NETL 2009 Workshop on Multiphase Flow Science,
Morgantown, WV, April 22-23, 2009

FCMOM: FROM POPULATION BALANCE EQUATIONS TO THE BOLTZMANN EQUATION (2-D)

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The Project & The Technology Roadmap

- Project Title: Dense Multiphase Flow Simulation: Continuum Model for Poly-dispersed Systems Using the Kinetic Theory Approach
- Participants: University of Puerto Rico – Mayaguez (Bogere); Illinois Institute of Technology (Arastoopour, Strumendo, Gidaspow)
- Poly-dispersity (size, density) & Kinetic theory

The Role of the Illinois Institute of Technology Unit

- Can the FCMOM be used in a kinetic theory approach? Can the FCMOM be used to solve the Enskog-Boltzmann equation for inelastic particles?
- Overall strategy: first 2-D systems (disks), afterwards 3-D systems (spheres).
- Derivation of governing equations.
- Validation through test cases (relaxation to the homogeneous equilibrium state, homogeneous cooling, impulsive start-up problem).

A Parallel between PBE and Kinetic Theory

How to predict the change of particle size, density, shape, composition?

How to describe the fluid dynamics of inelastic particles (in not too dense flows)?

particle size distribution function

$$f(\bar{\xi}, \bar{\mathbf{x}}, t)$$

particle velocity distribution function

Internal Variables

(Size, Density, Shape, etc.)

Components of Particle Velocities

Two Fundamental Equations

Population Balance Equation:

$$\frac{\partial f_r}{\partial t} + \frac{\partial \mathbf{v} \cdot f_r}{\partial \mathbf{x}} + \frac{\partial G \cdot f_r}{\partial r} = (B - D)$$

V is particle velocity

G is the growth rate

Aggregation, breakage

Enskog-Boltzmann Equation:

$$\frac{\partial f_c}{\partial t} + \frac{\partial \mathbf{c} \cdot f_c}{\partial \mathbf{x}} + \frac{\partial \mathbf{F}_{\mathbf{tot}} \cdot f_c}{\partial \mathbf{c}} = (B - D)_{coll}$$

Particle velocity

F_{tot} external forces

Collisions

Methods of Solution

Population Balance Equation:

Method of Classes, Methods of Moments (and MWR), Successive Approximations, Monte Carlo, Similarity Solutions

Enskog-Boltzmann Equation:

Discrete Ordinates, Methods of Moments (and MWR), Monte Carlo, Normal Solution methods

For Low Computational Effort (CFD applications):

Self-preserving Solutions, Methods of Moments

Normal Solution Methods, Methods of Moments

Quadrature Methods (QMOM, DQMOM)

FCMOM

New Methods of Moments for Enskog-Boltzmann eq.

Finite size domain Complete set of trial functions MOM (FCMOM)

1. PBE or Enskog-Boltzmann equation in a finite domain (moving boundary problem)
2. Efficient PSD reconstruction through orthogonal polynomials
3. Multivariate applications: domains always well defined

1. FCMOM for PBE: mono-variate PBE (Chemical Engineering Science, Solution of PBE by MOM in finite size domains, 63, 2624-2640, 2008) and bi-variate PBE (Industrial and Engineering Chemistry Research, Solution of bivariate PBE using the FCMOM, 48(1), 262-273,2009)
2. Work in progress on the application of FCMOM to the Enskog-Boltzmann eq.

FCMOM for mono-variate homogeneous processes

$f_r(r,t)$ is the particle size distribution (PSD)

$$\frac{\partial f_r}{\partial t}+\frac{\partial G\cdot f_r}{\partial r}=B-D$$

$r=[0,\infty]$

G = growth rate

Nucleation, breakage, aggregation

$r=\left[r_{\min}(t),r_{\max}(t)\right]$

Moving boundaries

$$\frac{\partial f_r}{\partial t}-\frac{\partial f_r}{\partial \bar{r}}\cdot\frac{1}{(r_{\max}-r_{\min})}\cdot\left[\left(\frac{dr_{\min}}{dt}+\frac{dr_{\max}}{dt}\right)+\bar{r}\cdot\left(-\frac{dr_{\min}}{dt}+\frac{dr_{\max}}{dt}\right)\right]+$$

$\bar{r}=[-1,1]$

$$+\frac{2}{(r_{\max}-r_{\min})}\cdot\left(\frac{\partial G\cdot f_r}{\partial \bar{r}}\right)=B-D$$

Correction term for change of reference frame

Dimensionless Moments Equations

Dimensionless moments $\mu_i = \int_{-1}^{1} \overline{f_r} \cdot \left(\bar{r}\right)^i \cdot d\bar{r}$

Term due to the change of reference frame

$$\frac{\partial \mu_i}{\partial \bar{t}} + i \cdot \mu_{i-1} \cdot \frac{1}{\left(r_{\max} - r_{\min}\right)} \cdot \left(\frac{dr_{\min}}{d\bar{t}} + \frac{dr_{\max}}{d\bar{t}}\right) + \left(i+1\right) \cdot \mu_i \cdot \frac{1}{\left(r_{\max} - r_{\min}\right)} \cdot \left(-\frac{dr_{\min}}{d\bar{t}} + \frac{dr_{\max}}{d\bar{t}}\right) -$$

$$-\left[\overline{f_1} - \left(-1\right)^i \cdot \overline{f_{-1}}\right] \cdot \frac{1}{\left(r_{\max} - r_{\min}\right)} \cdot \left(\frac{dr_{\min}}{d\bar{t}} + \frac{dr_{\max}}{d\bar{t}}\right) - \left[\overline{f_1} - \left(-1\right)^{i+1} \cdot \overline{f_{-1}}\right] \cdot \frac{1}{\left(r_{\max} - r_{\min}\right)} \cdot \left(-\frac{dr_{\min}}{d\bar{t}} + \frac{dr_{\max}}{d\bar{t}}\right) +$$

$$+ \frac{2 \cdot t_{sc}}{\left(r_{\max} - r_{\min}\right)} \cdot \left[G_1 \cdot \overline{f_1} - \left(-1\right)^i \cdot G_{-1} \cdot \overline{f_{-1}}\right] -$$

Boundary Conditions

$$- \frac{2 \cdot t_{sc}}{\left(r_{\max} - r_{\min}\right)} \cdot i \cdot \int_{-1}^{1} G \cdot \overline{f_r} \cdot \left(\bar{r}\right)^{i-1} \cdot d\bar{r} = \frac{t_{sc}}{f_{sc}} \cdot \int_{-1}^{1} \left(B - D\right) \cdot \left(\bar{r}\right)^i \cdot d\bar{r}$$

Integrals of growth, nucleation, aggregation, breakage

$\bar{t}, \bar{f}$ = dimensionless values $\quad t_{sc}, f_{sc}$ = scale factors

$G_1, \overline{f_1}, G_{-1}, \overline{f_{-1}}$ = boundary values

FCMOM: PSD vs. Moments

PSD as a series of Legendre polynomials:

$$\overline{f_r}\left(\bar{r},\bar{t}\right) \approx \sum_{n=0}^{M-1} c_n\left(\bar{t}\right)\cdot\phi_n\left(\bar{r}\right)$$

