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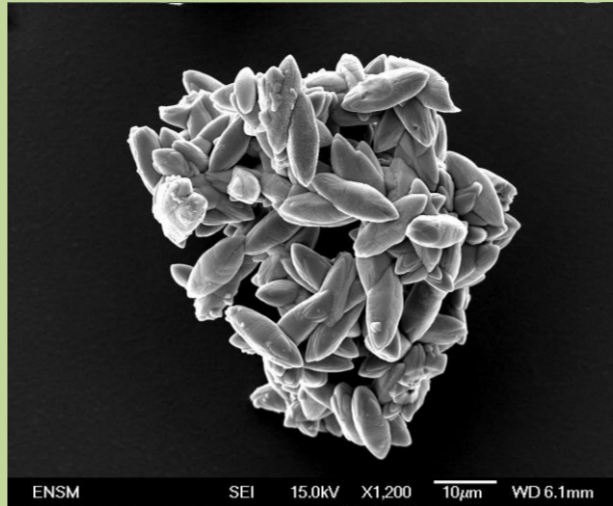
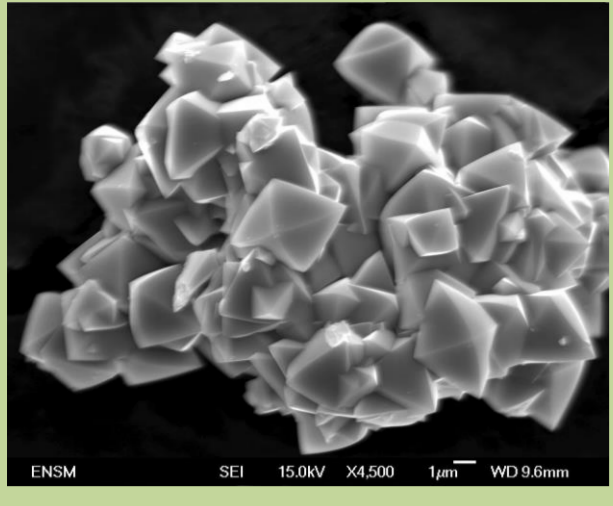
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# Modeling of strongly coupled particle growth and aggregation

## Introduction

**Topic:** Synthesis of fine particles by precipitation including nucleation, growth and aggregation

**Objective:** Modelize the dynamics of a suspension when the aggregation modifies the growth of the particles



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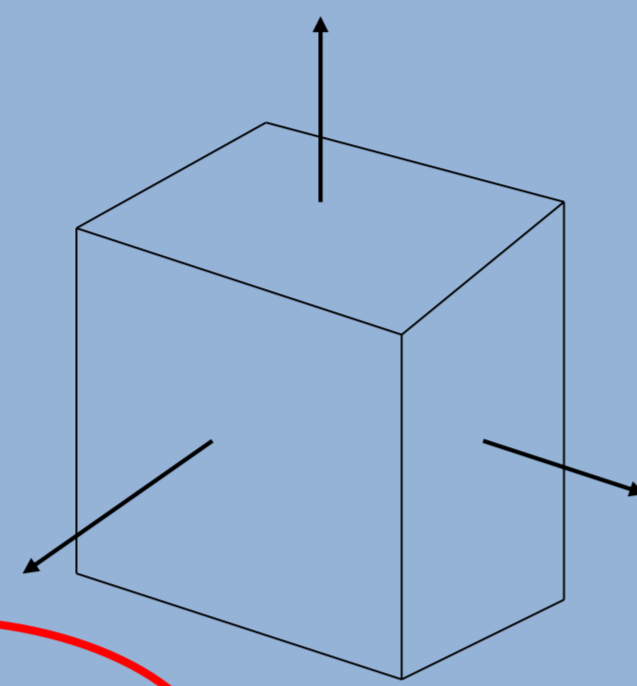
Ecole Nationale Supérieure des Mines  
158 cours Fauriel, Saint-Etienne, France

