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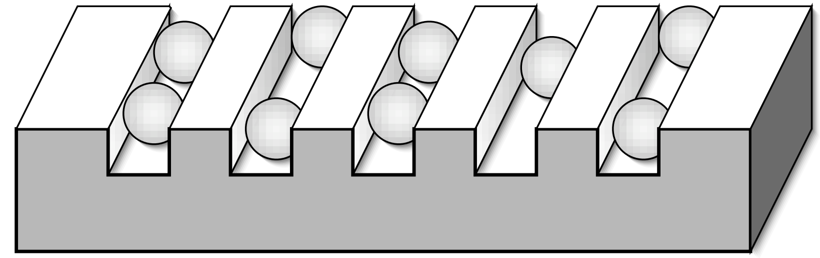
Mathematical Models for Self-Organization and Dissipation

Thanks to: Patrick Weidman (UC Boulder)
Steve Brueck & Deying Xia (CHTM,UNM)

D.D.Holm and V.P,
PRL **95**, 226106 (2005) http://arxiv.org/abs/nlin.PS/0501009
Physica D **220** (2), 183-196 (2006) http://arxiv.org/abs/nlin.PS/0506020
J Phys A (submitted) http://arxiv.org/abs/nlin.AO/0608011
Physica D (to appear, 2007) http://arxiv.org/abs/nlin.AO/0608054
D.D.Holm, VP and C.Tronci, Physica D, submitted
D.D.Holm, VP and C. Tronci, C.R.Acad.Sci Paris, to appear (2007).

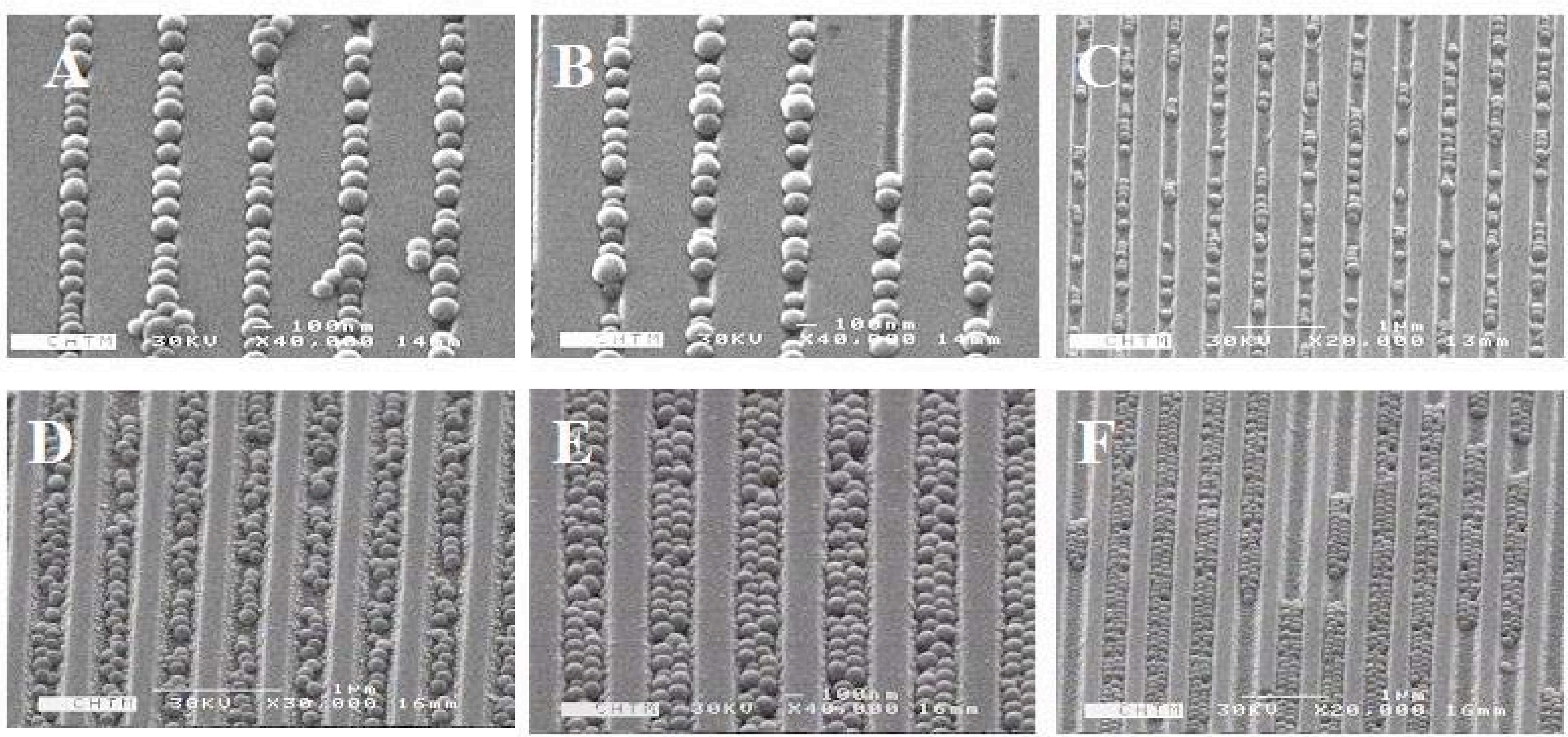
Motivation: Directed Self-Assembly at Nano-Scales



