Lecture 3: Topology and Geometry, and Coarsening

Rita M.C. de Almeida
Instituto de Física
Universidade Federal do Rio Grande do Sul

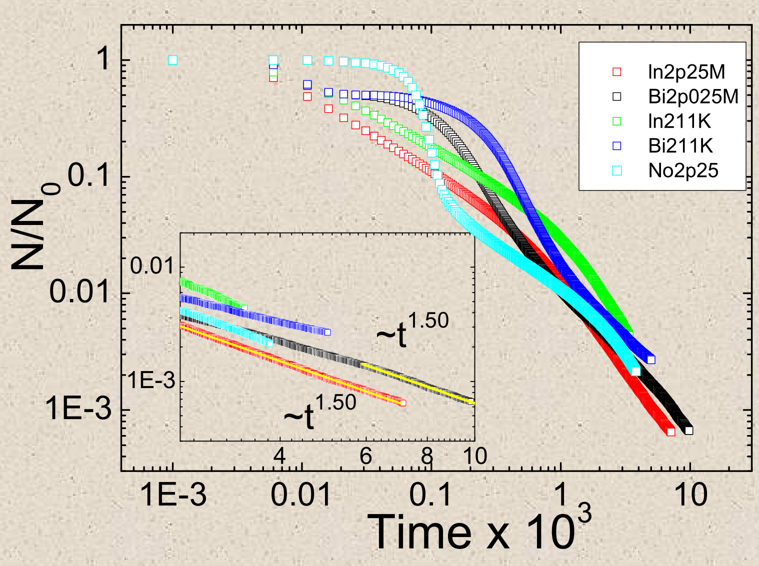
Plan of the lecture

- What is coarsening
- Mullins results for Scaling exponents
- Growth laws for bubbles, and for grains
- Potts model versus Surface Evolver: microscopic dynamics
- The scaling in 2D
- The 3D scaling in Evolver
- The 3D scaling in Potts
- Consequence for maximum entropy or free energy models.

Coarsening in foams

- Vertices move
- Pressure differences are created
- Gas diffusion through boundaries
- Low n/f bubbles shrink
- Large n/f bubbles growth
- T2 (disappearance) T1(neighbor switching)
- Average size increases.

How N goes with t?



It depends on the configuration of the froth.

But what about the scaling regime?

If it exists.

Thomas,de Almeida, and Graner
to appear

Mullins prediction for the scaling state

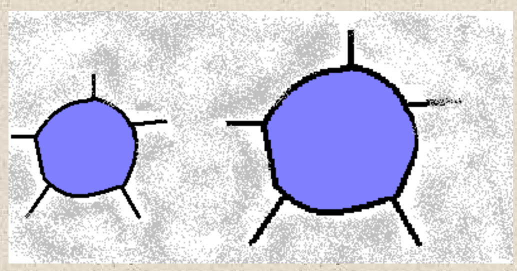
Consider a scaling state.

For each bubble: v and $\dot{v}$

In the scaling regime: v scales as $\bar{v}$

$\dot{v}$ scales as $\bar{v}^{\alpha}$

Depends on the system



$f(v,\dot{v},t)$ the probability at time t of finding a bubble with v and $\dot{v}$

scaling

$$f(v,\dot{v},t)=\frac{1}{\bar{v}^{(1+\alpha)}}\Phi\left(\frac{v}{\bar{v}},\frac{\dot{v}}{\bar{v}^{\alpha}}\right)$$

time independent

$$\frac{d\bar{v}}{dt}=C\bar{v}^{\alpha}$$

$$C=-\lim_{x\to 0}\int_{-\infty}^{0}\Phi(x,y)dy>0$$

# of disappearing bubbles

$$\frac{d\bar{v}}{dt} = C\bar{v}^{\alpha}$$ for $\alpha < 1$ it gives

$$[\bar{v}(t)]^{1-\alpha} - [\bar{v}(0)]^{1-\alpha} = (1-\alpha)Ct$$

In bubbles, $\dot{v} \propto v^{1/3}$ $\longrightarrow$ $\alpha = 1/3$

$$[\bar{v}(t)]^{2/3} = (1-\alpha)Ct + [\bar{v}(0)]^{2/3}$$

$$\bar{v}(t) \sim t^{3/2}$$ For large t

Mullins prediction

- In the scaling regime, for large t:

$\bar{v}(t) \sim t^{3/2}$ $N(t) \sim t^{-3/2}$

$\bar{s}(t) \sim t^{1}$

$\bar{\ell}(t) \sim t^{1/2}$

This is valid for the scaling regime and when $\dot{v} \propto v^{1/3}$

↗ Curvature driven systems

Many growth laws are compatible with Mullins predictions!

The quest for the soap froths 3D growth law is still there!

And there are other systems.

Mullins predictions are a test for the scaling state.

The scaling state in 2D

- No controversy.
- There is a scaling state where all distribution functions of non-dimensional variables are time independent.
- $\langle a \rangle \sim t$
- Theory, simulations and experiments.
- Review: J Stavans,
  Rep. Prog. Phys. 56 (1993) 733.

The scaling state in 3D

Consensus from experiments (not proven):

The systems tend to a unique state from any initial condition.

but

After long transients

Long Transients require

A large number of bubbles to guarantee that when the scaling regime is reached there is

1) Enough bubbles to yield good statistics.
2) Enough bubbles for long enough to measure the time evolution exponents
3) Enough bubbles to avoid finite size effects

Simulations in 3D: Surface Evolver

- Brakke in the 1990's.
- Represents a surface using triangulation, where the size of the elementary triangles may be reduced to increase .
- The code uses the gradient method to reduce the energy of the structure.

