clenshaw algorithm for the evaluation of the Legendre series as the heart of our proposed scheme. The present MREPDE reduced the order of computational complexity from O(M2) to O(M) with an accelerated implementation due to the low rank of the particle fusion matrix because of its tensorial decomposition. We implement the PBE and the MREPDE in a fully vectorized form, which results in a linear scaling of the CPU time with respect to M, instead of a cubic scaling using conventional methods. Therefore, our method is suitable for solving large-scale problems involving particle size distributions.

**Keywords**: Population Balances; Fast algorithm; Clenshaw; MREPDE.

* 1. Introduction

 The population balance equation (PBE) is a deterministic integro-partial differential equation with applications that spans many fields in pure and applied sciences. The PBE is known to admit analytical solutions only for a few cases with restricted forms of particle interaction rates and kinetics. Therefore, numerical-based solutions are required in case of general fusion and splitting rates when artificial intelligence supervising (Neuendorf et al., 2023) and real-time monitoring are required (Mickler et al., 2014). As a fast computational model (Drumm et al., 2010), the reduced two-equation population balance model OPOSPM is used in modelling real chemical engineering problems. This ranges from modelling and CFD simulation of pilot extraction columns (Drumm et al., 2010) to annular centrifugal extractors used to recover spent nuclear fuels, bubble column reactors and online monitoring and analysis of the multiphase ﬂow behaviour in industrial and chemical process engineering equipment (Mickler et al., 2014). Despite this, OPOSPM lacks the prediction of the full-size population distribution which is vital for online control purposes, estimation of individual particle physio-chemical properties and online inverse solution of the PBE (Mickler et al., 2014). To overcome this, we decoded the distribution behind OPOSPM by maximizing the Shannon entropy. The analytical form of this distribution is found to be the well-known Weibull distribution (Attarakih et al., 2020) which spreads as a function of time and space with mean particle size d30. The latter is a freely moving Lagrangian particle without bounds which is learned from the calculated moments of the corrected continuous solution of the PBE for which the Weibull distribution is used as prior information. The least biased posterior distribution, viewed as a correction to the prior information, is found by expanding the Kullback-Leibler divergence as a minimum solution to the relative entropy problem using a set of orthogonal Legendre polynomials. This allows us to derive the expansion coefficients in a closed form with integration quadrature based on careful sampling of the number concentration function.

The first challenge here is the complexity of the approximate continuous solution as it is represented by a series of orthogonal Legendre polynomials which has a summation complexity of O(M2) where M is the order of expansion which is repeated two times for each function evaluation. The second complexity comes from the quadratic source term for the formation of particles due to binary collisions with mechanisms embedded in the symmetric fusion rate. The complexity of this quadratic formation term depends on the used computational algorithm which in the order of O(M3). To overcome this challenge, we adapted the Clenshaw algorithm (Clenshaw, 1955) to evaluate the summation of Legendre polynomials series with a complexity of only O(M), while the evaluation of the quadratic source term is decomposed into two levels. The first one is the tensorial decomposition of the binary fusion rate using the singular value decomposition (SVD) which results in a low-order approximation O(2) for the Golovin fusion rate of turbulent diffusion and O(5) for the realistic fusion rate of Coulaloglou and Tavlarides based on the kinetic theory of gases. The second level is the complete vectorization of fusion and splitting source terms that are then implemented based on vectorized matrix computation techniques and popular vector-based software (e.g., MATLAB). This results in a compact algorithm which can be fast enough to meet the computational speed required when solving the PBE within real time monitoring and complex CFD environments.

