Stochastic weighted particle methods for fragmentation, coagulation and spatial inhomogeneity

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Introduction

- In this work, we develop stochastic particle methods to solve population balance models with multiple compartments.
- Two popular stochastic particle methods:
  - Direct simulation algorithm (DSA)
  - Stochastic weighted algorithm (SWA)
- Application of stochastic particle methods in problems with spatial inhomogeneity is relatively new
- In particular, this work presents a family of fragmentation algorithms for SWA

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Introduction

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- Two popular stochastic particle methods:
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- Application of stochastic particle methods in problems with spatial inhomogeneity is relatively new
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DSA (Direct Simulation Algorithm)

- Each computational particle represent the same number of real particles
- Coagulation events delete the original coalescing particles to create a new particle. This leads to a numerical issue where the ensemble will eventually deplete:
  - A **doubling algorithm** is used where the ensemble is duplicated when the number of particles falls below 3/8 of ensemble size
- Breakage increases number of particles
  - **Downsampling** may be necessary to avoid memory problems

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SWA (Stochastic Weighted Algorithm)

- A statistical weight is attached to each computational particle
- The statistical weight is representative of the number of particles
- Coagulation events do not change the number of computational particles, only the weights are adjusted
- No need for doubling algorithm – ideal for applications with high coalescence rates
- Inception (and breakage) introduce new particles and require **downsampling**

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Fragmentation: model definition

- A particle (*x*) breaks into particles (*y*) and (*x*-*y*) with the frequency *g*(*x*):

$$(x) \rightarrow (y), (x - y)$$

- The fragment particles (*y*) and (*x*-*y*) are defined by a probability density function

$$\beta(x, y)$$

- where (*y*) < (*x*).

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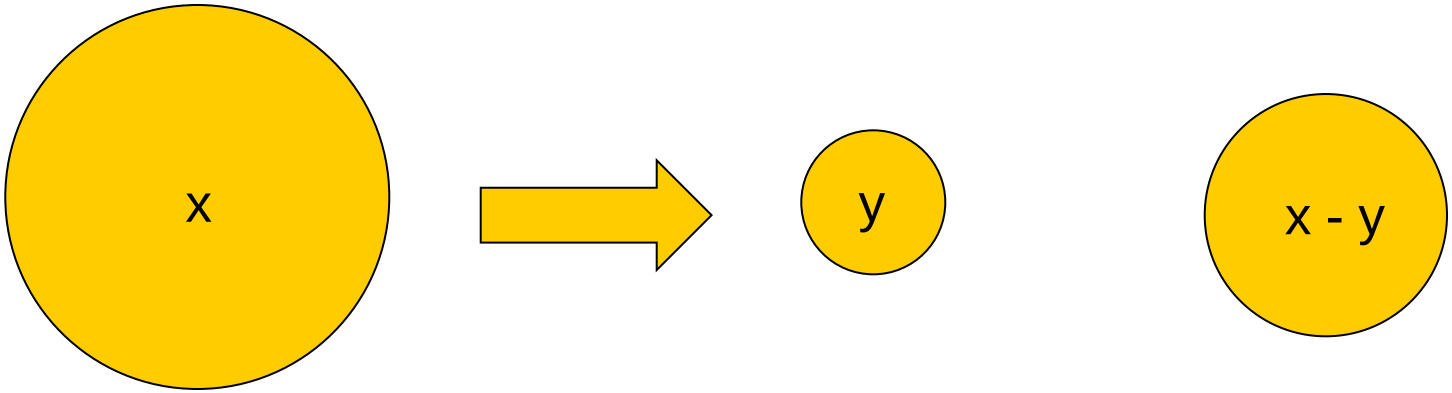
Fragmentation: DSA



Particles break at the frequency:

$$g(x)$$

Waiting time = $\sum g(x)$

Size of y is selected according to:

$$\beta(x, y)$$

(symmetric)

The second fragment is determined as a function of y:

$$x - y$$

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Fragmentation: SWA

- Particle weights are no longer identical
- Main purpose: Perform breakage processes which change one particle at a time, i.e.

$$(x, w_x) \rightarrow (y, w_y)$$

- In order to simulate the process accurately, we need to define an appropriate weight transfer function, γ, to calculate w_y

$$\begin{aligned} w_y &= \gamma(x, w_x, y) \\ &= w_x \alpha(x, y) \end{aligned}$$

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Fragmentation: SWA

- Our algorithm will have the correct approximation if alpha is defined according to the restriction below:

$$\frac{1}{\alpha(x,y)} + \frac{1}{\alpha(x,x-y)} = 1$$

- Two definitions are used in our studies:

SWA1	$\alpha(x,y) = 2$	Simplest solution but not efficient
SWA2	$\alpha(x,y) = \frac{m(x)}{m(y)}$	Conserves total mass

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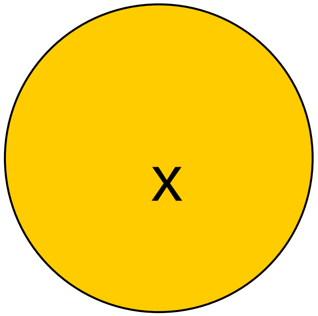
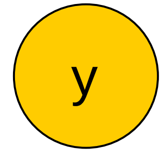
Fragmentation: SWA



$$w_x$$

Particles are tagged with statistical weights



$$w_y > w_x$$

$$w_y = w_x \times \alpha(x,y)$$

Fragmentation frequency: $g(x)$

Waiting time = $\sum g(x)$

Size of y is selected according to:

$$\frac{w_x}{w_y}\beta(x,y)$$

(No longer symmetric)