M = number of moments

Dependency on external variables → μ_i

Dependency on internal variables (size)

1) Good properties of convergence of Legendre series: PSD is well represented with few moments

2)PSD explicit: quadratures for growth/aggregation /breakage integrals can be optimized

3) Moments equations always closed

Validation Cases (Monovariate Distributions)

- Growth (linear, constant, diffusion-controlled): analytical solutions
- Growth (constant, diffusion-controlled) +Primary Nucleation: analytical solutions
- Growth (diffusion-controlled) +Nucleation (primary and secondary) +Solute mass balance: experimental data
- Dissolution: analytical solution
- Aggregation (constant, linear, product, Smoluchowski continuum kernels): analytical solutions and self-preserving solution for the Smoluchowski continuum kernel
- Aggregation and Growth (constant, linear kernels and constant and linear growth): analytical solutions
- Breakage (symmetric breakage, power-law breakage function, homogeneous type breakage kernels): analytical solutions

Chemical Engineering Science, Solution of PBE by MOM in finite size domains, 63, 2624-2640, 2008

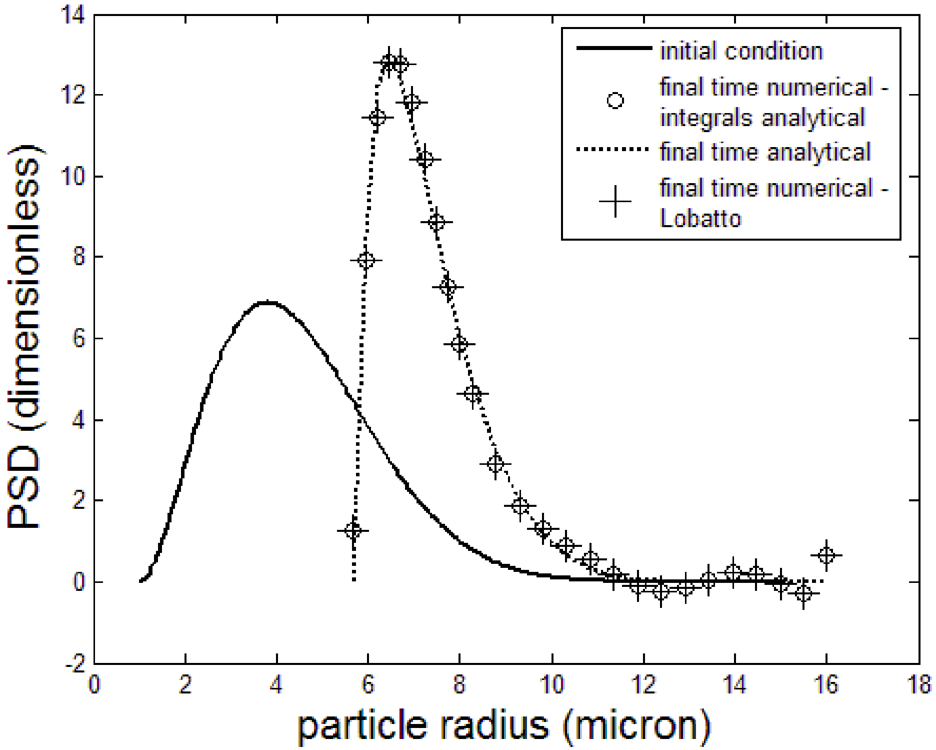
Diffusion Controlled Growth

$$G = \frac{dr}{dt} = \frac{K}{r}$$

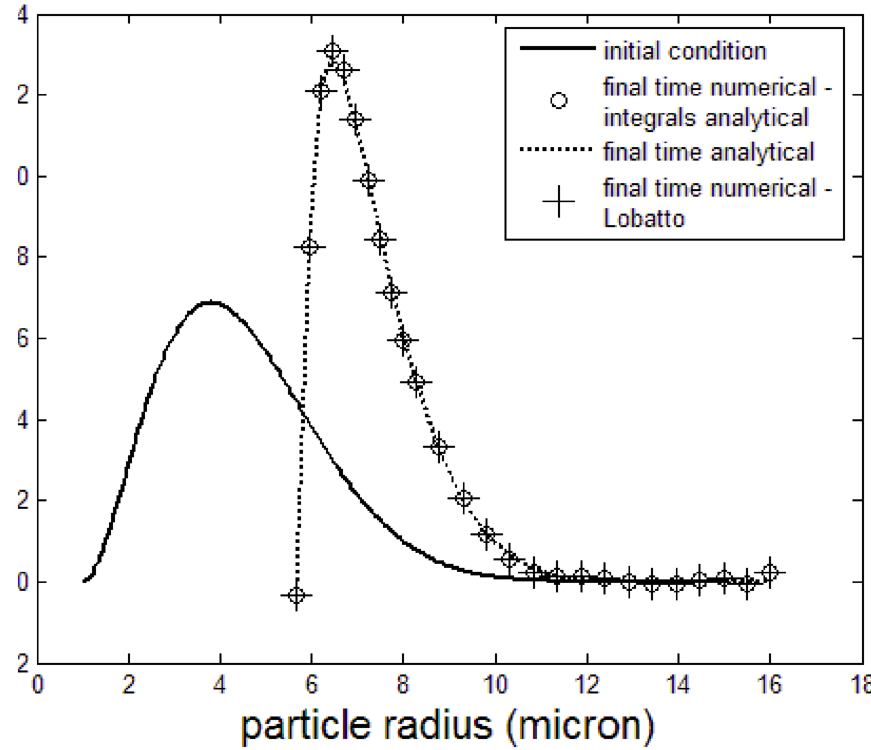
$$K = 0.78 \text{ micron}^2/\text{sec}$$

$$t_{fin} = 20 \text{ sec}$$

Clouds: particle radius > 1 micron (McGraw)



8 moments



10 moments

Aggregation models

1. **Smoluchowski equation:** particles of any size are produced and aggregate.

2. **Finite Smoluchowski equation:** a finite domain is defined. Particles of any size can be produced but not all the aggregations are possible: aggregations creating particles larger than the maximum size are neglected (similar to method of classes).