Surface Evolver: Basics

http://www.susqu.edu/facstaff/b/brakke/evolver/evolver.html

Basic elements

Vértices: points.

Edges: straight lines uniting points.

Facets: triangular surfaces uniting three vertices

(The surface to be worked on is the set of all facets.)

Body: defined by its limiting facets.

- Facets may be oriented.
- Each surface is associated to na Energy, that must be defined. Evolver minimizes this energy .
- Initial surface: defined in a text file.
- (Extension: .fe used for data files, meaning)

Example 1 : Initial file

```
// cube.fe
//Evolver data for cube with prescribe
   volume
Vertices /* given by coordinates */
1  0.0 0.0 0.0
2  1.0 0.0 0.0
3  1.0 1.0 0.0
4  0.0 1.0 0.0
5  0.0 0.0 1.0
6  1.0 0.0 1.0
7  1.0 1.0 1.0
8  0.0 1.0 1.0
```

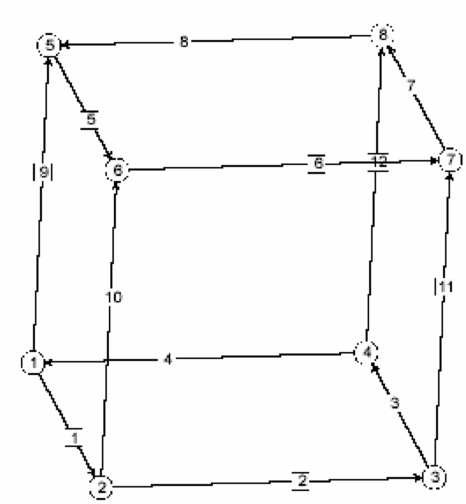


Figure 3.1: The cube skeleton.

Example 1 : Initial file

Edges /* given by endpoints */

1	1 2
2	2 3
3	3 4
4	4 1
5	5 6
6	6 7
7	7 8
8	8 5
9	1 5
10	2 6
11	3 7
12	4 8

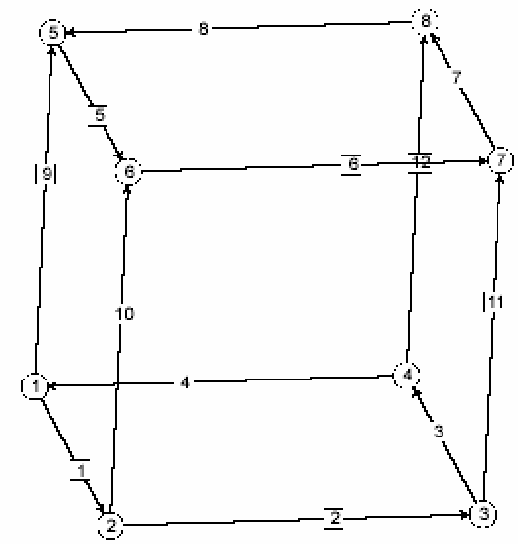


Figure 3.1: The cube skeleton.

Example 1 : Initial file

faces /* given by oriented edge loop */

1	1	10	-5	-9
2	2	11	-6	-10
3	3	12	-7	-11
4	4	9	-8	-12
5	5	6	7	8
6	-4	-3	-2	-1

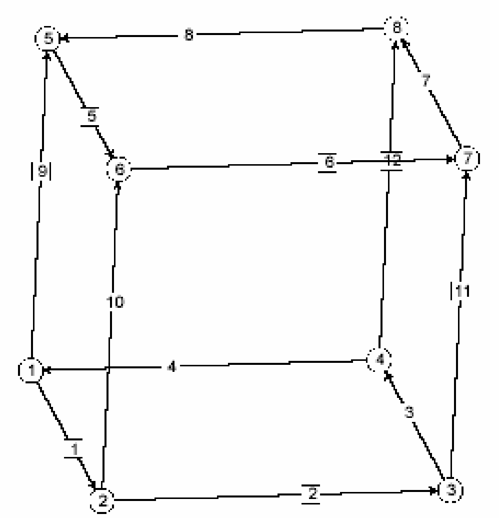


Figure 3.1: The cube skeleton.

Example 1 : Initial file

bodies /* one body, defined by its oriented faces*/

1   1   2   3   4   5   6   volume 1

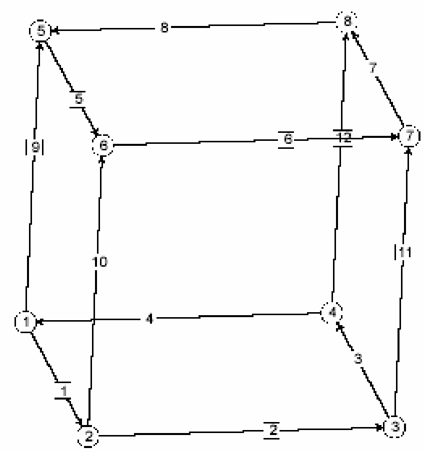
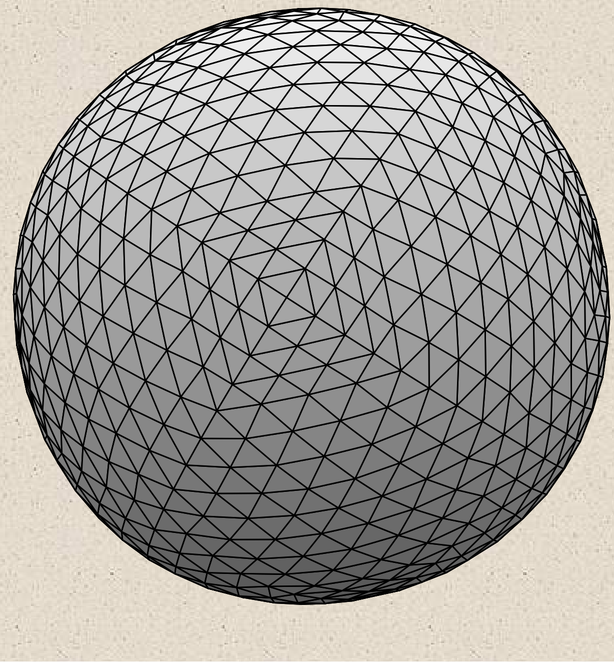


Figure 3.1: The cube skeleton.