w_y is determined by the weight transfer function

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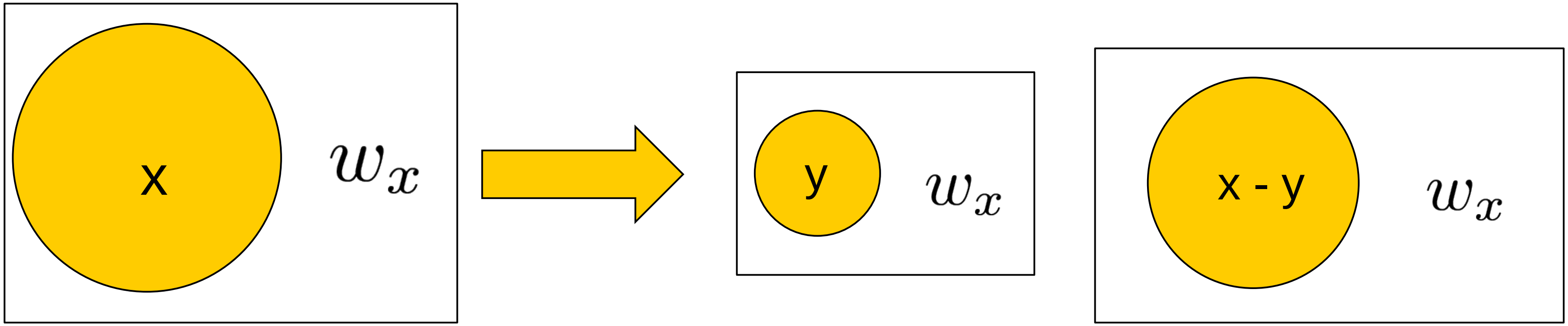
Fragmentation: SWA/DSA alternative



Fragmentation frequency: $g(x)$

Size of y is selected according to: $\beta(x, y)$

Waiting time = $\sum g(x)$

Fragments are given the same weights, but this jump process increase the number of particles

SWA3

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Fragmentation: simulation algorithm

	DSA	SWA1	SWA2	SWA3
Waiting time	$\sum g(x)$			
Selection of particle to break	$g(x)/\sum g(x)$			
Selection of fragment particles	$\beta(x,y)$	$\frac{w_x}{w_y}\beta(x,y)$		$\beta(x,y)$
Jump process	$(x) \to (y), (y-x)$	$(x, w_x) \to (y, w_y)$		$(x, w_x) \to (y, w_x), (y-x, w_x)$
Weight transfer function	N/A	$w_y = 2w_x$	$w_y = \frac{m(x)}{m(y)} w_x$	N/A

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Coagulation: model definition

- A particle (*x*) coagulates with particle (*y*) to form a larger particle (*x*+*y*):

$$(x), (y) \rightarrow (x+y)$$

- The rate is specified by a kernel

$$K(x,y)$$

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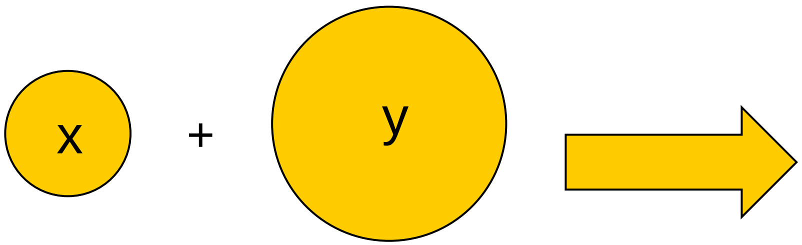
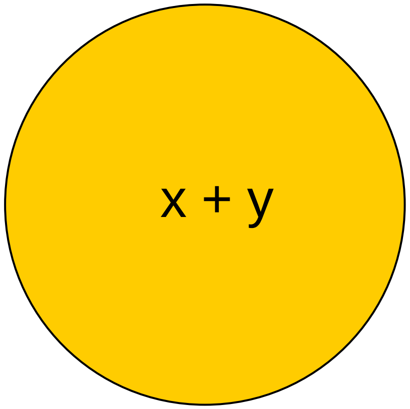
Coagulation: DSA





Both particles are selected uniformly

Each pair coagulates at the rate = $\frac{K(x,y)}{n}$

Total waiting time = $\frac{1}{2}\sum_{x \neq y} \frac{K(x,y)}{n}$

n = normalisation parameter

DSA depletes the number of particles

Doubling algorithm is necessary to prevent ensemble from depletion

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Coagulation: SWA

- Particle weights are no longer identical
- Main purpose: Perform coagulation jumps by changing one particle at a time, *i.e.*