3. **Oort-Hulst equation:** v' particles and v particles aggregate (v'< v); v' particles break in monomers and aggregate to v particles

$$\frac{\partial f(v,t)}{\partial t} = -\frac{\partial f(v,t)\cdot \int_0^v v' \cdot K(v,v')\cdot f(v',t)\cdot dv'}{\partial v} - \int_v^\infty K(v,v')\cdot f(v,t)\cdot f(v',t)\cdot dv'$$

Net gain of particles aggregating

Loss of particles breaking in monomers

Dubovski (J. Phys. A, 32, 781-793, 1999) compared 1) vs. 3):

in 1), aggregation front propagates at infinite rate;

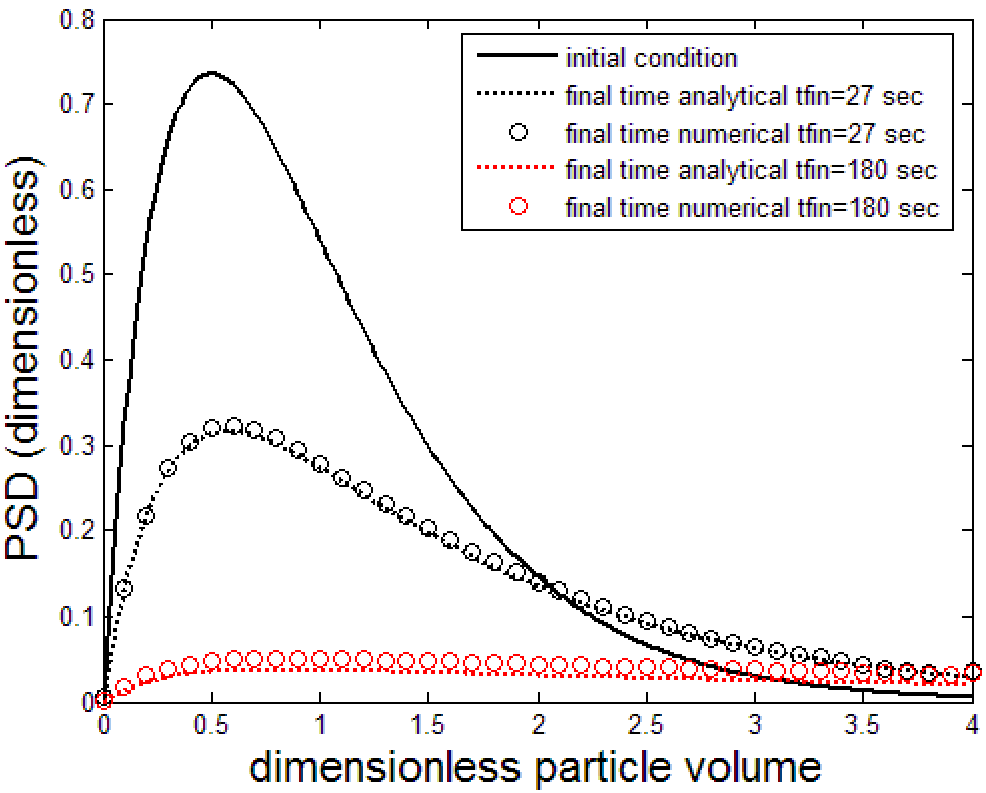
in 3), aggregation front moves at finite rate, unless mass conservation law breaks down

Aggregation: constant kernel $K=K_0$

Initial condition for PSD: Gaussian-like distribution

$$\overline{f} = \left(\frac{v_{\max}}{v_{av}}\right) \cdot \frac{(\upsilon+1)^{(\upsilon+1)}}{\Gamma(\upsilon+1)} \cdot \left(\frac{v}{v_{av}}\right)^{\upsilon} \cdot \exp\left[-\frac{v}{v_{av}} \cdot (\upsilon+1)\right]$$

$$\upsilon = 1, v_{av} = 4.189 \cdot (10)^{-15}\ \mathrm{m}^3, K_0 = 1.8 \cdot (10)^{-10}\ \frac{\mathrm{m}^3}{\mathrm{s}}, \left(\frac{v_{\max}}{v_{av}}\right) = 4, N_{in} = \frac{(10)^9}{4.189}\ \frac{\text{particles}}{\mathrm{m}^3}$$



For finite Smoluchowski equation:

- *Number of moments = 8*
- *Increasing the ratio $\left(\frac{v_{\max}}{v_{av}}\right)$ it converges to the solution of the Smoluchowski equation*

For Oort-Hulst equation:

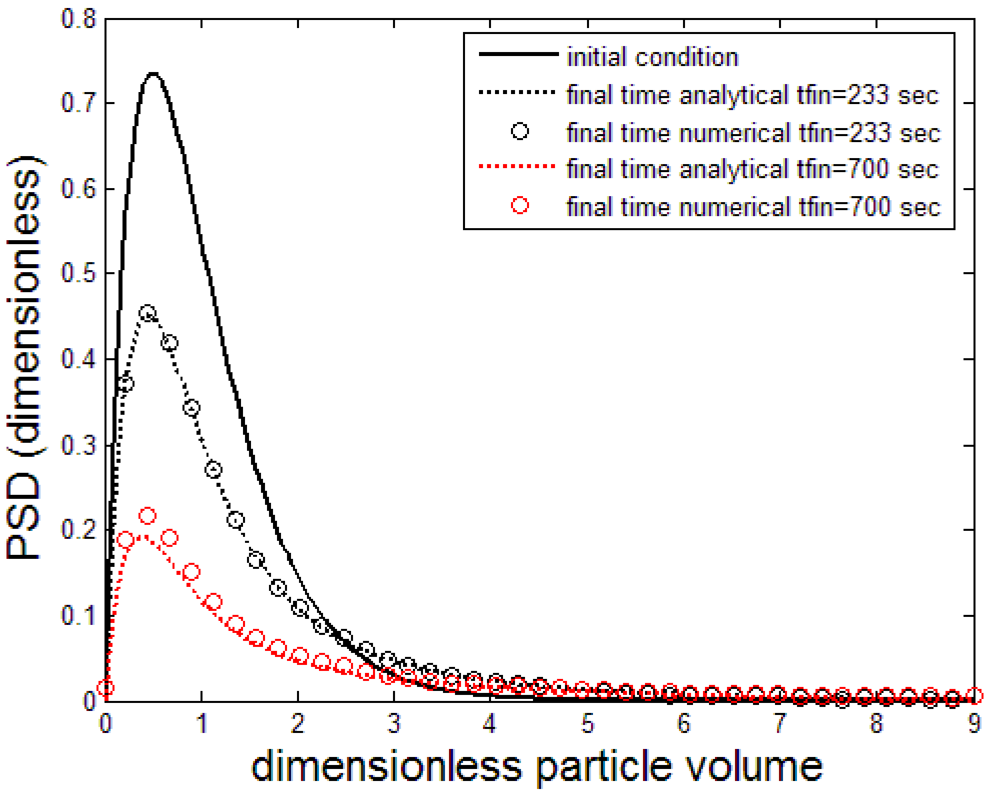
- *Number of moments = 10*
- *Aggregation front can be tracked*