1302 WAKAI *et al.*: MICROSTRUCTURAL EVOLUTION

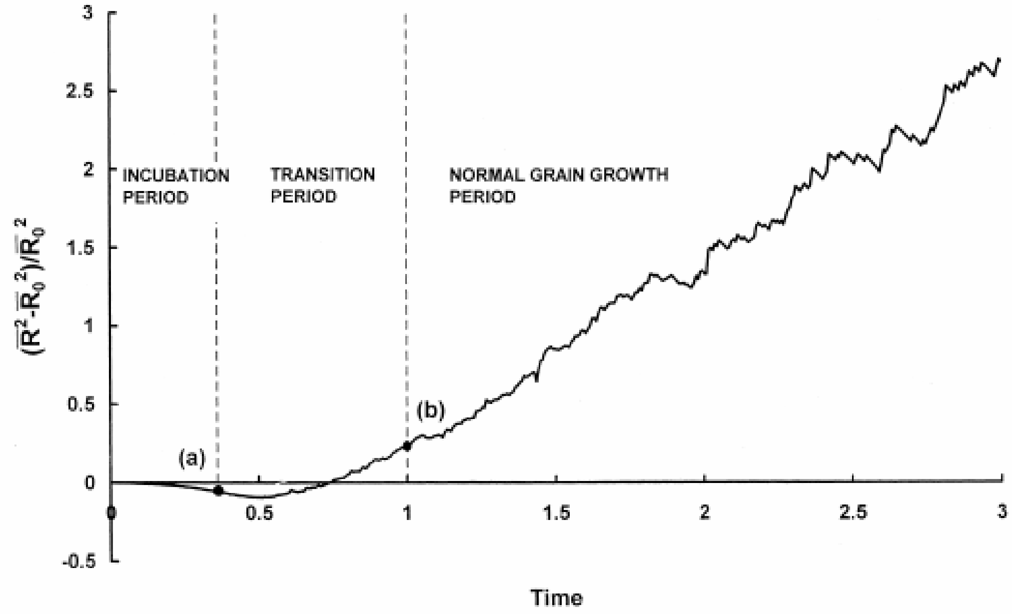


Fig. 6. Time dependence of a function $(\bar{R}_V^2 - \bar{R}_0^2)/\bar{R}_0^2$ of mean grain size.

- F.Wakai, N. Enomoto, H. Ogawa, Acta mater. 48, 1297-1311 (2000)

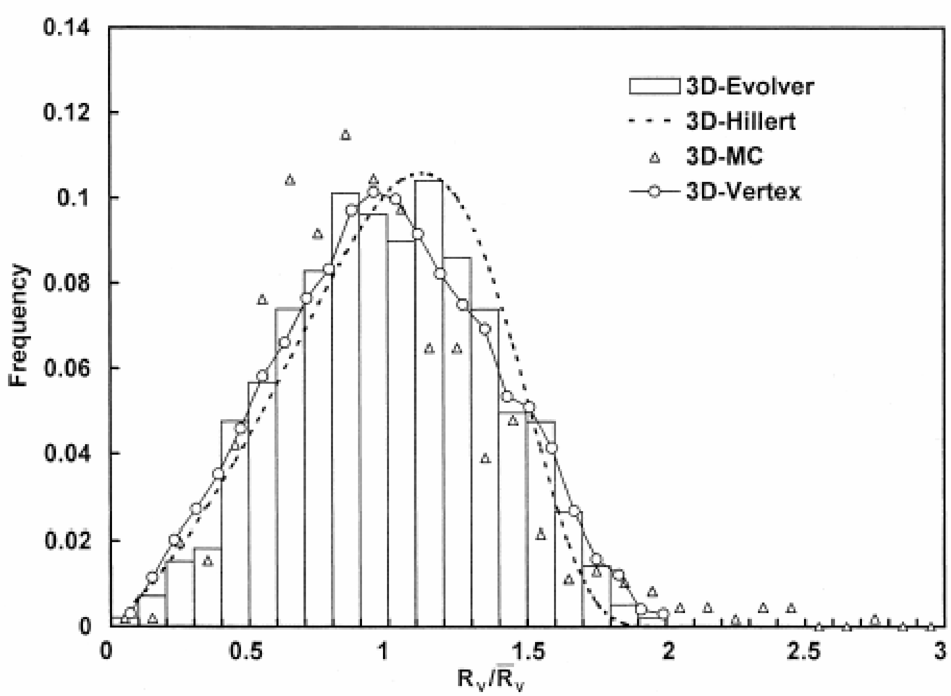


Fig. 8. Normalized grain size distribution of steady structure in normal grain growth period.