$$(x, w_x), (y, w_y) \to (x + y, w_{x+y}), (y, w_y)$$

- At the rate $\dfrac{\widehat{K}(x, w_x, y, w_y)}{n} = \dfrac{K(x, y) w_y}{n}$

- The weight w_{x+y} is defined as

$$w_{x+y} = w_x \times \frac{m(x)}{m(x+y)}$$

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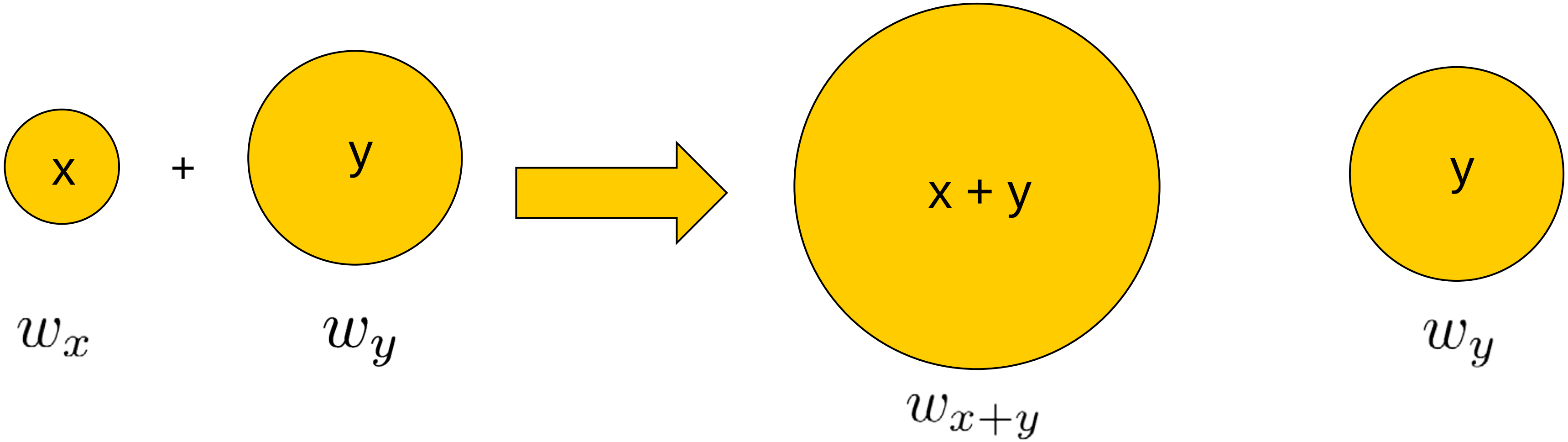
Coagulation: SWA



Each pair coagulates at the rate: $\frac{K(x,y)w_y}{n}$

Total waiting time = $\frac{\sum K(x,y)w_y}{n}$

n = normalisation parameter

w_{x+y} is determined by the weight transfer function

Only 1 particle is changed at a time

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Coagulation: simulation algorithms

	DSA	**SWA1/2/3**
Waiting time	$\frac{1}{2}\sum_{x\neq y}\frac{K(x,y)}{n}$	$\sum_{i\neq j}\frac{K(x,y)w_y}{n}$
Selection of particle 1	Uniform	Uniform
Selection of particle 2	Uniform	$\frac{w_y}{\sum w}$
Jump process	(x), (y) (x + y)	(x, w_x), (y, w_y) $(x + y, w_{x+y})$, (y, w_y)
Weight transfer function	N/A	$w_{x+y} = \frac{m(x)}{m(x+y)} w_x$

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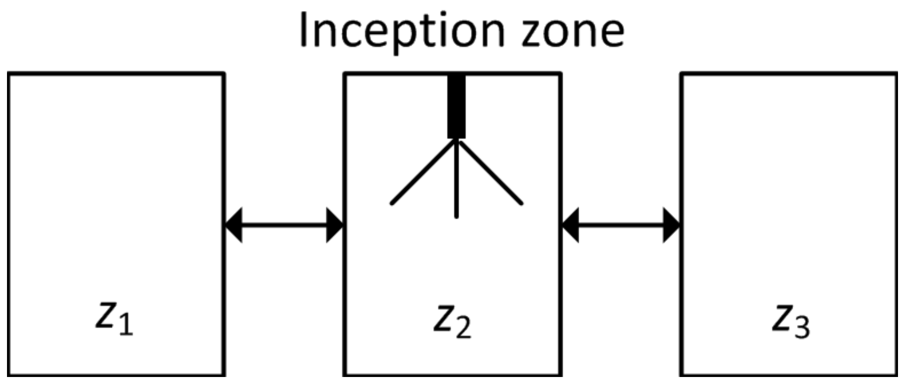
Compartmental model - Transport



Normalisation parameter	$n(z_1)$	$n(z_2)$	$n(z_3)$
Residence time	$\tau(z_1)$	$\tau(z_2)$	$\tau(z_3)$
Rate of particle leaving	$\frac{1}{\tau(z_1)}$	$\frac{1}{\tau(z_2)}$	$\frac{1}{\tau(z_3)}$
Particle destination	100% to z_2	50% to z_1 50% to z_3	100% to z_2

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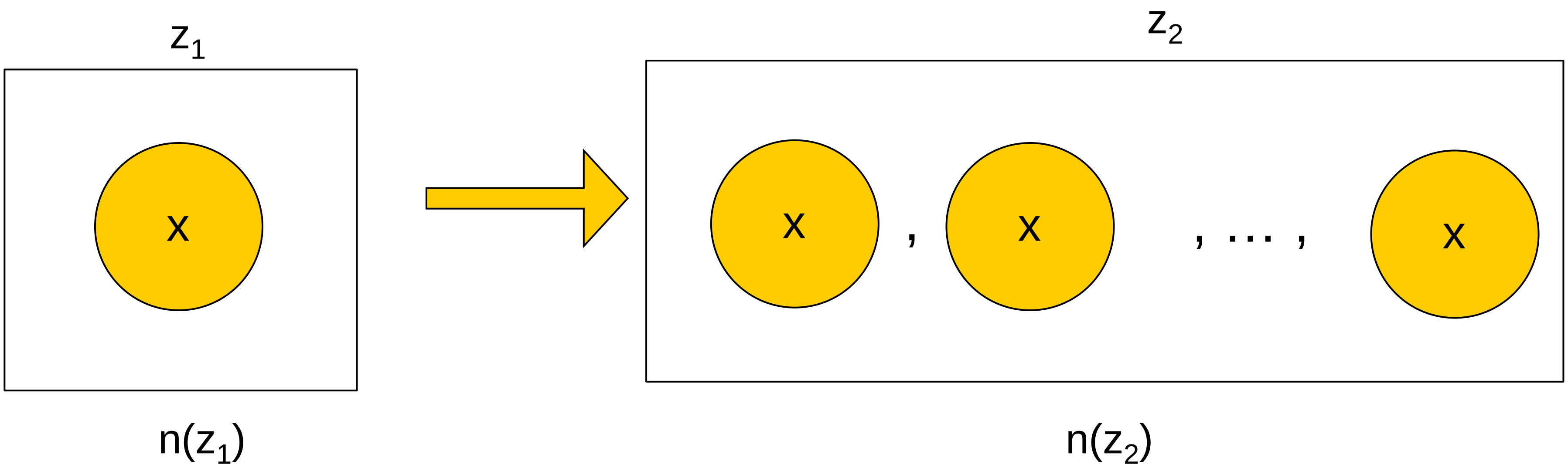
Transport: DSA