Aggregation: sum kernel $K=K_0*(v+v')$

Initial condition for PSD: Gaussian-like distribution

$$\overline{f} = \left(\frac{v_{\max}}{v_{av}}\right)\cdot\frac{(\upsilon+1)^{(\upsilon+1)}}{\Gamma(\upsilon+1)}\cdot\left(\frac{v}{v_{av}}\right)^{\upsilon}\cdot\exp\left[-\frac{v}{v_{av}}\cdot(\upsilon+1)\right]$$

$$\upsilon=1, v_{av}=4.189\cdot(10)^{-15}\ \mathrm{m}^3, K_0=1.53\cdot(10)^3\frac{1}{\mathrm{s}}, \left(\frac{v_{\max}}{v_{av}}\right)=9, N_{in}=\frac{(10)^9}{4.189}\frac{\text{particles}}{\mathrm{m}^3}$$



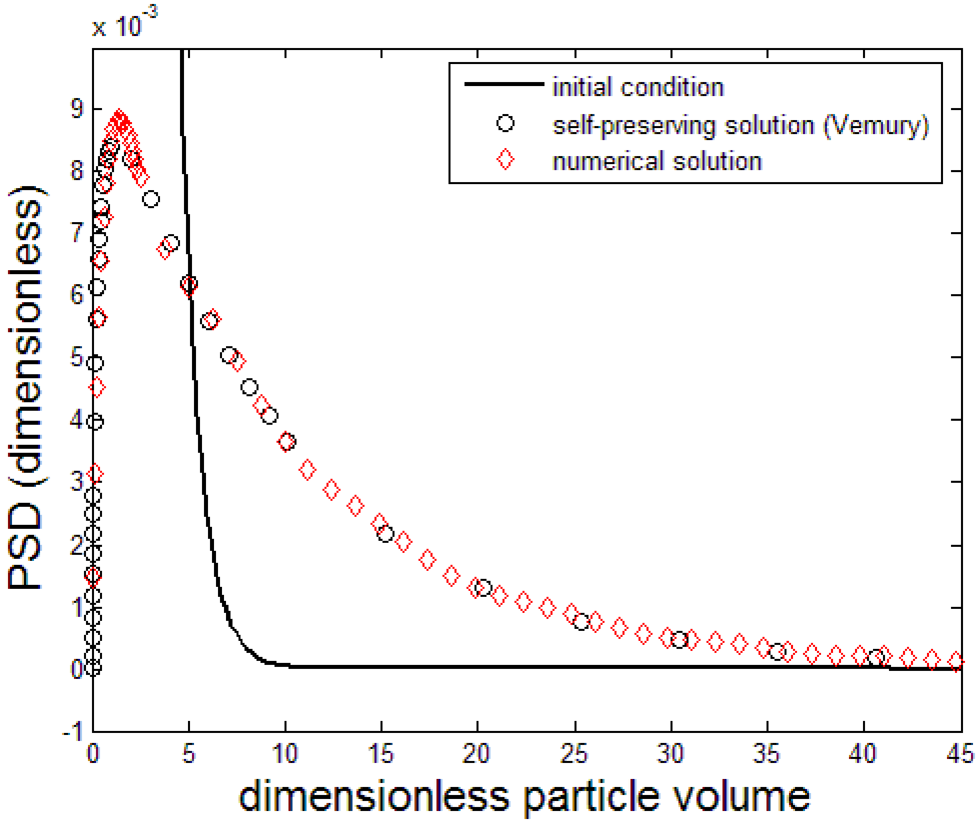
For finite Smoluchowski equation:

- *Number of moments = 12*
- *Increasing the ratio $\left(\frac{v_{\max}}{v_{av}}\right)$ it converges to the solution of the Smoluchowski equation*

Aggregation: Smoluchowski Kernel - Continuum Regime

$$K = \frac{2 \cdot T \cdot K_{BOLTZ}}{3 \cdot \mu} \cdot \left[2 + \left(\frac{v_i}{v_j} \right)^{\frac{1}{3}} + \left(\frac{v_j}{v_i} \right)^{\frac{1}{3}} \right]$$

Initial condition for PSD: Exponential distribution

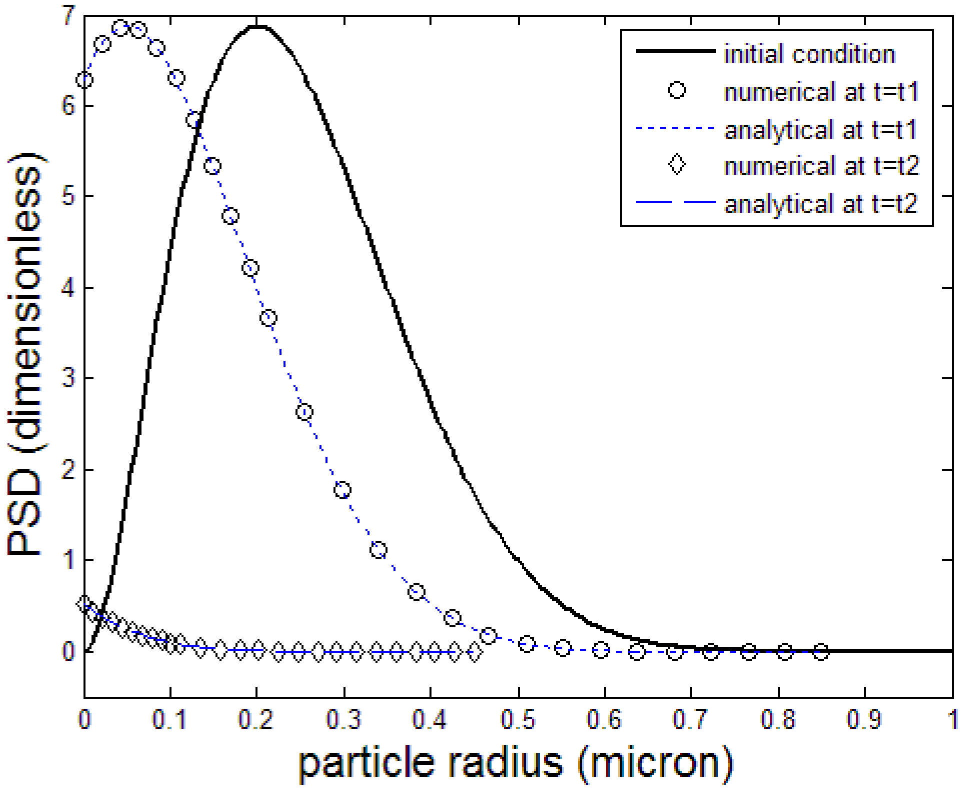


For finite Smoluchowski equation:

- *Increasing the ratio* $\left(\frac{v_{\max}}{v_{av}} \right)$ *it converges to the solution of the Smoluchowski equation*
- *With Smoluchowski kernel,* $\left(\frac{v_{\max}}{v_{av}} \right)$ *must be high (50)*

Particle Dissolution

Constant dissolution rate, 10 moments



1) *Solution with other MOM is problematic for particle dissolution*

2) *Even in this case, results are excellent with FCMOM*

Validation Cases (Bivariate Distributions)