## Classical modeling: Weakly Coupled Growth & Aggregation

### Growth

1st system: crystal + supersaturated solution

Growth law:  $\frac{dm}{Adt} = \varphi = k S^j \rightarrow \frac{dv}{dt} = G(v)$



**The growth law only depends on the instantaneous state of the system**

2nd system: population of crystals + supersaturated solution

Population balance equation (PBE) for population density  $n(t,v)$

PBE 1D: one internal variable  $v$

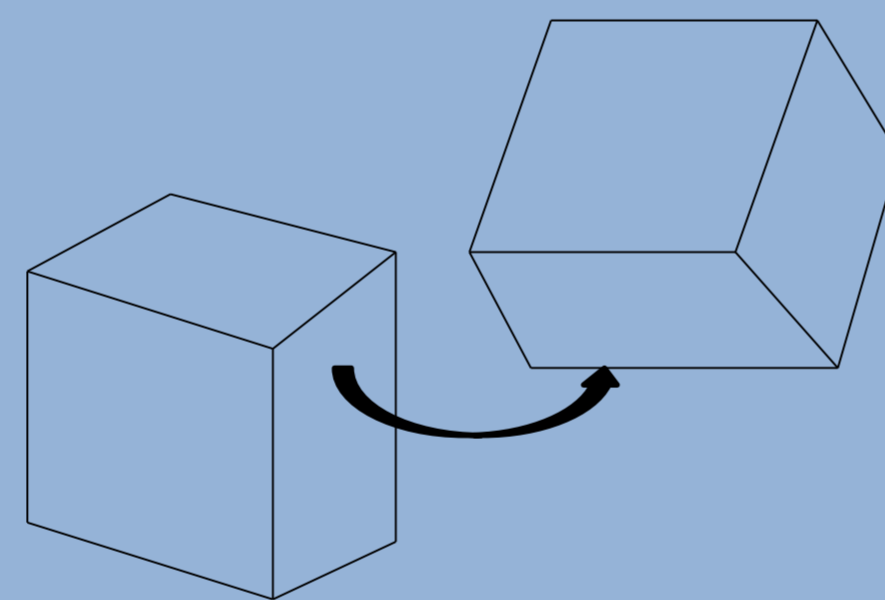
$$\frac{\partial n}{\partial t} = - \frac{\partial G(v)n}{\partial v}$$

### Binary collision – aggregation

Smoluchowski equation

PBE 1D: one internal variable  $v$

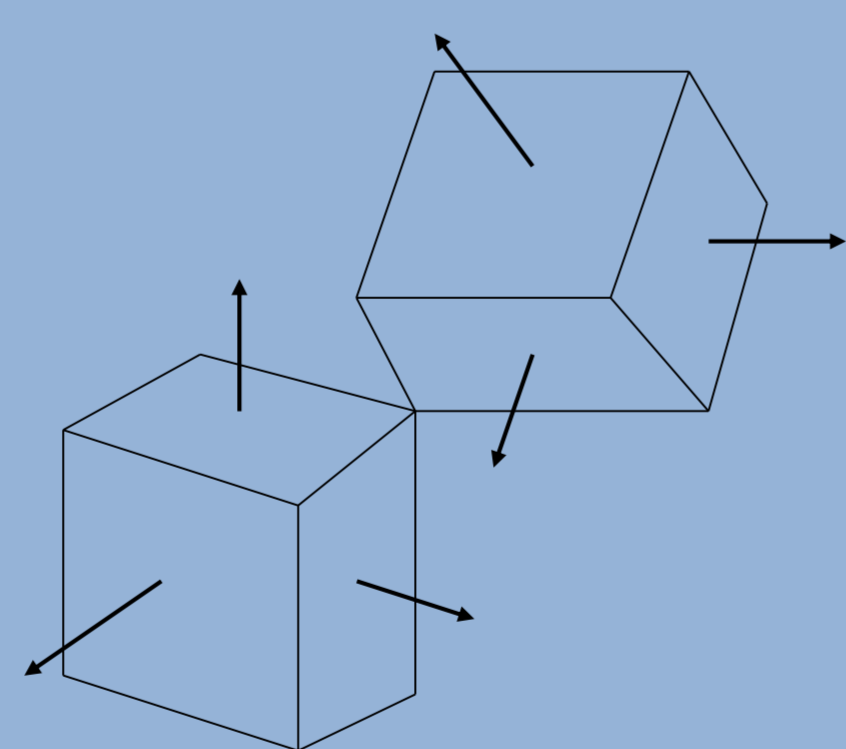
$$\frac{\partial n}{\partial t} = \frac{1}{2} \int_0^v K(\bar{v}, v-\bar{v}) n(\bar{v}) n(v-\bar{v}) d\bar{v} - n(v) \int_0^\infty K(v, \bar{v}) n(\bar{v}) d\bar{v}$$