Number of copies is determined randomly by the ratio of normalisation parameters

$$n_c \approx \frac{n(z_2)}{n(z_1)} \longrightarrow$$ Usually not an integer

Rate = $\dfrac{1}{\tau(z_1)}$

Decide randomly between $\lfloor \frac{n(z_2)}{n(z_1)} \rfloor + 1, \lfloor \frac{n(z_2)}{n(z_1)} \rfloor$

$$u < \frac{n(z_2)}{n(z_1)} - \lfloor \frac{n(z_2)}{n(z_1)} \rfloor$$

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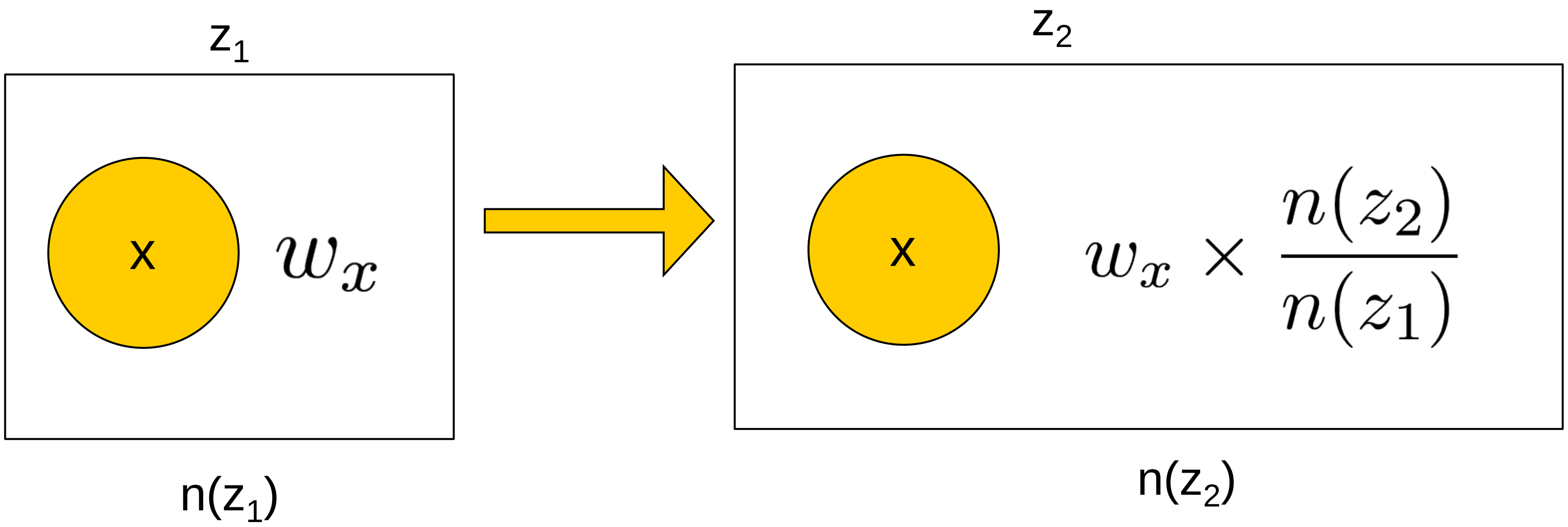
Transport: SWA



Rate = $\frac{1}{\tau(z_1)}$

No need to determine the number of copies randomly with the presence of statistical weights

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Test system

- Type space $\mathcal{X} = \{1, 2, 3, \ldots\}$
- So the system can be written as a series of ODEs
- Analysed the performances of the algorithms at different rates
- Constant coagulation kernel (only differ in different compartments):

$$K(z, x, y) = k_{\text{coag}}(z)$$

- Fragmentation: Frequency proportional to size and a fragmentation probability density β

$$g(z, x) = x k_{\text{frag}}(z) \qquad \beta(x, y) = \frac{1}{x - 1}$$

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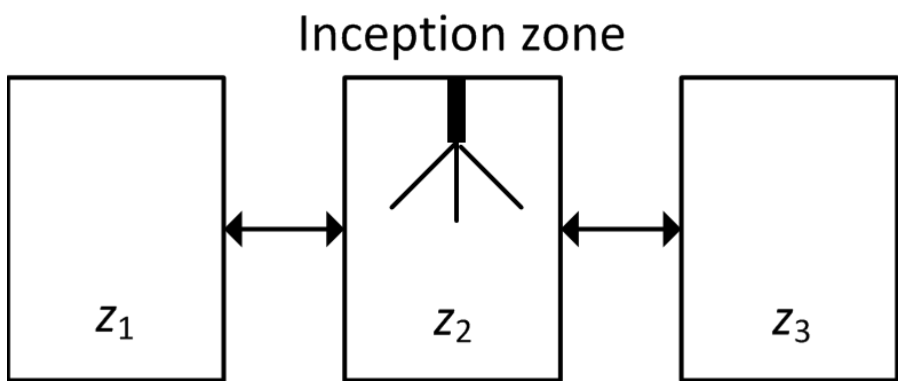
Test system: compartmental model



Normalisation parameter	$n(z_1)$	$n(z_2)$	$n(z_3)$
Residence time	$\tau(z_1)$	$\tau(z_2)$	$\tau(z_3)$
Rate of particle leaving	$\frac{1}{\tau(z_1)}$	$\frac{1}{\tau(z_2)}$	$\frac{1}{\tau(z_3)}$
Particle destination	100% to z_2	50% to z_1 50% to z_3	100% to z_2