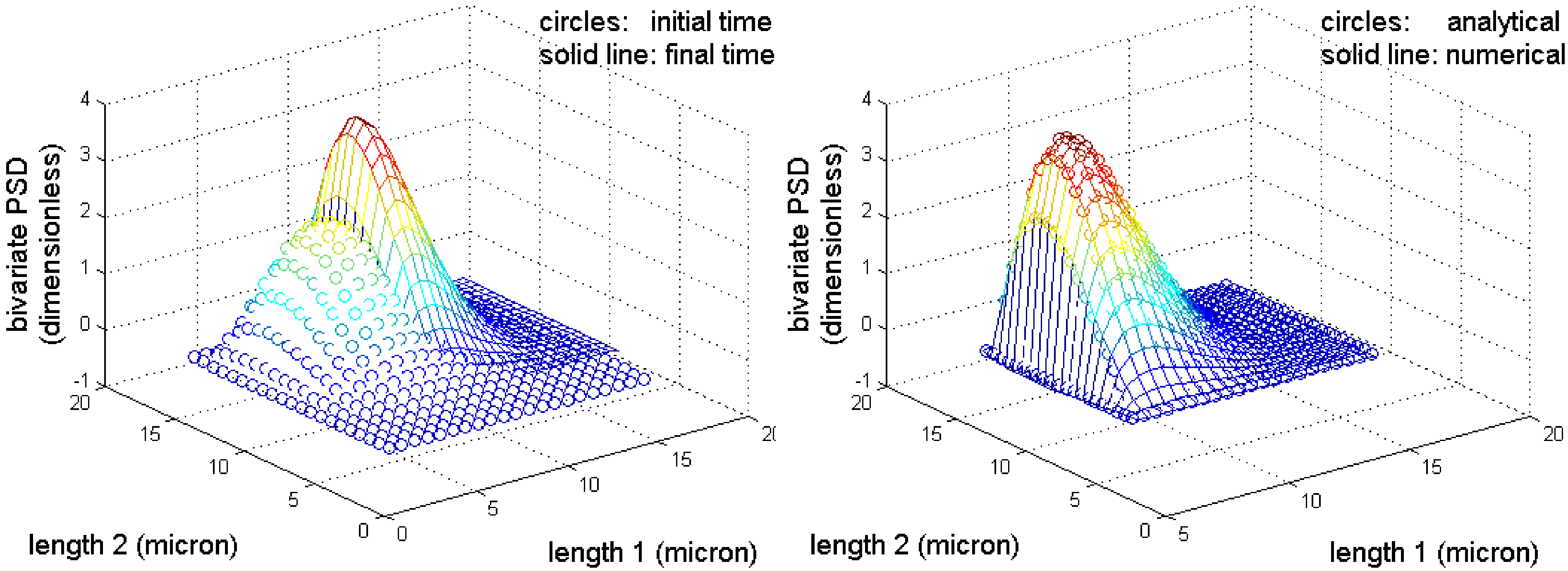
- Growth (linear, constant, diffusion-controlled): analytical solutions
- Dissolution: analytical solution
- Aggregation (constant kernel): analytical solution
- Aggregation + Growth (constant kernel and linear growth rate): analytical solution

Industrial and Engineering Chemistry Research, Solution of bivariate PBE using the FCMOM, 48(1), 262-273, 2009

Bivariate PBE: Diffusion Controlled Growth

Different crystal growth on two different axes:

$$K_1 = 1 \text{ micron}^2/\text{sec} \; K_2 = 0.5 \text{ micron}^2/\text{sec}$$



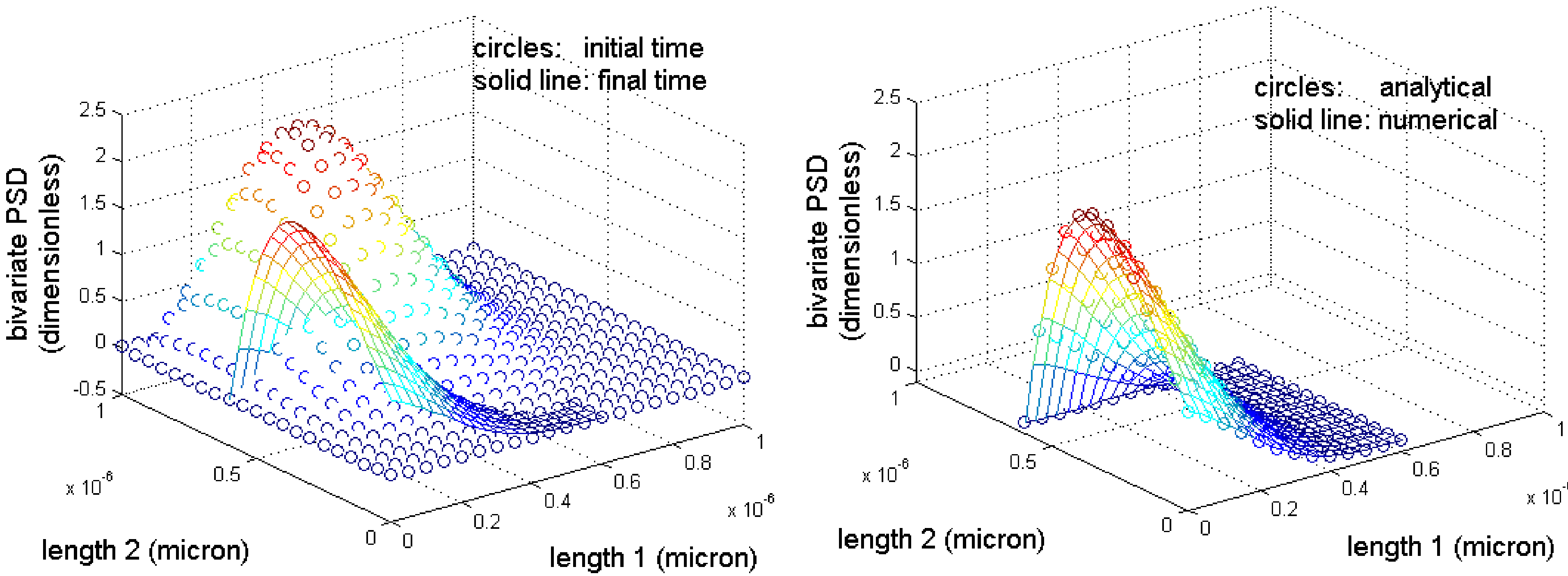
Algorithm is still efficient as in monovariate case

(Computational time about 2-3 bigger than monovariate case)