### Weakly coupled growth & aggregation

Growth & aggregation separately contribute to the PBE

$$\frac{\partial n}{\partial t} + \frac{\partial (G(v)n)}{\partial v} = \frac{1}{2} \int_0^v K(\bar{v}, v-\bar{v}) n(\bar{v}) n(v-\bar{v}) d\bar{v} - n(v) \int_0^\infty K(v, \bar{v}) n(\bar{v}) d\bar{v}$$

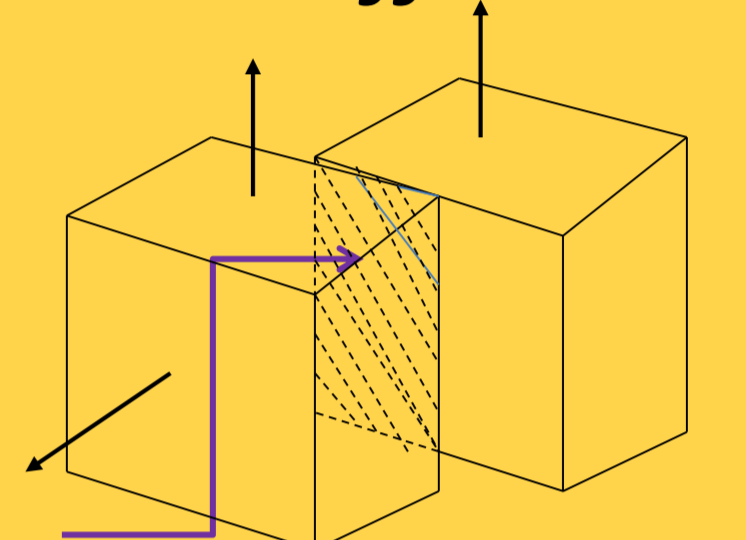


$S$ : supersaturation  $\varphi$ : mass flux  $A$ : area  $G$ : growth rate  $K$ : kernel

## Non classical modeling: Strongly Coupled Growth & Aggregation

### Growth

- Growth is perturbed by the collision event
- Cause of the crystal growth is yet the same (supersaturation), but the mass increase becomes different



Growth law:  $\varphi = k S^j \quad \frac{dm}{dt} = (A - \alpha A_0) \varphi \quad A \propto v^{2/3}$