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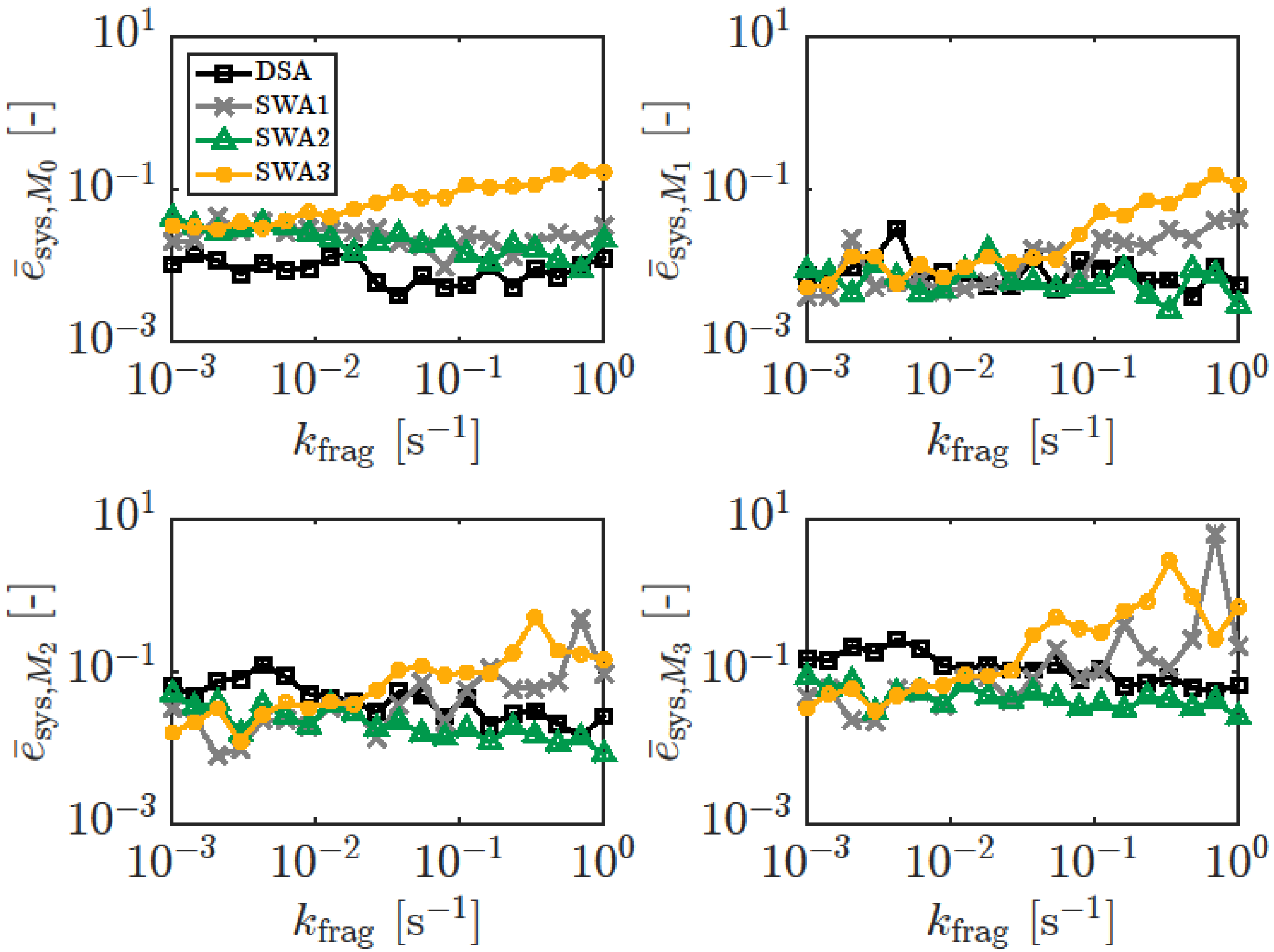
Errors at different frag. rates for each algorithm