* 1. Mathematical Model
		1. The Discrete Population Balance Equation

 Let the continuous number concentration function f(x,t) that describes the population of particles in a homogeneous physical space at any given point in time be sampled M times with points i = 0,1, …M-1 that are represented along the real line of the discrete particle space as ξi with a point population sample Ni = f(xi,t). Then, the discrete population balance model which accounts for binary particle fusion and splitting is written as:

where D(t) is the particle dilution rate, Ω is the discrete matrix of binary particle fusion rate per unit volume of the physical space. The upper triangular matrix B represents the discrete rate of binary particle splitting that depends on the given daughter particle distribution function and splitting rate. The discrete rate of birth of particles (Si) due to binary fusion depends on the discretization schemes that is used to reduce the continuous source term into its discrete form which can be written in two distinctive forms:

The difference is due to the discrete representation of the stretched particle phase space as presented by the product f(x,t)f(x-u,t). In the above formulation Ni represents the particle sample at ξi and N`i is the respective sample at (ξi-uj). Accordingly, Ψ and Π are the binary fusion rates (Ω) modified by the method of discretization. Note that the superscripts (|i〉 and 〈i〉) represent the ith row and column vectors of the given matrix respectively. Also, both terms appearing in Eq.(2) are quadratic birth terms with complexity in the order of O(M2) at any given discrete point i. Hence the overall complexity for M grid points is in the order of O(M3) (Attarakih et al., 2004).

* + 1. The Minimum Relative Entropy Population Density Estimator (MREPDE)

In our previous work (Attarakih et al., 2020) the general continuous solution of the PBE based on minimizing the relative entropy using the Kullback-Leibler divergence was presented. In this regard, the prior information (0 & 3rd moments) is decoded from the solution of the two-moment equation model (OPOSPM) using the maximum entropy principle. The posterior information is supplied from the local discrete samples (Ni) which were obtained from the solution of M-transport equations. The MREPDE has four striking advantages: Firstly, it is a continuous approximate solution satisfying the positivity physical conditions, secondly, it is consistent with total number and mass concentrations of the particles, thirdly, it supplies the local details of the number concentration function and fourthly, it is consistent with the low-order moments of the population density function. The main challenge in the original density estimator is the complexity arising from the Legendre series as the backbone of the functional estimator with order of complexity 2O(M2) per sampling point. Two distinctive features were introduced to the present MREPDE: firstly, the Clenshaw algorithm (Clenshaw, 1955) is extended from evaluating the Chebyshev series to that of Legendre one and secondly, the MREPDE is completely vectorized to exploit the elegant representation of the complex discrete PBE in complete vectorized form (see Fig.(1)). This enables efficient and parallel execution of numerical algorithms on TPUs (Tensor Processing Units) by exploiting the inherent structure of vectors and matrices. The MREPDE initial learning phase starts by OPOSPM distribution followed by a learning phase that samples the discrete local information in a reinforcement loop. At the heart of the MREPDE is the Clenshaw algorithm which computes the series of Legendre polynomials using a backward recurrence formula based on the information stored in the expansion coefficients (λ) as shown in Fig.(1). The order of complexity is now only O(M) thanks to the Clenshaw algorithm.

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Figure (1): Minimum Relative Entropy Population Density Estimator (MREPDE).

* + 1. *Tensorial Decomposition of the binary fusion rate*

To further enhance the computational speed of the discrete PBE model as given by Eq.(1), it is clear that the other cost of computation lies in the fusion rate matrix Ω (Matveev et al., 2015). In this work we used the tensorial decomposition of Ω to reduce its rank based on the singular value decomposition (SVD). This allows us to express Ω as a sum of rank-one tensors with set of coordinates arranged according to its decreasing magnitude.

* 1. Results and discussion
		1. Low-order fusion rate approximation

A sample of results is presented to show the low order approximation of two popular fusion rates using the SVD. The first one is the tensorial decomposition of the Golovin fusion rate for turbulent diffusion which results in an exact low-order approximation of order two. The second case is the most realistic fusion rate of Coulaloglou and Tavlarides based on the kinetic theory of gases to model droplet and bubble coalescence. A five-rank approximation with an error in order of machine precision is found. Fig.(2) shows the contours of the exact (15×15 gris points) and approximate fusion rates ((5×5 grid points)) for a wide range of operating conditions prevailing in an industrial scale mixer used for liquid-liquid dispersions (Alopaeus et al., 1999). On the other hand, the information contents as represented by the singular values is shown in Fig.(3)-Left. This reduction in the rank of fusion rate matrix results in an accelerated computational time.