Anisotropic Dissolution

Different crystal dissolution rates on different axes

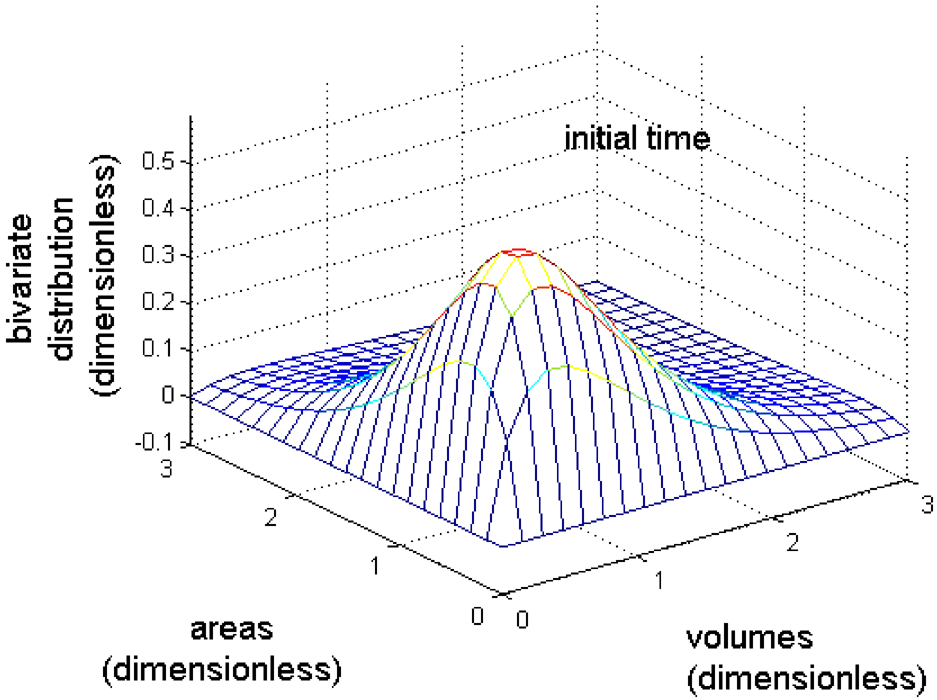
$$K_1, K_2 \cong 10^{-1} \text{ micron/sec}$$

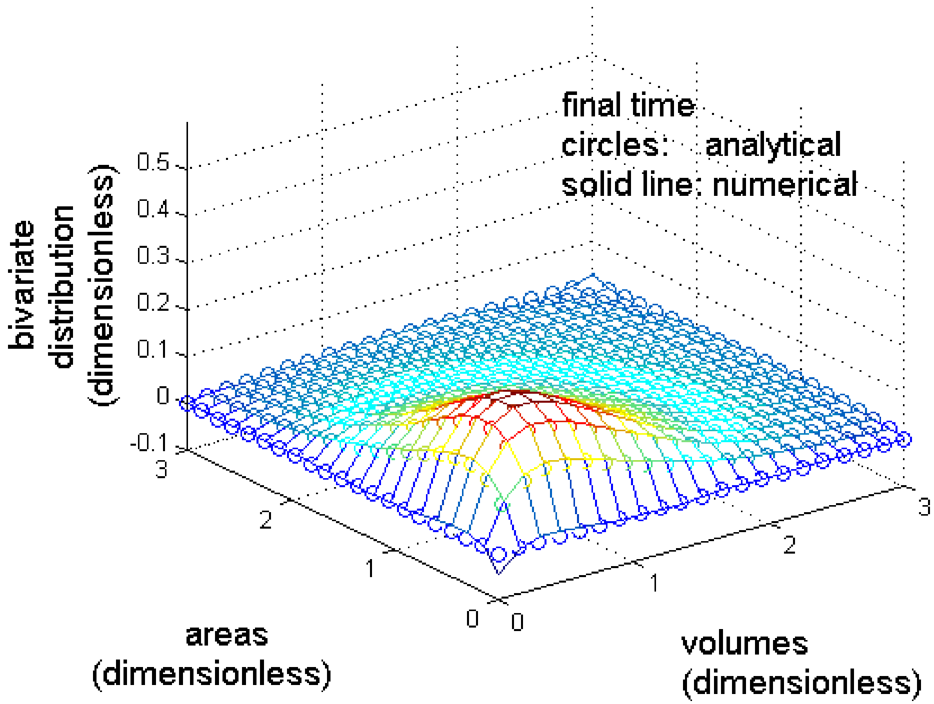


Bivariate aggregation (constant kernel)

Nano-aggregates production: particle volume and surface area

Initial condition: gamma distribution

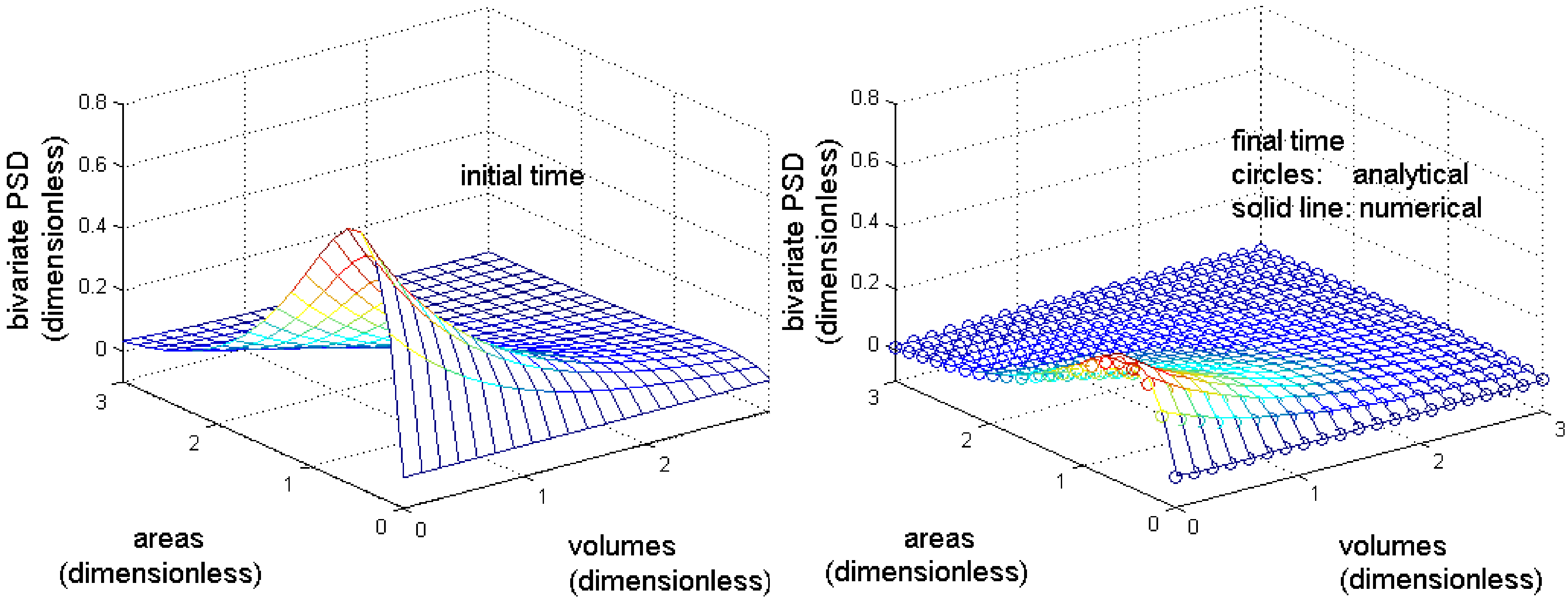




Again, comparison is excellent and the domains are well defined

Bivariate aggregation (constant kernel)