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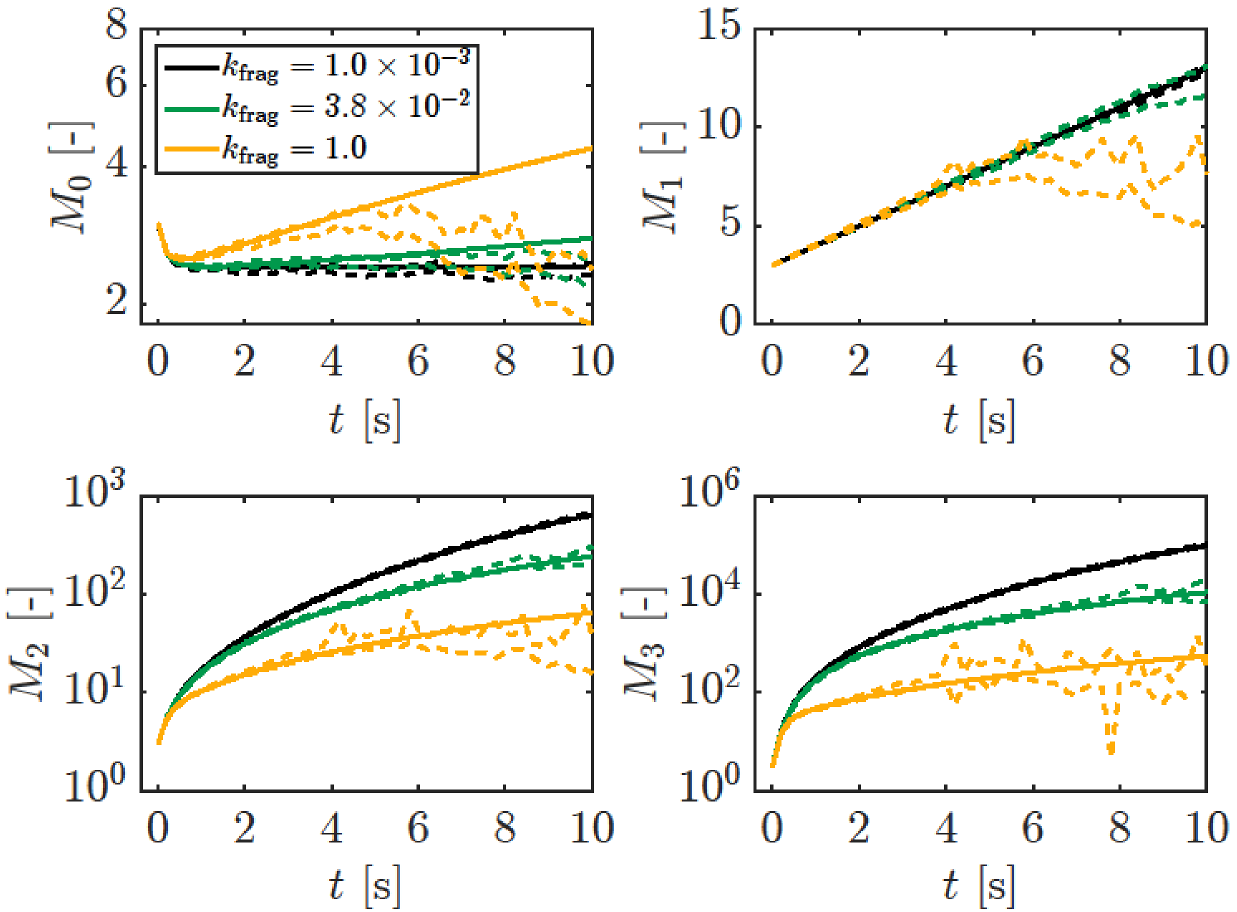
SWA3 – worst algorithm
errors increase with frag. rate



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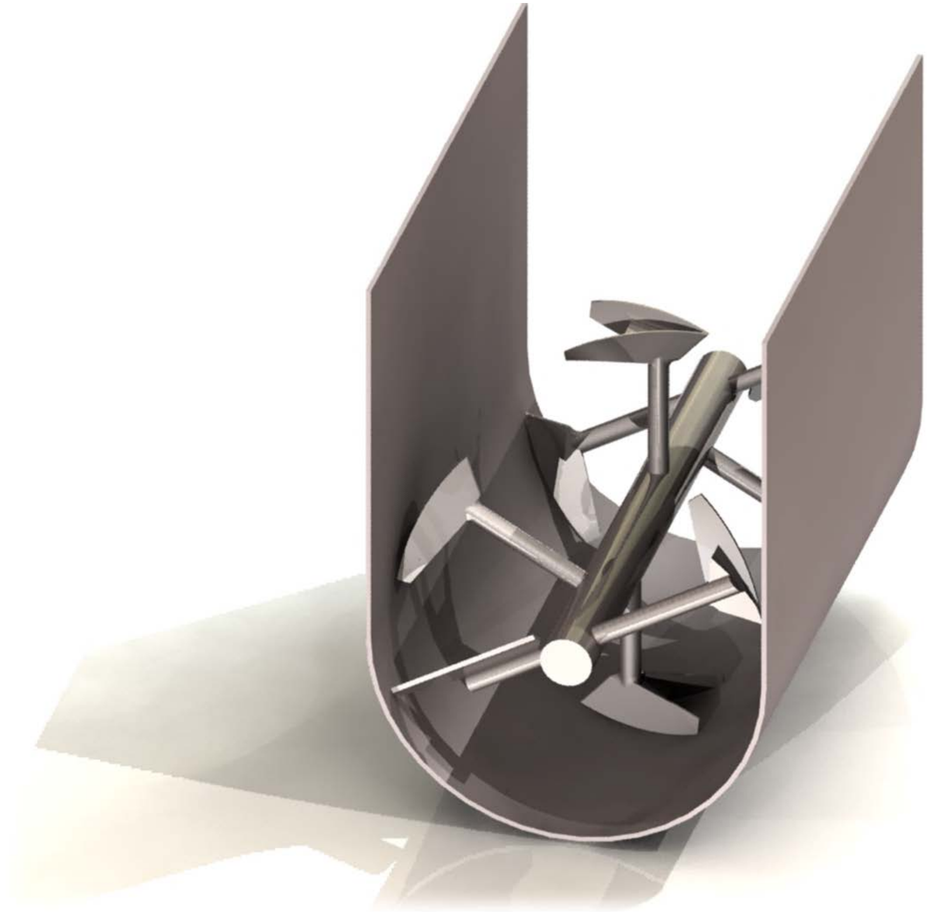
Experimental system