WAKAI *et al.*: MICROSTRUCTURAL EVOLUTION 1307

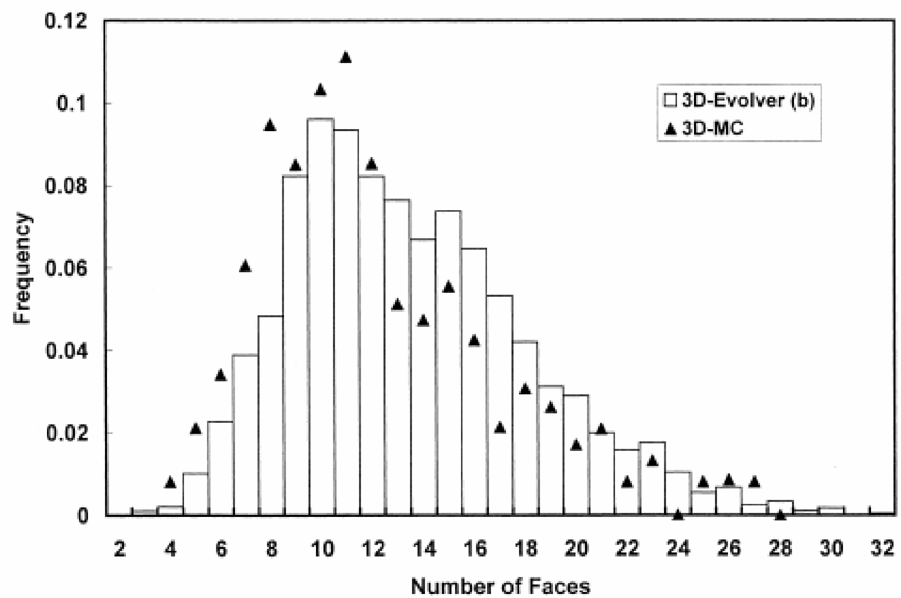


Fig. 15. Frequency of the number of faces in steady structure.

Growth law

$$\left\langle \frac{1}{R_V} \frac{\mathrm{d}V}{\mathrm{d}t} \right\rangle = M\gamma G_1(f) G_2(f)$$

$$G_1(F) = \pi/3 - 2\arctan[1.86(f-1)^{1/2}/(f-2)]$$

$$G_2(F) = 5.35 f^{2/3}\left[(f-2)/2(f-1)^{1/2} - \frac{3}{8} G_1(f)\right]^{-1/3}.$$

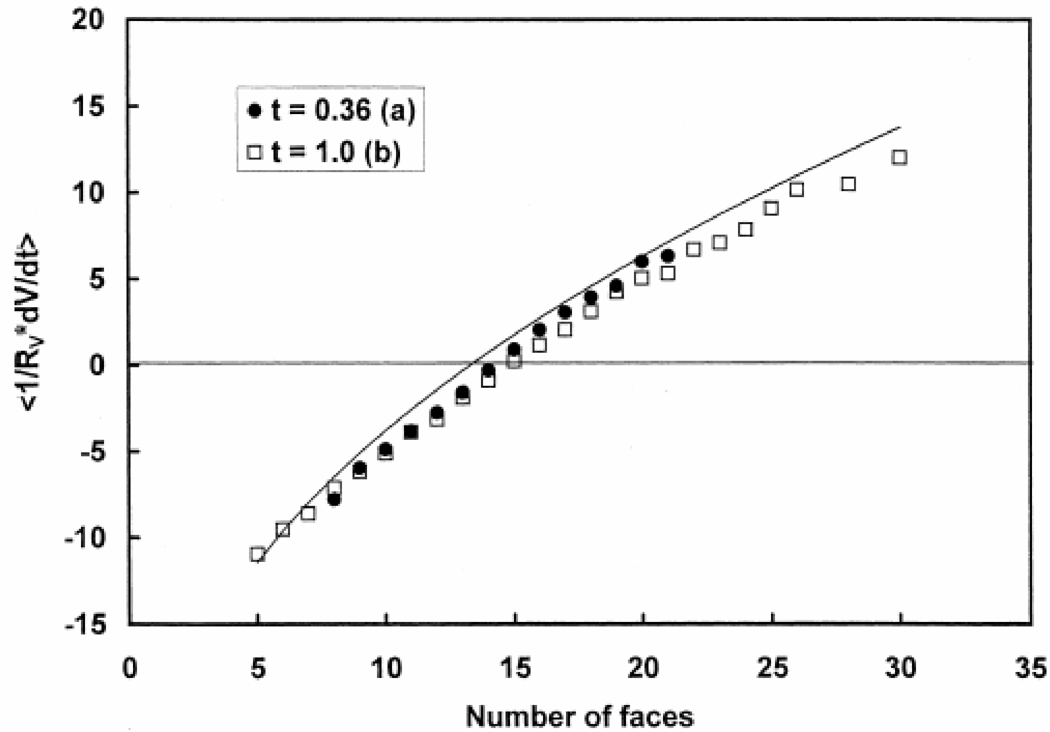


Fig. 19. Relationship between the number of faces f and product $\langle (1/R_V)(dV/dt) \rangle$. The solid line shows the von Neumann–Mullins law.