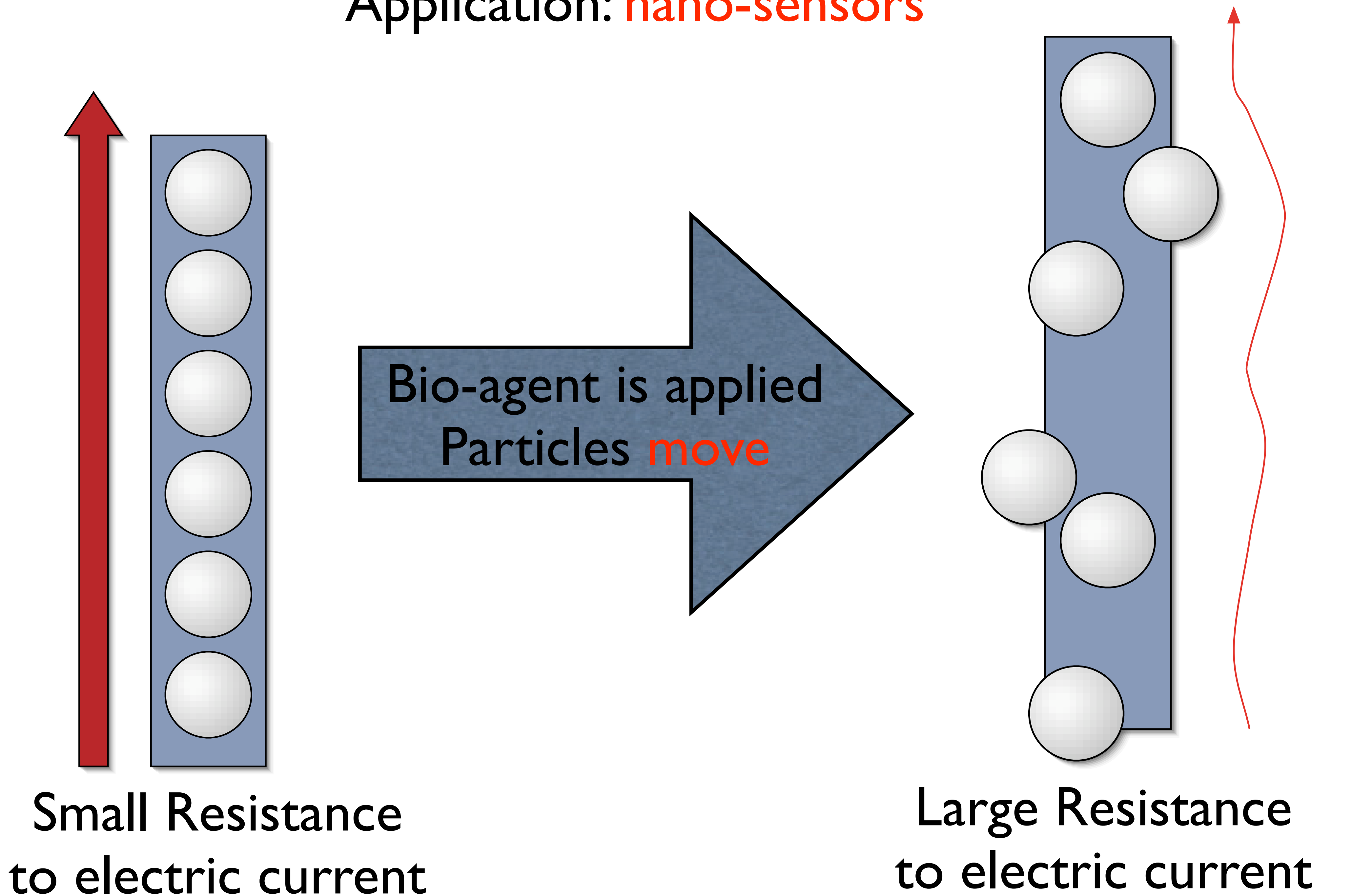
Colloidal solution of 50nm particles deposited on a grooved substrate