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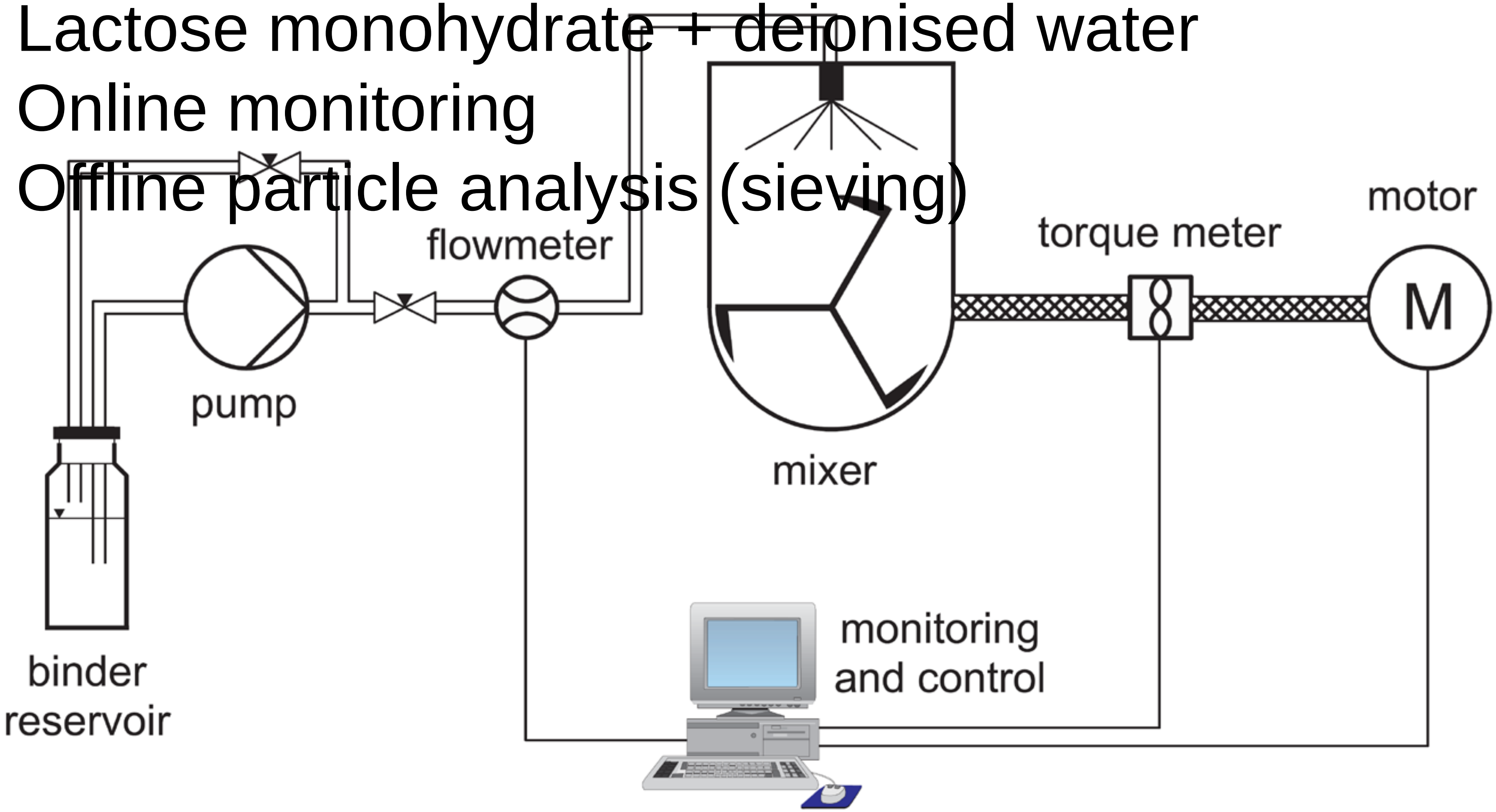
Experimental system

- Bench scale system
- Lactose monohydrate + deionised water
- Online monitoring
- Offline particle analysis (sieving)



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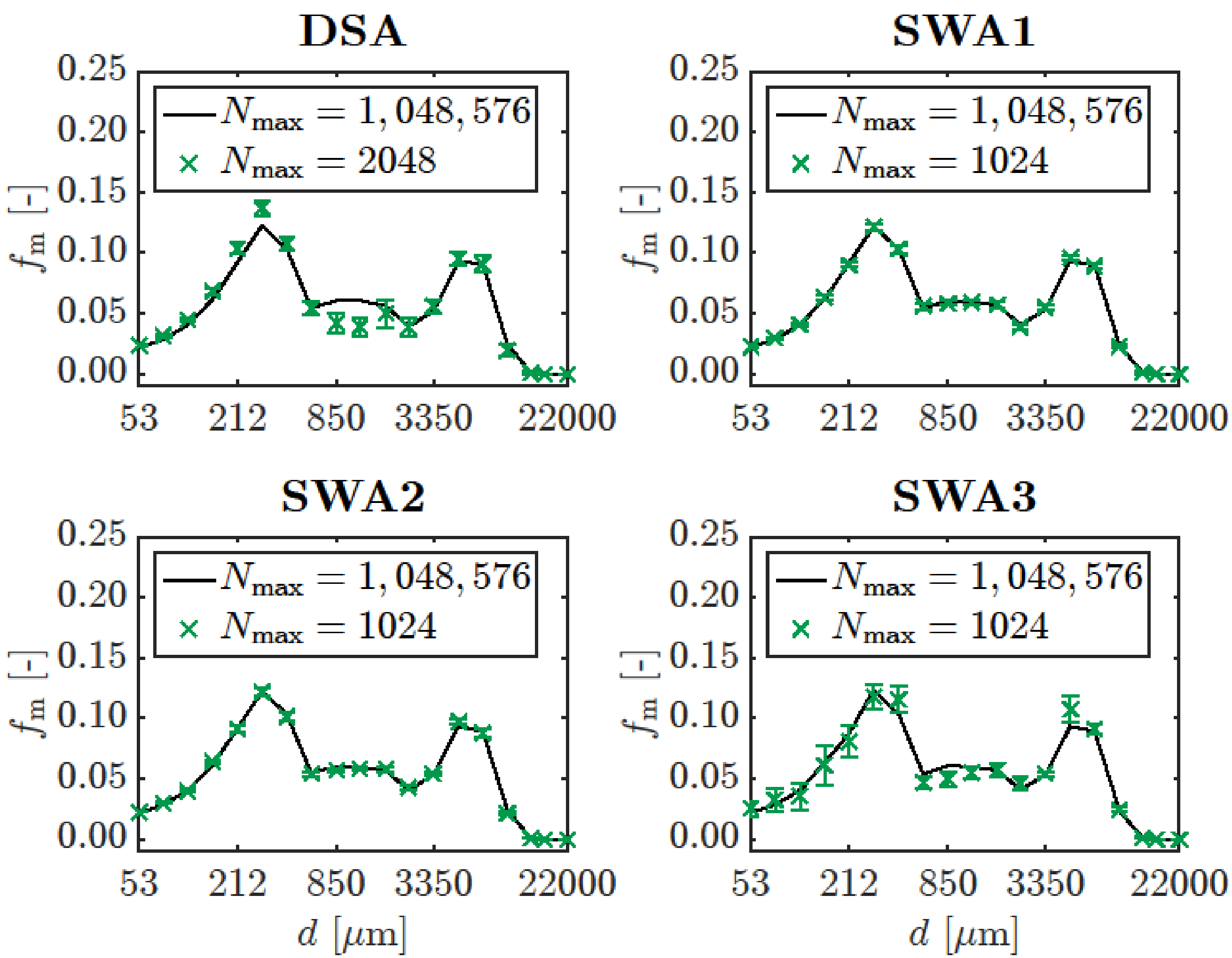
Computational efficiency



