POPULATION BALANCE EQUATION FOR COLLISIONAL FRAGMENTATION

Arijit Das

Friedrich-Alexander-Universität
DYNAMICS, CONTROL, MACHINE LEARNING AND NUMERICS

FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

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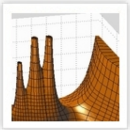

X Partial differential equations, optimal design and numerics
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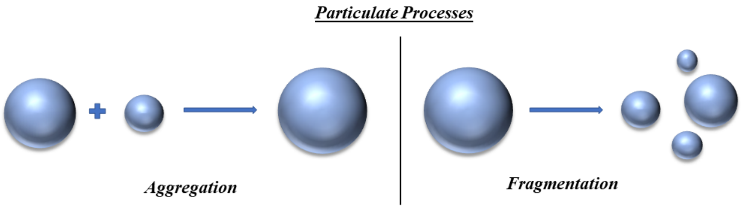
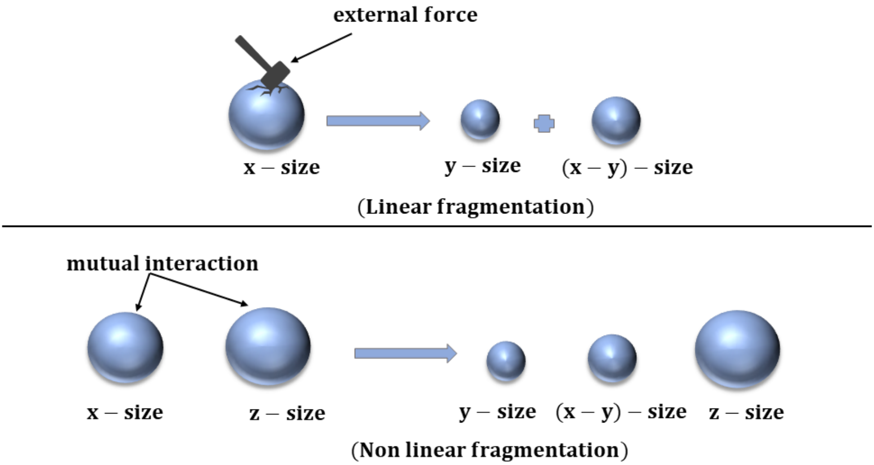
Outline of the presentation

- General introduction: The nonlinear collisional fragmentation model
- Existence, uniqueness and asymptotic analysis
- Finite volume discretization: A mass conserving number preserving scheme
- Numerical test for mass conservation and shattering transition
- Conclusions and future scopes

General introduction



Linear and nonlinear fragmentation



Collisional breakage equation

The pure binary nonlinear collisional breakage equation is given by

$$\frac{\partial \varphi(x,t)}{\partial t} = \int_0^\infty \int_x^\infty \mathcal{B}(x|y,z)\mathcal{K}(y,z)\varphi(y,t)\varphi(z,t)\mathrm{d}y\mathrm{d}z - \int_0^\infty \mathcal{K}(x,y)\varphi(x,t)\varphi(y,t)\mathrm{d}y \quad (1)$$

Supported with the initial data:

$$\varphi(x,0) = \varphi_0(x)(\geq 0) \quad \text{for all} \quad x \in (0,\infty) \quad (2)$$

$\mathcal{B}$ satisfies the following properties:

$$\mathcal{B}(x|y,z) = 0 \quad \text{for all} \quad x \geq y, \quad \text{and} \quad \int_0^y x\mathcal{B}(x|y,z)\mathrm{d}x = y; \quad (3)$$

$$\int_0^y \mathcal{B}(x|y,z)\mathrm{d}x = \nu(y,z) < \infty \quad \text{for all} \quad y > 0, z > 0. \quad (4)$$

Moment functions

The $p-$th order moment of the solution to the fragmentation equation:

$$\mathcal{M}^{(p)}(t) = \int_0^\infty x^p \varphi(x,t)\mathrm{d}x, \qquad \text{and} \qquad \mathcal{M}_m^{(p)}(t) = \int_m^\infty x^p \varphi(x,t)\mathrm{d}x.$$

- Total mass of the particles present in the system:

$$\mathcal{M}^{(1)} = \int_0^\infty x\varphi(x,t)\mathrm{d}x.$$

- Total number of the particles present in the system:

$$\mathcal{M}^{(0)} = \int_0^\infty \varphi(x,t)\mathrm{d}x.$$

The system obeys the mass conservation law:

$$\frac{\mathrm{d}\mathcal{M}^{(1)}(t)}{\mathrm{d}t} = 0 \implies \mathcal{M}^{(1)}(t) = \mathcal{M}^{(1)}(0).$$

Solution

We consider the solution space

$$\Psi_{r,\sigma} := L^1\left[(0,\infty)\,;\left(x^r + x^{-2\sigma}\right)\mathrm{d}x\right] \qquad \text{for} \qquad r \geq 1, \sigma > 0.$$

Also $\Psi^+_{r,\sigma}$ be the positive cone of the space $\Psi_{r,\sigma}$.