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Figure (2): Exact and reduced contours of Coulaloglou and Tavlarides fusion rate using the SVD.

* + 1. CPU time for the fast MREPDE

For comparison between the new MREPDE with enhanced vectorized features in terms of computational time (as measured by the CPU time), we performed a standard test on the implementation of the Golovin fusion rate for turbulent diffusion with 0.05/s dilution rate and 0.025/s pre-frequency factor. The particle size domain x∈[a = 0.01, b = 4] with a grid that is distributed according to the distribution of Gauss-Legendre quadrature nodes. The initial condition is normal distribution with μ = 1.20 mm and σ = 0.30 mm.

* + 1. Reference solution

To validate the MREPDE model (Eq.(3)) in terms of the conserved moments; namely, the zero and third moments as well as higher order moments, the Chebyshev-QMOM is used with InvQMOM to reconstruct the particle size distribution (Attarakih et al., 2021).

In Eq.(3) w is the Weibull pdf and ϕ is a Legendre polynomial. The system of Eqs.(1,2 and 3) were solved in the standard summation forms with the MREPDE in its classical form with no vectorization except for the calculation of the vector λ. On the other hand, the fully vectorized form of Eqs.(1 and 2) and the MREPDE with Clenshaw algorithm (see Fig.(1)) were also solved under the same conditions listed in section 3.2.

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Figure (3): (Left) Information content (Singular values) of the Coulaloglou and Tavlarides fusion rate, (Right) CPU time ratio between the fast (vectorized) and slow (nonvectorized) algorithms.

Fig.(3)-Right shows the CPU time ratio between the vectorized MREPDE with Clenshaw algorithm and the classical nonvectorized PBE. It is obvious that as the order of approximation is increased, the CPU time ratio increases as well. This indicates the reduction in complexity from O(M2) to O(M) per sampling point. Actually the CPU time for the fast vectorized MREPDE with Clenshaw algorithm shows linear dependency on the order of approximation (Fig.(4)-Left) while the classical nonvectorized one shows cubic dependency on the order of approximation as shown in Fig.(4)-Right.

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Figure (4): (Left) CPU time for the fast algorithm, (Right) CPU time for the classical algorithm.

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Figure (5): (Left) Estimated density with 30 nodes, (Right) Estimated low-order moments.

Fig.(5)-Left shows the estimated population number concentration at final simulation time of 20 seconds as calculated using the MREPDE (sloid line) and compared to the reconstructed solution (bars) using the InvQMOM (Attarakih et al., 2021) with 8 nodes. The cross symbols show the distribution of the Gauss-Legendre sampling nodes. The accuracy of the solution is not only demonstrated by the number concentration function, but also by the calculated low-order moments from the number density at each instant of time (Fig.(5)-right) as calculated by Chebyshev-QMOM (Attarakih et al., 2021). Also, the root mean square error in successive approximations of the number concentration function is found to decrease rapidly as the order of approximation is increased.

* 1. Summary and conclusions

We proposed the MREPDE model with its backbone is the fast Clenshaw algorithm. The MREPDE is coupled with the fully vectorized source term of the discrete PBE and is accelerated by reducing the rank of the fusion rate matrix using the SVD. With this SVD of the popular Coulaloglou and Tavlarides fusion rate, it is found a rank of order 5 is sufficient to produce accurate approximation of the exact matrix. On the other hand, the Clenshaw algorithm is extended and used to evaluate the Legendre series in the MREPDE which reduced the order of complexity from O(M2) to O(M). Based on this, the CPU time average ratio between the fast and standard implementation of the MREPDE is found up to 7 times as the number of sampling points approaches 50 nodes. Our fast implementation is found extremely accurate in estimating the population density and its global moments when compared to the InvQMOM.

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