Growth laws

Glazier and Prause 2000

$$\frac{dv^{2/3}}{dt} = v^{-1/3}\frac{dv}{dt}$$

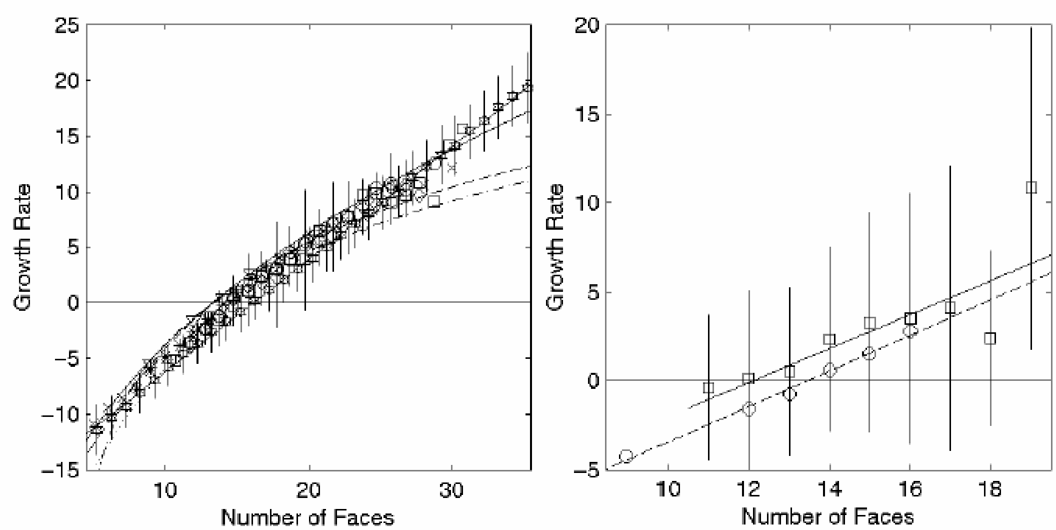


Figure 2a. Growth rates as a function of number of faces for Fortes' edge and vertex models (Dashed lines), Mullins' model (Solid Line), Kawasaki's vertex model (Squares, Circles and Diamonds), Weygand's vertex model (Dotted Line), Monnereau *et al.*'s boundary dynamics model (Triangles), Wakai's boundary dynamics model (Xs and Stars) and Glazier's Potts model (Star of David). 2b. Monnereau *et al.*'s optical tomography experiments (Circles) and our MRI experiments (Squares).

Scaling states: Theory

- Time independent distribution functions of dimensionless quantities.
- The relevant variables are bubble volume, surface, and number of faces.
- Maximization entropy, subject to energy, topology and geometry constraints. (Rivier)

Method

- Equilibrium statistical mechanics.
- Phase space➔ representing all possible configurations of the froth.
- Suppose N bubbles filling volume V.
- Each bubble i: v_i, s_i, f_i
- The whole froth: $v_1,s_1,f_1;v_2,s_2,f_2;\ldots,v_N,s_N,f_N$

The constraints: possible configurations

Non-holonomic constraint:

There is a maximum possible volume for a given surface.

The regular polyhedron

Or

The Isotropic Plateau Polyhedron

???

The calculations

$$\rho_N = \rho_N\left(f_1, f_2, \ldots, f_N; s_1, s_2, \ldots, s_N; v_1, v_1, \ldots, v_N;\right)$$

$$\Phi = \sum_{f_1=f*}^{\infty} \ldots \sum_{f_N=f*}^{\infty} \int_0^{\infty} ds_1 \ldots \int_0^{\infty} ds_N \int_0^{v_1^{max}} dv_1 \ldots \int_0^{v_N^{max}} dv_N$$

$$S = -k_B \Phi \rho \ln(\lambda^N \rho)$$

$$\Phi \rho = 1$$

$$\Phi \rho \sum_{i=1}^{N} \frac{\sigma}{2} s_i = < E >$$

$$\Phi \rho \sum_{i=1}^{N} f_i = 2F$$

$$\Phi \rho \sum_{i=1}^{N} \delta(f_i - f)[s_i - < s >_f] = 0$$

Results

$$P(f) = \frac{3\sqrt{\pi}}{4\lambda Q}(\frac{2e}{5})^{\frac{5}{2}}\langle s\rangle^{\frac{5}{2}} \exp(-gf - h\frac{\langle s\rangle_f}{\langle s\rangle})k(f)(\frac{\langle s\rangle_f}{\langle s\rangle})^{\frac{5}{2}}$$

$$Q = \frac{3\sqrt{\pi}}{4}(\frac{2e}{5})^{\frac{5}{2}}\langle s\rangle^{\frac{5}{2}} S_{5/2}$$

$$S_{5/2} = \sum_f^{\infty} \exp -gf - h\frac{\langle s\rangle_f}{\langle s\rangle}k(f)(\frac{\langle s\rangle_f}{\langle s\rangle})^{\frac{5}{2}}.$$

$$S_4 = \sum_f^{\infty} \exp(-gf - h\frac{\langle s\rangle_f}{\langle s\rangle})k^2(f)(\frac{\langle s\rangle_f}{\langle s\rangle})^4$$

$$S_3 = \sum_f^{\infty} \exp(-gf - h\frac{\langle s\rangle_f}{\langle s\rangle})k^{\frac{4}{3}}(f)(\frac{\langle s\rangle_f}{\langle s\rangle})^3.$$

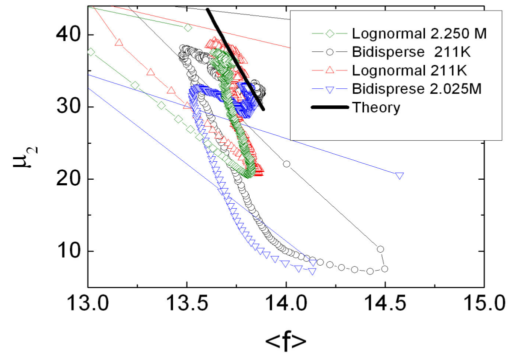
Results

$$\frac{\langle v\rangle_f}{\langle v\rangle} = k(f)(\frac{\langle s\rangle_f}{\langle s\rangle})^{\frac{3}{2}}\frac{S_{5/2}}{S_4}$$