Definition

Let $T \in (0,\infty)$. A solution of the IVP (1)-(2) is a function $\varphi : [0, T] \longrightarrow \Psi^+_{r,\sigma}$ such that for $x > 0$ a.e.

1. $\varphi(x,\cdot)$ is continuous on $[0, T]$,
2. for all $t \in [0, T]$, $\int_0^t \int_0^\infty \int_0^\infty \mathcal{K}(y,z)\varphi(y,t)\varphi(z,t)\mathrm{d}y\mathrm{d}z\mathrm{d}s < +\infty$,
3. for all $t \in [0, T]$,

$$\varphi(x,t) = \varphi_0(x) + \int_0^t \left[\int_0^\infty \int_x^\infty \mathcal{B}(x|y,z)\mathcal{K}(y,z)\varphi(y,t)\varphi(z,t)\mathrm{d}y\mathrm{d}z - \int_0^\infty \mathcal{K}(x,y)\varphi(x,t)\varphi(y,t)\mathrm{d}y\right]\mathrm{d}s.$$

Assumptions

(A1) The collisional kernel $\mathcal{K}(x,y) \leq k\dfrac{(1+x+y)^{\lambda}}{(x+y)^{\sigma}}$, for some constants k, $\lambda, 0 \leq \sigma < \frac{1+\nu}{2}$ satisfying $\sigma \leq \lambda \leq \min\{1+\nu+\sigma, r-1\}$, is nonnegative and continuous on $(0,\infty)^2$;

(A2) The fragmentation kernel $\mathcal{B}(x|y,z)$ is nonnegative and continuous on $(0,\infty)^3$ and satisfies the 'power-law' rates given by

$$\mathcal{B}(x|y,z) = \begin{cases} (\nu+2)\,\dfrac{x^{\nu}}{y^{\nu+1}}, & \text{when} \quad y > x, \\ 0, & \text{when} \quad x \geq y, \end{cases}$$

for $-1 < \nu \leq 0$.

Well-posedness [1]

Theorem (Existence)

Let the functions $\mathcal{K}(x,y)$ and $\mathcal{B}(x|y,z)$ satisfy the assumptions $(A1)$ and $(A2)$ respectively. If the initial data $\varphi_0(x)$ is continuous and belongs to $\Psi^+_{r,\sigma}$, then the IVP (1)-(2) *has at least one mass conserving solution in $\mathcal{C}\left([0,T];\Psi^+_{r,\sigma}\right)$ for some $T>0$.*

Theorem (Uniqueness)

Let the functions $\mathcal{K}(x,y)$ and $\mathcal{B}(x|y,z)$ be nonnegative and continuous $(0,\infty)^2$ and $(0,\infty)^3$ respectively, and satisfy the conditions $(A1)-(A2)$ with $\sigma=0$ and $0\le\lambda\le\min\{1,r-1\}$. If the initial data $\varphi_0(x)$ is continuous and belongs to $\Psi^+_{r,0}$, then the IVP (1)-(2) *has a unique solution in $\mathcal{C}\left([0,T];\Psi^+_{r,0}\right)$ for some $T>0$.*

[1] Das, A. Saha, J. Mass-Conservation and Finite-Time Shattering transition in a Nonlinear Collisional Fragmentation with Singular Kinetic Rates, *submitted*, (2024).

Sketch of the proof

- **Kernel truncation:**

$$\mathcal{K}_n(x,y) \begin{cases} = \mathcal{K}(x,y), & \text{when} \quad x, y \geq \frac{1}{n}, \text{ and } x, y \leq n, \\ \leq \mathcal{K}(x,y), & \text{otherwise.} \end{cases}$$

- **Relative compactness:** The sequence of solution $\{\varphi_n\}_{n=1}^{\infty}$ is relatively compact over a compact rectangular subset of

$$\Xi = \{(x,t) : 0 < x < \infty, 0 \leq t \leq T\}.$$

  - uniform boundedness of the sequence $\{\varphi_n\}_{n=1}^{\infty}$ is obtained over a compact subset of Ξ.
  - equi-continuity of the sequence $\{\varphi_n\}_{n=1}^{\infty}$

Combining all these results along with the Arzelà-Ascoli theorem ensure that

$$\lim_{n\to\infty} \varphi_n = \varphi$$

uniformly on each compact subset $\Xi_1 = \{(x,t) : \frac{1}{X} < x < X, 0 \leq t \leq T\}$ of Ξ.