Initial condition: mixed gamma and exponential distribution



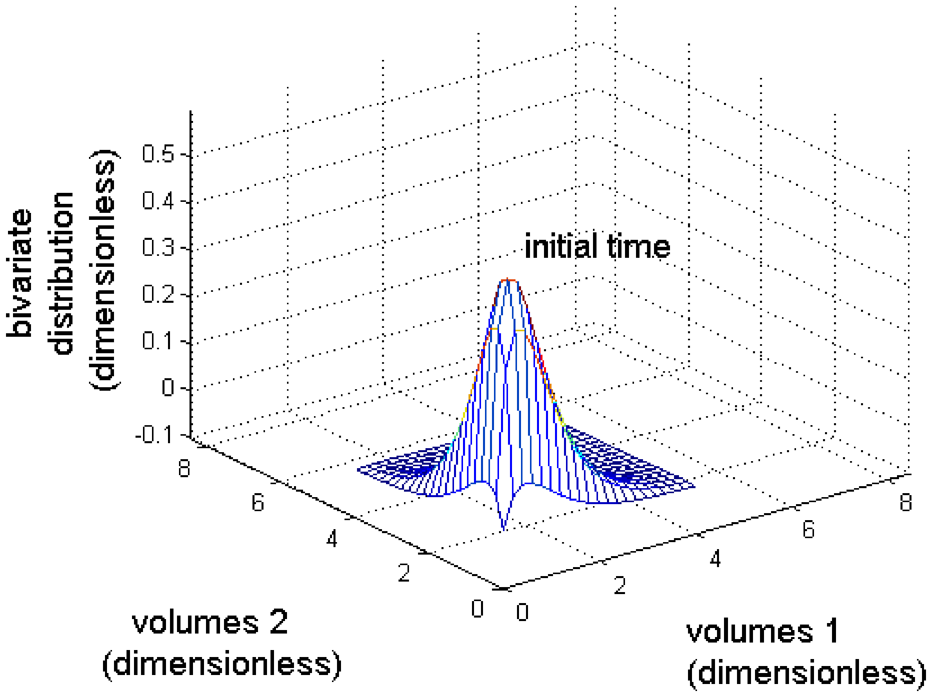
Aggregation and Growth

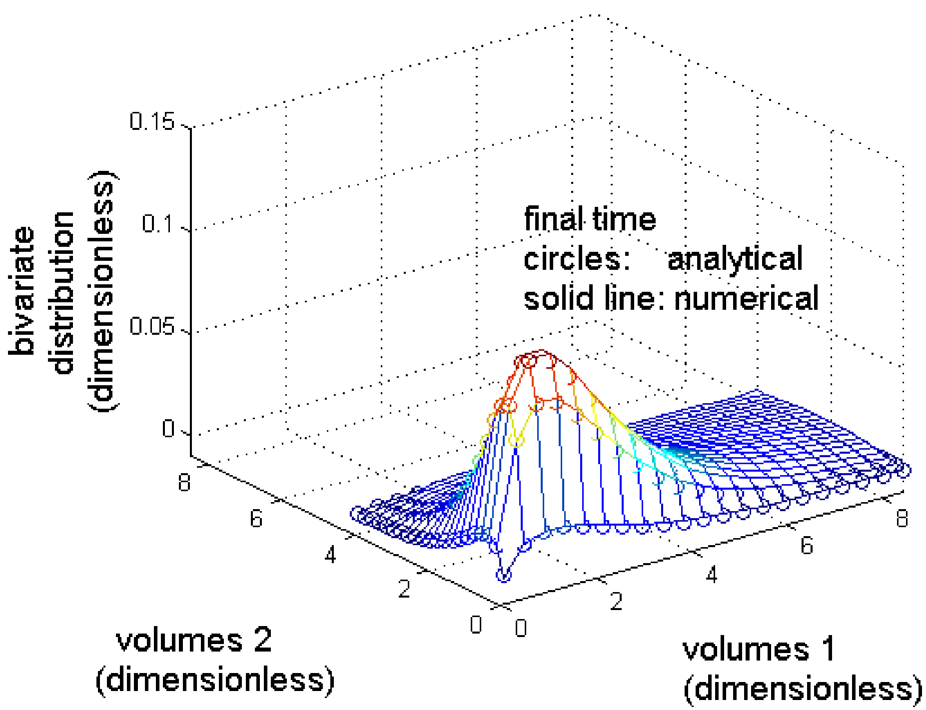
Constant kernel, linear growth rate (chemical reaction on the particle is controlling)

Internal variables: particle volumes of each of 2 components

Initial condition: gamma distribution

Analytical solutions by Gelbard & Seinfeld





2-D Boltzmann Equation

$$\frac{\partial f_c}{\partial t}+\frac{\partial \mathbf{c}\cdot f_c}{\partial \mathbf{x}}+\frac{\partial \mathbf{F}_{\mathbf{tot}}\cdot f_c}{\partial \mathbf{c}}=\left(B-D\right)_{coll}$$

Particle velocity *F_{tot} external forces* *Collisions*

Terms of B-D

(due to collisions) are:

$$B=\int\limits_{\mathbf{g}\bullet\mathbf{k}>0}\int\left[\frac{1}{e^2}\cdot f_c\left(\mathbf{c}',\mathbf{x},t\right)\cdot f_c\left(\mathbf{c}_1',\mathbf{x},t\right)\right]\cdot D_P\cdot\left(\mathbf{g}\cdot\mathbf{k}\right)\cdot d\mathbf{k}\cdot d\mathbf{c}_1$$

$$D=\int\limits_{\mathbf{g}\bullet\mathbf{k}>0}\int\left[f_c\left(\mathbf{c},\mathbf{x},t\right)\cdot f_c\left(\mathbf{c}_1,\mathbf{x},t\right)\right]\cdot D_P\cdot\left(\mathbf{g}\cdot\mathbf{k}\right)\cdot d\mathbf{k}\cdot d\mathbf{c}_1$$

D_P = particle diameter; $\mathbf{g}$ = relative velocity; $\mathbf{k}$ = unit vector

e = restitution coefficient; $\mathbf{c}_1$ = second particle velocity;

$\mathbf{c}',\mathbf{c}_1'$ = pre collision velocities leading to $\mathbf{c},\mathbf{c}_1$

2-D Boltzmann equation is a bi-variate PBE, in which:

- *Internal variables are particle velocities and, therefore, the "growth rates" are the external forces F_{tot}*