Water evaporates, contact line is pinned at grooves

Particles dragged into the grooves and self-organize



Application: nano-sensors



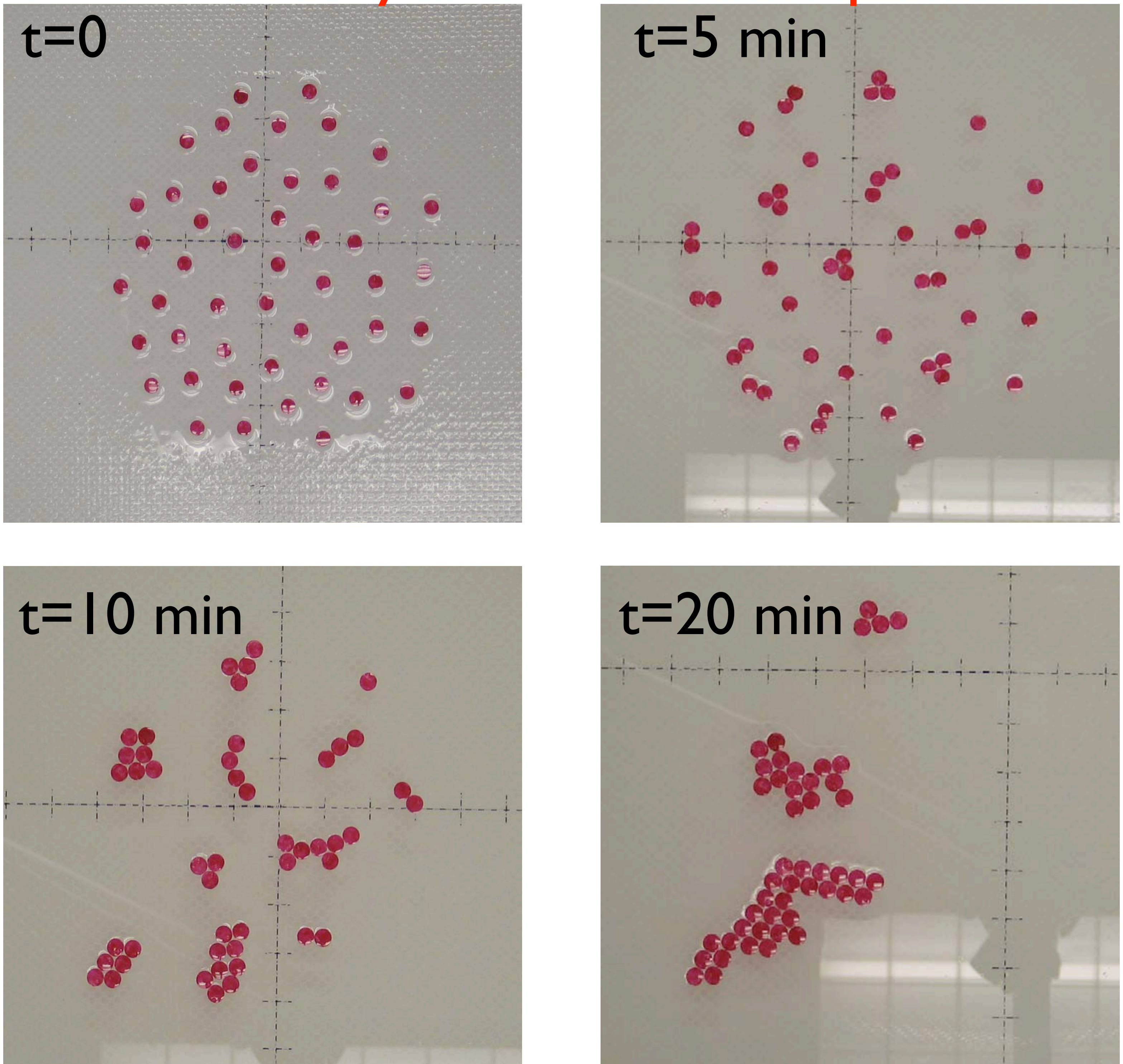
Everything is self-assembly

It would be nice to figure out how Nature works:
G. M. Whitesides and B. Grzybowski, Self-assembly at all scales, *Science*, **295**, 2418–2421 (2002).