Large time analysis [2]

Proposition (Formation of dust particles)

Let the assumptions $(A1)$ *and* $(A2)$ *on the kinetic kernels* $\mathcal{K}$ *and* $\mathcal{B}$ *holds good and in addition, the initial data* $\varphi_0(x)$ *is continuous and belong to* $\Psi^{+}_{r,\sigma}$*, then* $\mathcal{M}^{(0)}(t)$ *is a nondecreasing function. Moreover,* $\mathcal{M}^{(0)} \longrightarrow \infty$ *as* $t \longrightarrow \infty$*.*

[2] Das, A. Saha, J. Mass-Conservation and Finite-Time Shattering transition in a Nonlinear Collisional Fragmentation with Singular Kinetic Rates, *submitted*, (2024).

Finite time shattering

Theorem

Let the kinetic kernels $\mathcal{K}$ and $\mathcal{B}$ have the same growth rate (A1) and (A2) respectively. If the initial data $\varphi_0(x)$ is continuous and belongs to $\Psi^+_{r,\sigma}$ with $\mathcal{Q} := \xi_1(0) < \infty$. There is a constant κ depending on λ and k_0 such that the nonlinear collisional equation (1) has a unique mass conserving solution φ on $[0, T_0)$, where

$$T_0 := \frac{\mathcal{M}_\lambda^{(-\sigma)}(\varphi_0)}{\mathcal{D}(r,\sigma,\lambda)}. \tag{5}$$

where $\mathcal{D}(r,\sigma,\lambda) := \kappa \bar{M}_0 \left(\bar{M}_0 + 2\bar{M}_r\right)$. In particular, $T_{sh} \geq T_0$.

Sketch of the proof

If possible let, there exist a mass conserving solution to the given problem (1)-(2) on $\mathcal{C}\left([0, T^*); \Psi^{+}_{r,\sigma}\right)$ for some $T^* < T_0$.

- Multiplying the equation (1) by the test function $\phi_m(x) := x^m \chi_{[\lambda,\infty]}(x)$ and using the moment estimations, we can obtain

$$\frac{\mathrm{d}\Theta_m^\lambda(t)}{\mathrm{d}t} \geq \frac{\Lambda (1-m)\, \mathcal{Q}^{\frac{-\sigma}{1-m}}}{m+\nu+1} \Theta_m^\lambda (t)^{\frac{1+\sigma-m}{1-m}}. \tag{6}$$

  where

$$\Theta_m^\lambda (\varphi)(t) := \mathcal{A}(r,\sigma,\lambda) + \frac{\Lambda (1-m)\, \mathcal{Q}^{\frac{-\sigma}{1-m}}}{m+\nu+1} \int_0^t \left[\mathcal{M}_\lambda^{(m)}(\varphi(s))\right]^{\frac{1+\sigma-m}{1-m}} \mathrm{d}s,$$

  with $\mathcal{A}(r,\sigma,\lambda) := \mathcal{M}_\lambda^{(-\sigma)}(\varphi_0) - \mathcal{D}(r,\sigma,\lambda)\, T^*$.

- $$t \leq \frac{(m+\nu+1)}{\sigma\Lambda} \mathcal{Q}^{\frac{\sigma}{1-m}} \mathcal{A}(r,\sigma,\lambda)^{\frac{-\sigma}{1-m}}. \tag{7}$$

- Now by taking the limit $t \longrightarrow T^*$ and then $m \longrightarrow -\nu - 1$ on the above relation, we can obtain $T^* = 0$, a contradiction.

Divergence form and discretization

The mass conserving form of nonlinear collisional breakage equation:

$$\frac{\partial (x\varphi(x,t))}{\partial t} = \frac{\partial}{\partial x}\int_0^\infty \int_x^\infty \int_0^x u\mathcal{B}(u|v,w)\mathcal{K}(v,w)\varphi(v,t)\varphi(w,t)\mathrm{d}u\mathrm{d}v\mathrm{d}w, \quad (8)$$

with the initial data $\varphi(x,0) = \varphi_0(x)$.