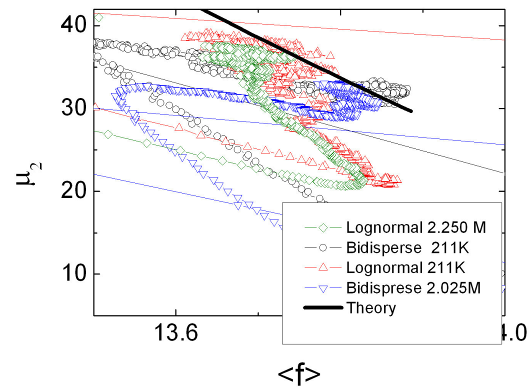
$$\phi_v(\frac{v}{\langle v\rangle}) = \frac{16}{3\pi}\frac{S_4}{S_{5/2}^2}\sum_f^{\infty} \exp(-gf - h\frac{\langle s\rangle_f}{\langle s\rangle})\frac{\langle s\rangle_f}{\langle s\rangle}\exp(-\frac{5}{2}\frac{\langle v\rangle^{\frac{2}{3}}}{k^{\frac{2}{3}}(f)\langle s\rangle_f}(\frac{v}{\langle v\rangle})^{\frac{2}{3}}),$$

$$\phi_s(\frac{s}{\langle s\rangle}) = \frac{4}{3\pi}(\frac{5}{2})^{\frac{5}{2}}\frac{1}{S_{5/2}}\sum_f^{\infty} \exp(-gf - h\frac{\langle s\rangle_f}{\langle s\rangle})k(f)(\frac{\langle s\rangle_f}{\langle s\rangle})^{\frac{3}{2}}\exp(-\frac{5s}{2\langle s\rangle_f})$$

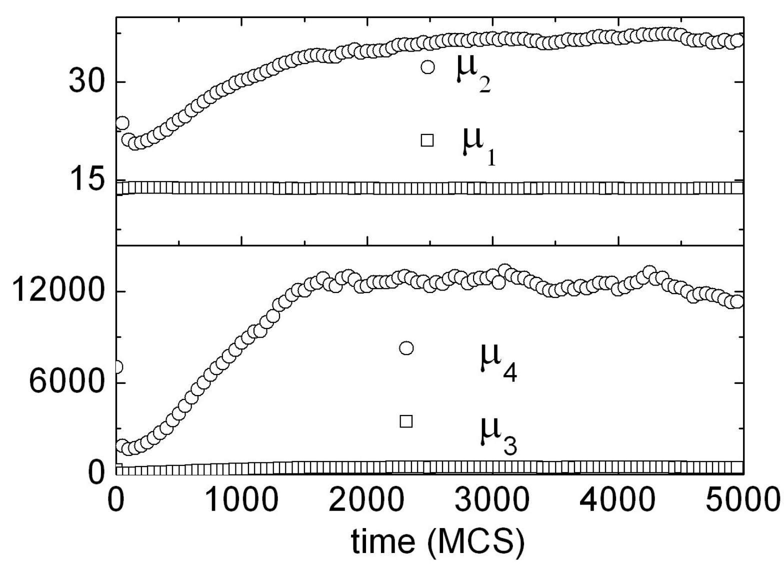
$$\phi_{v^{1/3}}(\frac{\langle v^{\frac{1}{3}}\rangle}{\langle v\rangle^{\frac{1}{3}}}) = 3\frac{\langle v^{\frac{1}{3}}\rangle}{\langle v\rangle^{\frac{1}{3}}}(\frac{v}{\langle v\rangle})^{\frac{2}{3}}\phi_v(\frac{v}{\langle v\rangle})$$

