Presentation of the DQMOM

The reference method to computationally solve a bivariate PBE equation is the Direct Quadrature Method of Moments (DQMOM). The DQMOM make an approximation of the distribution function $f(n_A, n_D)$ by a quadrature of N points (Marchisio et al. 2005, Fox 2006).

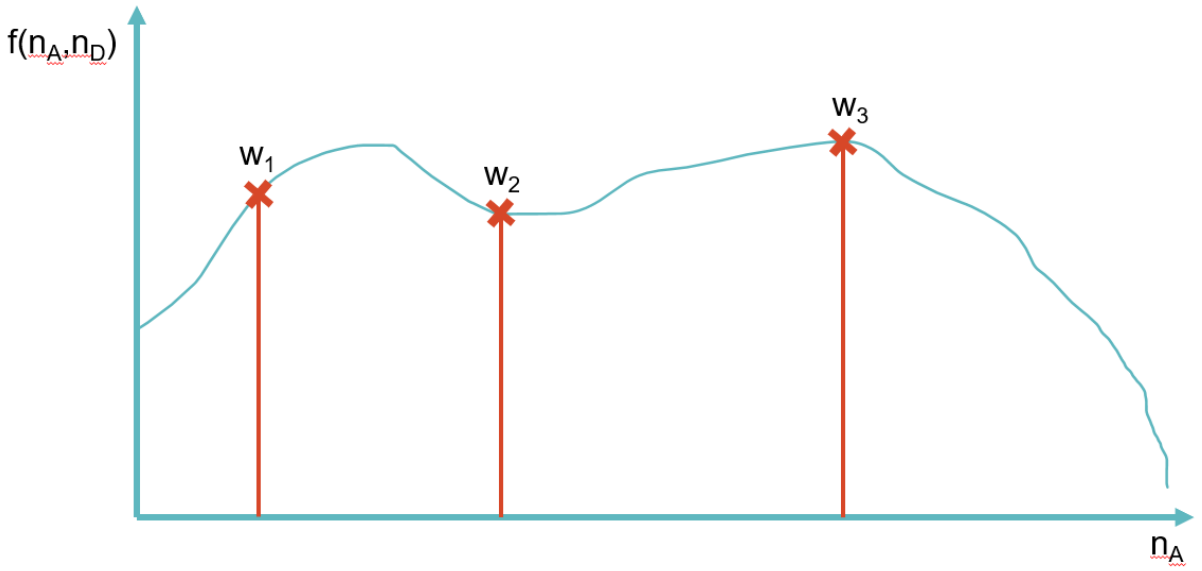

Figure 1: Schematic representation of a quadrature of N=3 points of the distribution function $f(n_A,n_B)$.

As you can see on the figure 1, with $f(n_A,n_D)$ giving the proportion of aggregates containing n_A strains A and n_D strains D, the distribution is represented by 3 weighted points w_1 to w_3, so here in each time step, only 9 equations will be calculated in place to all couples (n_A,n_D) possible.
In other words, each weight w_1 to w_3 corresponds to a couple of numbers of particles on aggregates (n_{A1}, n_{D1}) to (n_{A3}, n_{D3}). These initial weights and abscissas represent couples of numbers (n_A,n_B). From an initial distribution, weights can be chosen wisely to represent hot points of the distribution such as the mean, the maximum, the variance or the symmetry of the distribution.

The DQMOM will calculate moments of a distribution function, not solve directly the proposed equation, so the whole distribution function on an instant t will be synthesized into N nodes representing N weights corresponding to N couples of particle numbers (n_A,n_D) following the next equation:

$$f(n_A, n_B) = \sum_{i=1}^{N} w_i(n_A, n_B)\delta(n_A - n_{Ai})\delta(n_D - n_{Di}) \qquad (1)$$

with δ the Dirac function, $\delta(n - n_i) = 1$ when $n = n_i$ and $\delta = 0$ in other cases and $w_i(n_A, n_B)$ the weight associated with the Dirac (Marchisio et al. 2005).