A Finite Boltzmann Equation Model

Homogeneous conditions

$$B = \int\limits_{\mathbf{g}\bullet\mathbf{k}>0} \int \left[\frac{1}{e^2} \cdot f_c\left(\mathbf{c}', \mathbf{x}, t\right) \cdot f_c\left(\mathbf{c}_1', \mathbf{x}, t\right) \right] \cdot D_P \cdot \left(\mathbf{g} \cdot \mathbf{k}\right) \cdot d\mathbf{k} \cdot d\mathbf{c}_1$$

$$\frac{\partial f_c}{\partial t} = \left(B - D\right)_{coll}$$

$$D = \int\limits_{\mathbf{g}\bullet\mathbf{k}>0} \int \left[f_c\left(\mathbf{c}, \mathbf{x}, t\right) \cdot f_c\left(\mathbf{c}_1, \mathbf{x}, t\right) \right] \cdot D_P \cdot \left(\mathbf{g} \cdot \mathbf{k}\right) \cdot d\mathbf{k} \cdot d\mathbf{c}_1$$

1. Classical Boltzmann Equation (CBE): particles of any velocity range can collide and are obtained by collisions.
2. Finite Boltzmann Equation (FBE): a finite domain is defined. Particles of any velocity range can be produced but not all the collisions are possible: collisions creating particle velocities larger than the maximum velocity are neglected.

Increasing the finite domain, the solution of the FBE converges to the solution of the CBE

Computation of Collision Integrals

Homogeneous conditions

$$\frac{\partial \mu_{i_1,i_2}}{\partial t} = \int (B-D)_{coll} \cdot (\xi_x)^{i_x} \cdot (\xi_y)^{i_y} \cdot d\boldsymbol{\xi}$$

$$\int D_{coll} \cdot (\xi_x)^{i_x} \cdot (\xi_y)^{i_y} \cdot d\boldsymbol{\xi} \propto \int \overline{f_c{}'(\boldsymbol{\xi}^{\mathbf{1}},t)} \cdot \overline{f_c{}'(\boldsymbol{\xi},t)} \cdot (\xi_x)^{i_x} \cdot (\xi_y)^{i_y} \cdot (\mathbf{g}\cdot\mathbf{k}) \cdot d\mathbf{k} \cdot d\boldsymbol{\xi}^{\mathbf{1}} \cdot d\boldsymbol{\xi}$$

$\boldsymbol{\xi}, \boldsymbol{\xi}^{\mathbf{1}}$ = dimensionless velocities of the 2 colliding particles; $\mathbf{k}$ = unit vector

Integration in finite domain is more difficult than in infinite domains; classical manipulations cannot be used

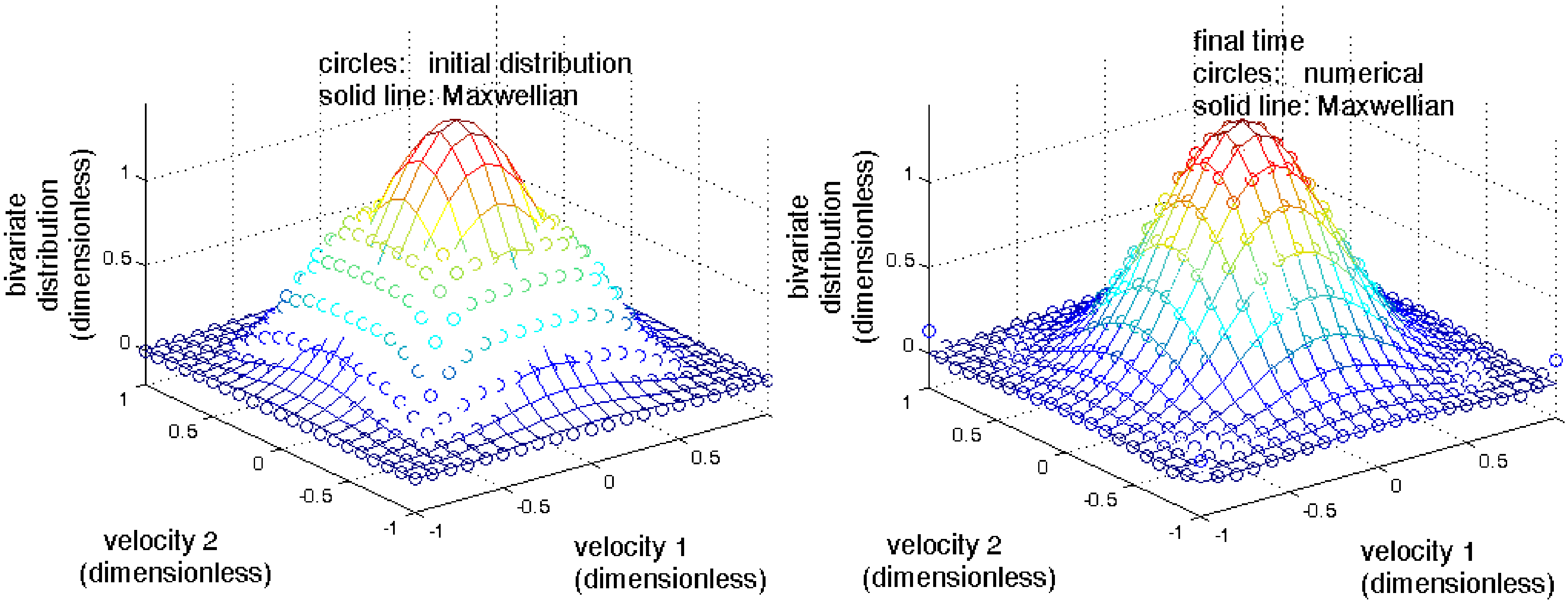
Procedure to pre-compute automatically collision integral coefficients

Solutions in Homogeneous Conditions

1. Elastic Particles: the system relaxes to the Maxwellian state (from an initial condition which can be not-Maxwellian).
2. Inelastic Particles: after sufficiently long times, the system approaches the Homogeneous Cooling State solution (for 2-D systems: Brey, Cubero, Ruiz-Montero, Physical Review E, 59 (1), 1256-1258, 1999).

Elastic Particles

$D_P = 100\mu$, Granular Temperature $\square$ $0.2\frac{m^2}{s^2}$, Solid fraction (Area) $\square$ 0.01



With 7-8 moments, there are still some oscillations but there is a good agreement.

Simple application, but not trivial: no assumption of Maxwellian distribution in the FCMOM

Conclusions

1. The FCMOM is an efficient (low computational effort) MOM to solve PBE and provides accurate PSD reconstruction.
2. The FCMOM is efficient and accurate also for bivariate distributions; besides in bivariate applications the domains of the internal variables are always well defined.
3. The FCMOM was applied to the 2-D Boltzmann equation. Application to the relaxation to equilibrium of elastic particles showed good agreement.
4. Future plan: validation of the FCMOM for the 2-D Boltzmann equation will be extended (homogeneous cooling of inelastic particles, impulsive start up problem).