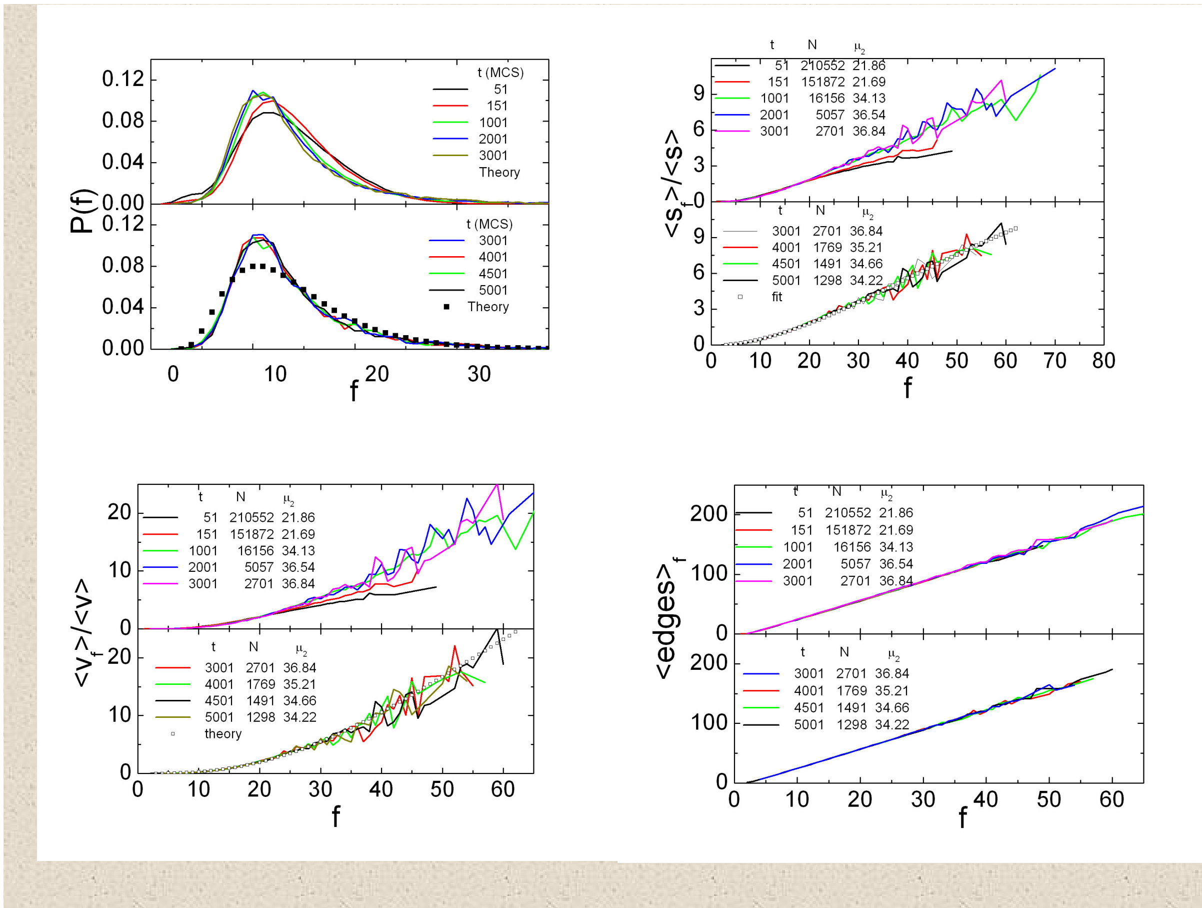


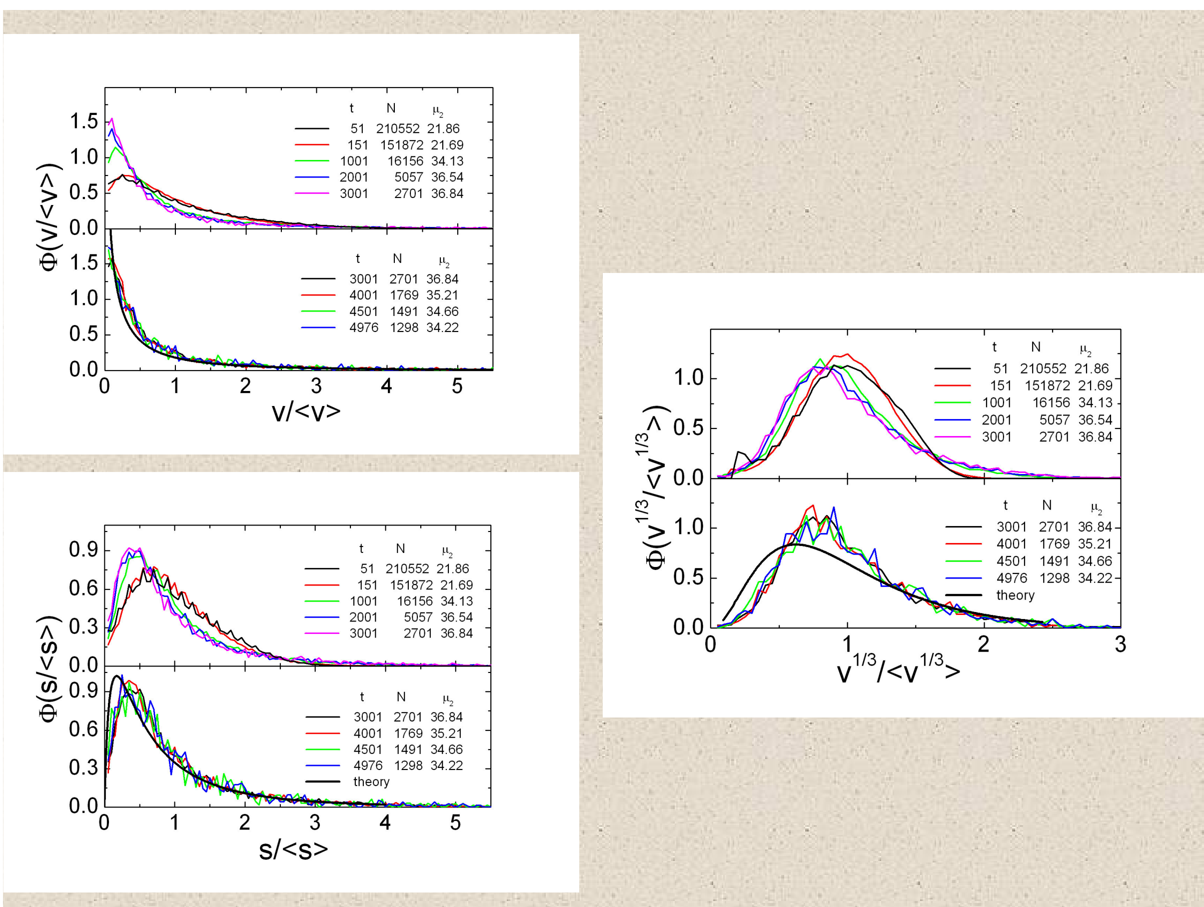
Thomas,de Almeida, and
Graner
to appear



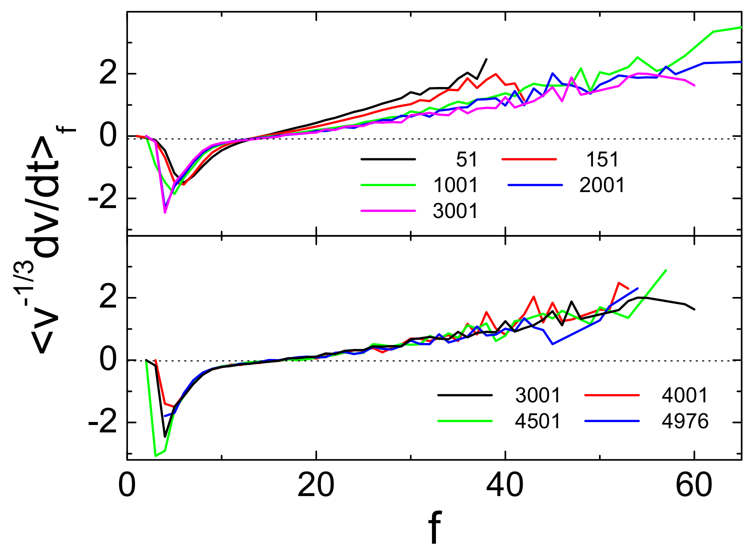
Reaching the scaling state



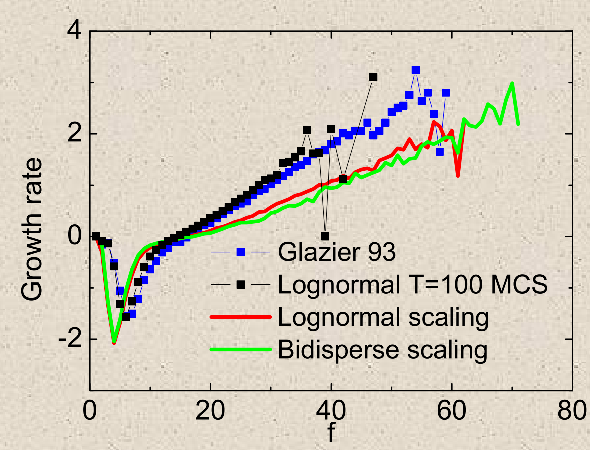

P(f)
f
t (MCS)
Theory
<s_f>/<s>
<v_f>/<v>
<edges>_f
t N μ2
51 210552 21.86
151 151872 21.69
1001 16156 34.13
2001 5057 36.54
3001 2701 36.84
4001 1769 35.21
4501 1491 34.66
5001 1298 34.22
fit
theory


Φ(v/<v>)
v/<v>
Φ(s/<s>)
s/<s>
Φ(v^1/3/<v^1/3>)