$\rightarrow \frac{dv}{dt} = G(v, v_0)$  Effective growth rate

### Strongly coupled growth & aggregation

The presence of  $v_0$  in  $G(v, v_0)$  leads to a new version of the PBE

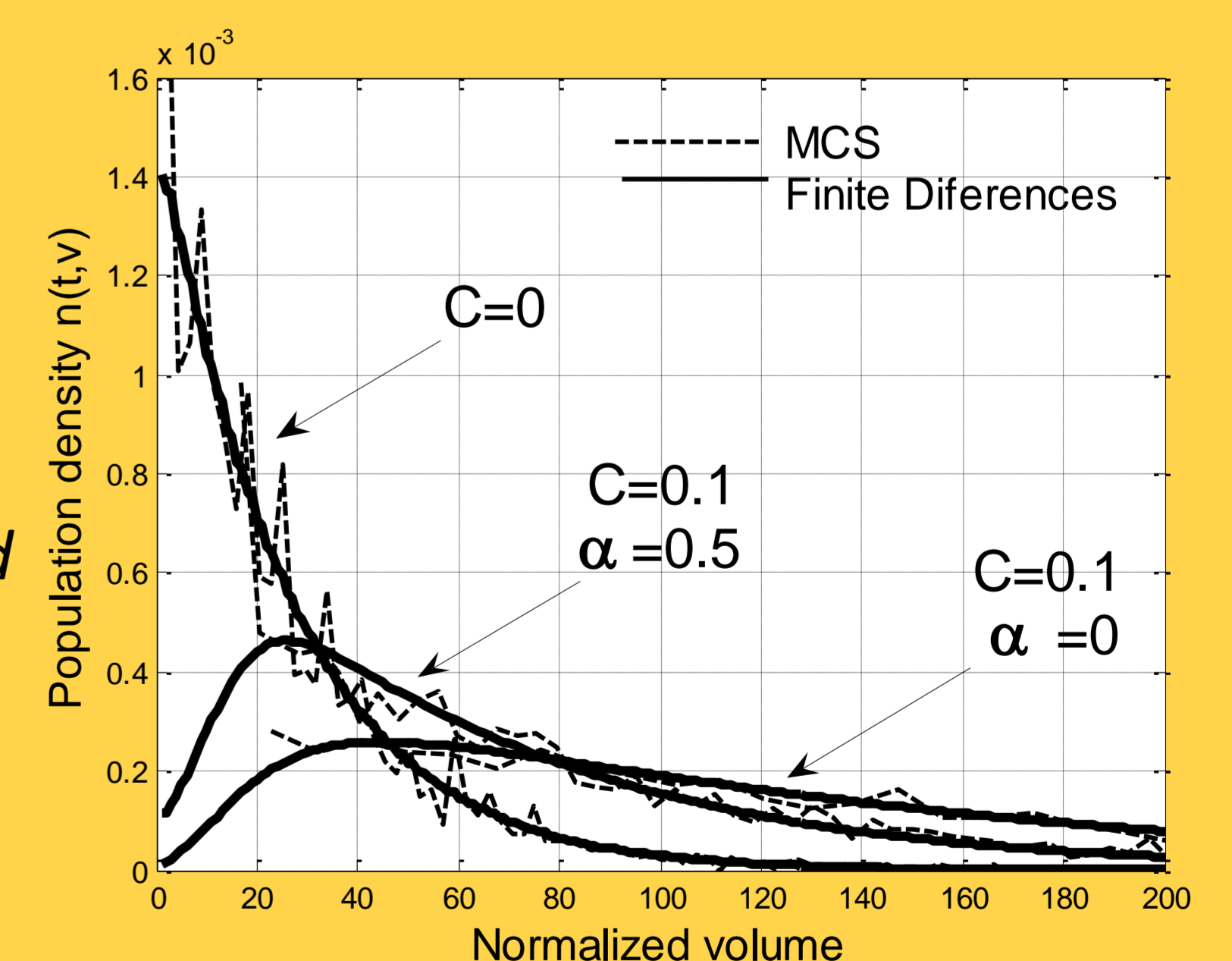
- PBE 2D: two internal variables:  $(v, v_0) \rightarrow (t, v, v_0)$
- New densities:  $n(t, v) = \int_0^v N(t, v, v_0) dv_0 \quad N(t, v < v_0, v_0) = 0$
- New PBE:

$$\frac{\partial N(t, v, v_0)}{\partial t} + \frac{\partial G(v, v_0) N}{\partial v} = \delta(v - v_0) J_{v_0} - N(t, v, v_0) \int_0^\infty K(v, \bar{v}) n(t, \bar{v}) d\bar{v} \quad v \geq v_0$$

$$J_{v_0} = \frac{1}{2} \int_0^{v_0} K(\bar{v}, v_0 - \bar{v}) n(t, \bar{v}) n(t, v_0 - \bar{v}) d\bar{v}$$

- Solving:

- by Monte Carlo Simulation
- by Finite difference method



$$G(v, v_0) = B(A - \alpha A_0) = C(v^{2/3} - \alpha v_0^{2/3})$$

$$K = 0.5$$

## Outlook & Application

- Application to realistic (perikinetic, orthokinetic) aggregation kernels:  
*aggregation of crystal suspension in a turbulent medium*
- Application to various growth kinetics (involving adsorbed molecules ...):  
*crystal growth in presence of surfactant or impurity*
- Application to PBE with other internal parameters (porosity ...):  
*aggregation with restructuring*