Let $\Lambda :=]0, x_{\max}]$ be the computational domain and $\Lambda_i := \left]x_{i-1/2}, x_{i+1/2}\right]$, $i = 1,2,\ldots,I$ with $x_{1/2} = 0$, $x_{I+1/2} = x_{\max}$ and $\Delta x_i := x_{i+1/2} - x_{i-1/2}$.

The discrete number density function over the cell Λ_i is calculated as

$$N_i(t) \approx \int_{x_{i-1/2}}^{x_{i+1/2}} \varphi(x,t)\mathrm{d}x.$$

Discrete scheme

The mass conserving finite volume scheme of equation (8) is written as

$$x_i \frac{\mathrm{d}N_i}{\mathrm{d}t} = \mathcal{G}_{i+1/2}(t) - \mathcal{G}_{i-1/2}(t), \tag{9}$$

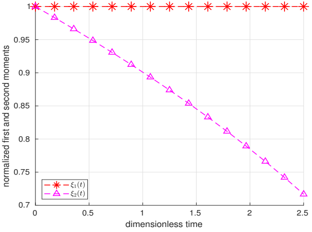
where $\mathcal{G}_{i+1/2}$ is the numerical flux at the right end of i^{th} cell Λ_i and is defined as

$$\mathcal{G}_{i+1/2} := \sum_{p=1}^{I} \sum_{q=i+1}^{I} \sum_{r=1}^{i} \beta_{r,q}^{p} \mathcal{K}_{q,p} N_q(t) N_p(t), \tag{10}$$

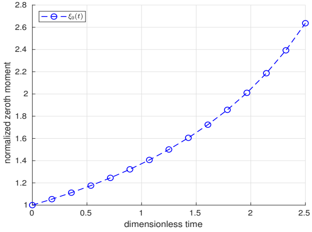
with, $\beta_{r,q}^{p} := \int_{\Lambda_r} x\mathcal{B}(x|x_q, x_p)\mathrm{d}x$, denoting the splitting of particles of size x_q in the interval $\left[x_{r-1/2}, x_{r+1/2}\right]$. The numerical flux at the boundaries of domain $\mathcal{D}$ are taken as

$$\mathcal{G}_{1/2} = 0 \quad \text{and} \quad \mathcal{G}_{I+1/2} = 0. \tag{11}$$

Test case I: $\mathcal{K} = \frac{(x+y)^{2.5}}{(xy)^{0.3}}$, $\mathcal{B} = \frac{2}{y}$ and $\varphi_0(x) = xe^{-x}$



(a)



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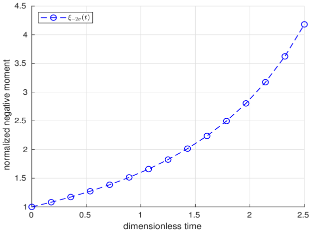

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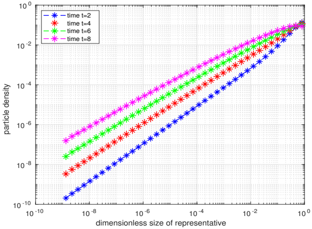
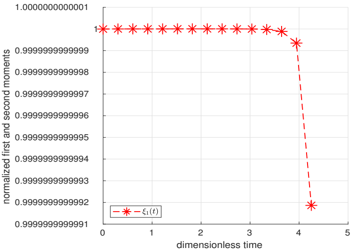


(d)

Finite time shattering and blowup of moments



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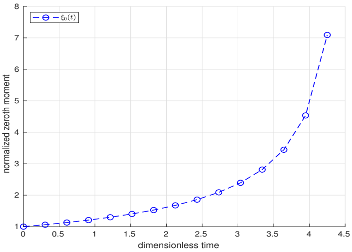

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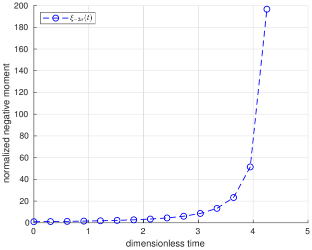


(c)

Predict the other moments with low accuracy

Scheme 1 (MC):

$$x_i \frac{\mathrm{d}N_i}{\mathrm{d}t} = \mathcal{G}_{i+1/2}(t) - \mathcal{G}_{i-1/2}(t), \tag{12}$$

with weight function $\mathcal{G}_{i+1/2} := \sum_{p=1}^{I} \sum_{q=i+1}^{I} \sum_{r=1}^{i} \beta_{r,q}^{p} \mathcal{K}_{p.q} N_q(t) N_p(t).$

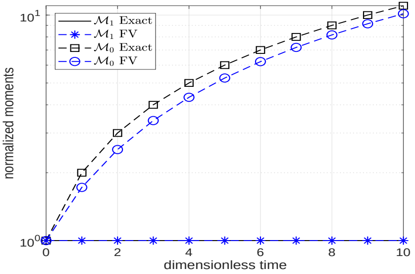


Figure: Comparison of zeroth and first moments predicted by MC scheme for $\mathcal{B}(x|y,z) = \delta(x - 0.4y) + \delta(x - 0.6y)$ and $\varphi_0(x) = \delta(x - 1)$.