v^1/3/<v^1/3>
t N μ2
51 210552 21.86
151 151872 21.69
1001 16156 34.13
2001 5057 36.54
3001 2701 36.84
4001 1769 35.21
4501 1491 34.66
4976 1298 34.22
theory

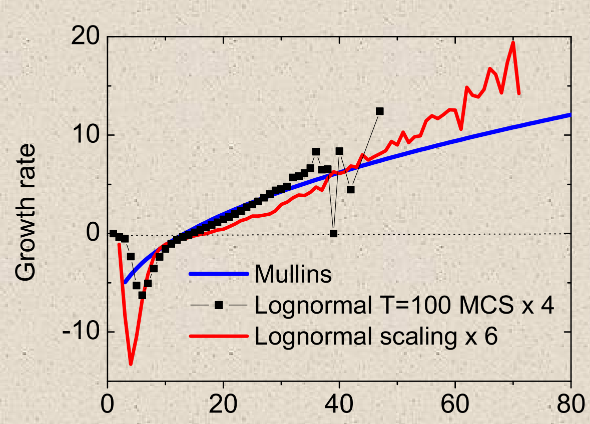
Growth law



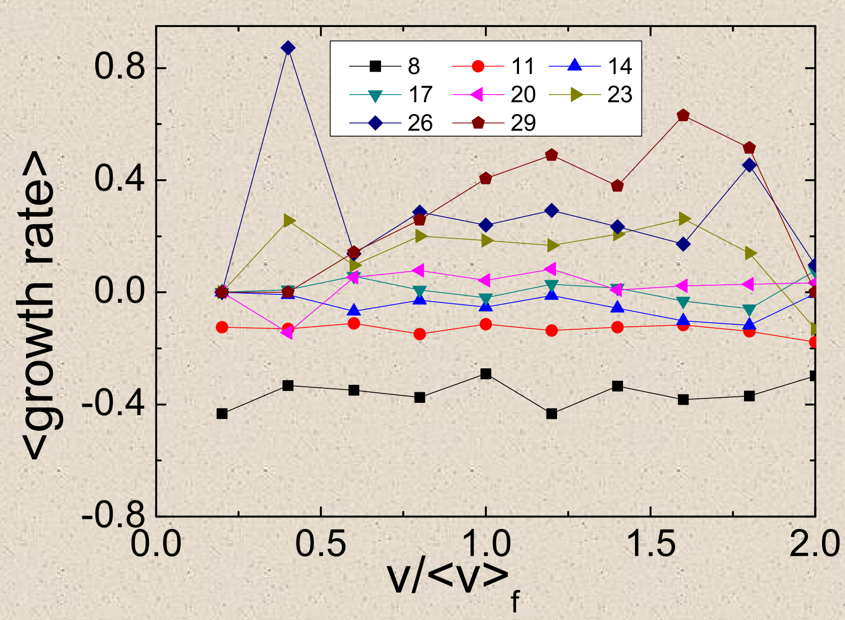
$<v^{-1/3}dv/dt>_f$
f
51
151
1001
2001
3001
3001
4001
4501
4976



Growth rate
f
Glazier 93
Lognormal T=100 MCS
Lognormal scaling
Bidisperse scaling



Growth rate
Mullins
Lognormal T=100 MCS x 4
Lognormal scaling x 6



Thank you !