Then we define a moment of the distribution:

$$m_{ij} = \sum_{k=1}^{N} w_k n_{Ak}^{i} n_{Dk}^{j} \qquad (2)$$

With this equation, we are able to evaluate 4 moments, all with a physical signification (Zucca et al. 2007):

$$m_{00} = \sum_{k=1}^{N} w_k \quad (3)$$

Represents the sum of weights chosen.

$$m_{10} = \sum_{k=1}^{N} w_k n_{Ak}^{i} \qquad (4)$$

Represents the mass conservation of strains A on the system.

$$m_{01} = \sum_{k=1}^{N} w_k n_{Dk}^{j} \qquad (5)$$

Represents the mass conservation of strains D on the system.

$$m_{11} = \sum_{k=1}^{N} w_k n_{Ak} n_{Dk} \qquad (6)$$

Represents the mean number of particles on aggregates.

The DQMOM calculates our equation in the form of moments, so the equation to be solved becomes (Marchisio et al. 2005):

$$\frac{dm_{ij}(n_A, n_B)}{dt} = \frac{1}{2} \sum_{k=1}^{N} \sum_{l=1}^{N} w_k w_l \beta \Gamma [(n_{Ak} + n_{Al})^{i} (n_{Dk} + D_{Dl})^{j} - n_{Ak}^{i} n_{Dk}^{j} - n_{Al}^{i} n_{Dl}^{j}] \qquad (7)$$

On the right hand-side of the equation is our model proposed in the moment form. To become a linear equation, and solve it by matrix inversion, the left-hand side has to be built as follows (Fox 2006):

$$\frac{dm_{ij}(n_A, n_B)}{dt} = \sum_{k=1}^{N} (1 - i - j) n_{Ak}^{i} n_{Dk}^{j} + i n_{Ak}^{i-1} n_{Dk}^{j} + j n_{Ak}^{i} n_{Dk}^{j-1} \qquad (8)$$

For a preliminary assay, we have chosen N=2 so 6 equations have to be solved to find for each time step two weights w_1, w_2 and four abscissas n_{A1}, n_{A2}, n_{D1}, n_{D2}. In that way 6 couples of power (i,j) have to be chosen wisely to create 6 different equations of moments. We have chosen the following set for numeric calculations because it takes into account all outstanding interest moments (3-4-5-6) (Fox 2006).

$$v_i = [0\ 1\ 0\ 1\ 2\ 1] \qquad (9)$$

$$v_j = [0\ 0\ 1\ 1\ 0\ 2] \qquad (10)$$

Equations (7) and (8) are assembled on matrices A and D. On each time step the following matrix equation is solved to find numbers on the α matrix containing abscissas and weights at the time step considered.

$$A\alpha = D \Leftrightarrow \alpha = A^{-1}D \quad (11)$$

The DQMOM takes input points representing a certain distribution of aggregates, and does not allow zero-values. In that way, we had to choose two weights (w_1,w_2) and two pairs of abscissas (n_{A1},n_{A2}) and (n_{D1},n_{D2}). To represent a punctual distribution with an ideal concentration ratio supposed to be $\frac{n_A}{n_D} = 1$ corresponding to the smallest aggregate possible, so for the particle with one strain A and one strain D, the first weight was fixed to 0.99%, and the second was fixed to 0.005% to represent an aggregate with two strains A and two strains D. In that way, when we integrate along abscissas, we obtain the overall proportion of strains A equal to 1 (likewise for strains D). In that way the proportion of all particles is 2.

The number of nodes, weights and abscissas chosen for all simulations to solve the PBE with the DQMOM are on the following table:

Variable	Name of the variable	Variable on Matlab	Value(s)
N	Number of nodes	N	2
n_A	Number of strains A considered on the first aggregate	L11	1
n'_A	Number of strains A considered on the second aggregate	L12	2
n_D	Number of strains D considered on the first aggregate	L21	1
n'_D	Number of strains D considered on the second aggregate	L22	2
w_1	Percentage of the first aggregate considered	w1	0.99
w_2	Percentage of the second aggregate considered	w2	0.01