Improved formulation with weighted numerical flux[3]

Scheme 2 (MCNP):

$$x_i \frac{\mathrm{d}N_i}{\mathrm{d}t} = \tilde{\mathcal{G}}_{i+1/2}(t) - \tilde{\mathcal{G}}_{i-1/2}(t). \qquad (13)$$

Here, $\tilde{\mathcal{G}}_{i+1/2}$ is the revised weighted numerical flux at the i^{th} cell and is defined as

$$\tilde{\mathcal{G}}_{i+1/2} := \sum_{p=1}^{I} \sum_{q=i+1}^{I} \sum_{r=1}^{i} \beta_{r,q}^{p} \Theta_{q,p} \mathcal{K}_{q,p} N_q(t) N_p(t), \qquad (14)$$

where, the weight function $\Theta_{q,p}$ is defined as,

$$\Theta_{q,p} := \frac{x_q\left(\nu(x_q, x_p) - 1\right)}{\sum_{j=1}^{q} (x_q - x_j) \int_{\Lambda_j} \mathcal{B}(x|x_q, x_p)\mathrm{d}x}, \qquad (15)$$

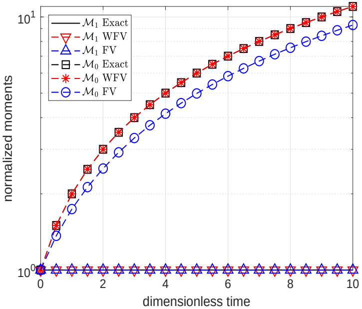
with $\Theta_{1,p} = 0$ and $\tilde{\mathcal{G}}_{1/2} = \tilde{\mathcal{G}}_{I+1/2} = 0$.

[3] Das, A. Kushwah, P. Saha, J. Singh, M. Improved higher-order finite volume scheme and its convergence analysis for collisional breakage equation, *Applied Numerical Mathematics 196 (1), (2024).*

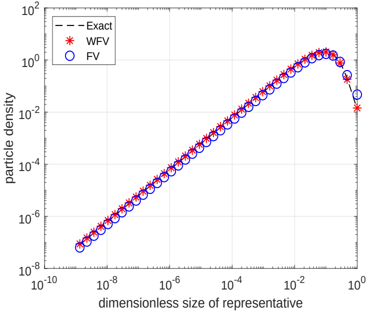
Test case II:

Problem: $\mathcal{B}(x|y;z) = \frac{2}{y}$, $\mathcal{K}(x,y) = xy$ and $n_0(x) = \delta(x-1)$.

Exact solution: $n(t,x) = \exp(-tx)[2t + t^2(1-x)] + \delta(x-1)\exp(-t)$



(a) Dimensionless moments



(b) Number density

Figure: A comparison of numerical results of Test problem I

Concluding discussion

- **Analytical study of the nonlinear fragmentation equation**.
  - Existence of mass conserving solution for a class of unbounded singular collision kernels,
  - The existing mass conserving solution is unique,
  - Due to pure fragmentation, the particles become dust after a large time.

- **Numerical approximation of the nonlinear collisional fragmentation equation**
  - Formulation of a mass conserving number preserving finite volume scheme,
  - Numerical simulations of test problem
  - Finite time shattering.

Future scopes

- Collisional fragmentation with source term

$$\partial_t \varphi(x,t) = \mathcal{Q}(\varphi)(x,t) + \underbrace{V(\varphi,t)}_{source},$$

with the initial condition

$$\varphi(x,0) = \varphi_0(x).$$

Our interest is to find such V for which there exist a sharp time T such that

$$\int_0^\infty x\varphi(x,t) = \int_0^\infty x\varphi_0(x)\mathrm{d}x \quad \text{for} \quad t \geq T.$$

- Being a pure fragmentation model, to achieve the steady state is not possible, however a self similar profile can be obtain for large time scale.

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Thank you