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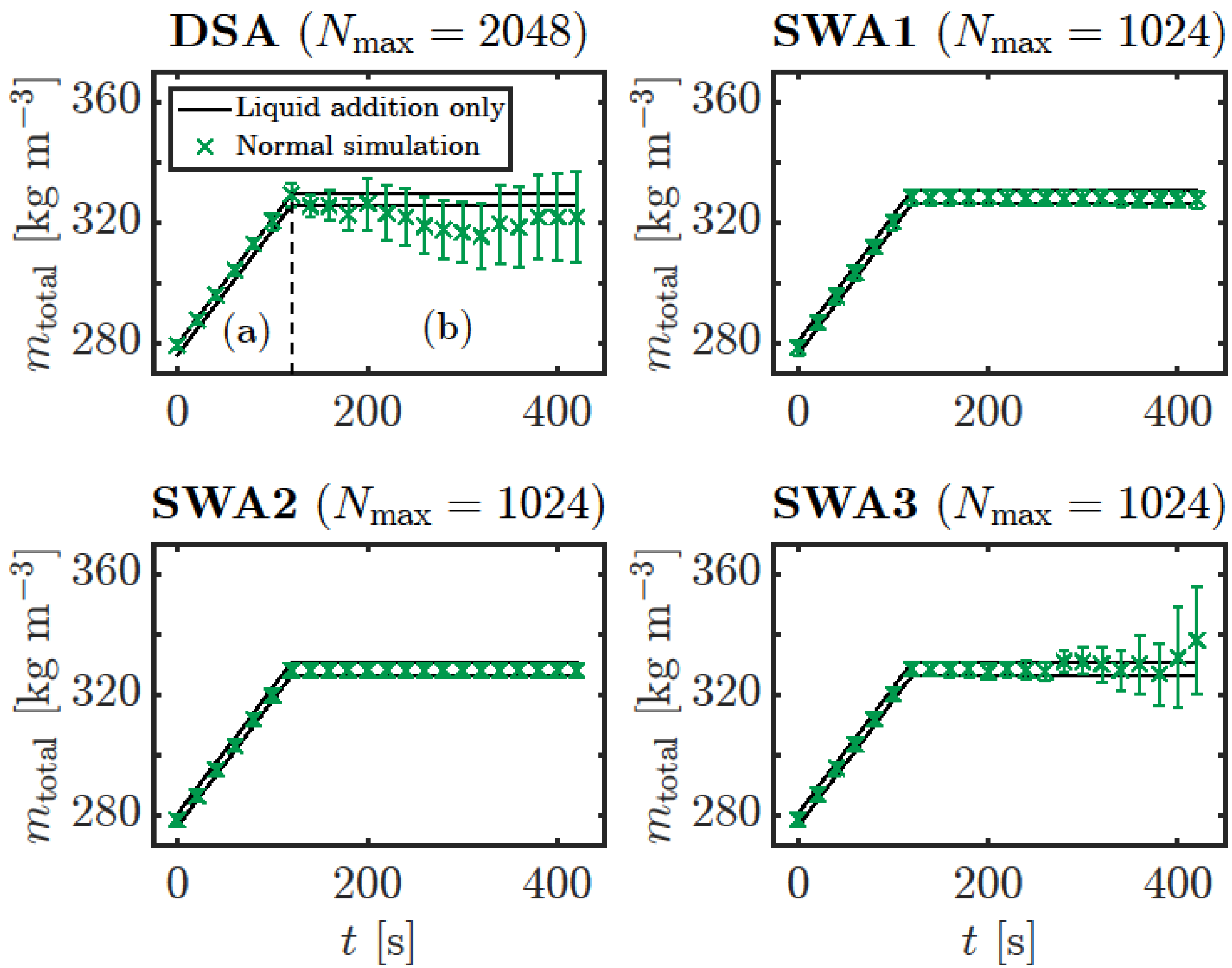
Problems with DSA and SWA3 - fluctuation of mass



DSA: Error mainly from transport

SWA3: Error mainly from particle deletions

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Conclusions

- A new family of fragmentation algorithms for weighted particles have been introduced in the context of granulation models
- All the algorithms converge to the same solution, but the new algorithms are more efficient
- The fragmentation algorithms are applied to a multi-dimensional population balance model
- It is found that the new algorithms provide significant numerical stability (e.g. negligible fluctuation in total mass)

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Acknowledgements

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