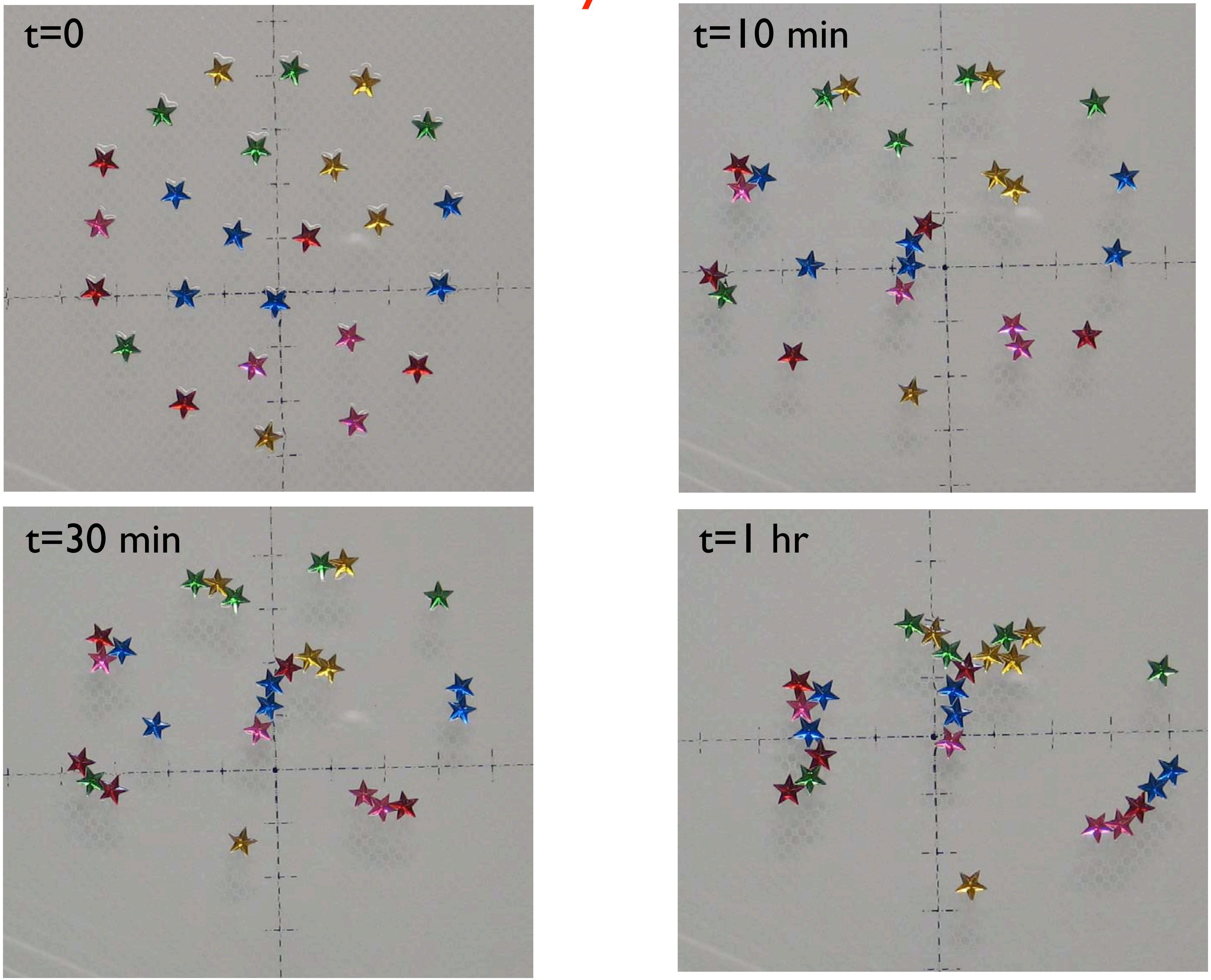
Macro-scales I (many many km): Stars, galaxies *etc*.
Macro-scales II (many km-km): Clouds, river networks *etc*.
Macro-scales III (meters-cm): Forests, schools of fish *etc*.
Meso-scales IV (mm-100 microns): micro-devices, bugs *etc*.
Micro-scales V (microns- nanometers): nano-devices, proteins *etc*.

Macro-nano scales: Life on Earth

Self-assembly of round 2mm particles



Self-assembly of 4 mm stars



Round particles, Linear energy, singular solutions

Mathematical modeling framework:

Density is advected with velocity proportional to gradient of (potential of interaction, concentration of chemical ...)

Interacting particles + Diffusion:

P.J.M. Debye and E. Huckel, *Zur Theorie der Elektrolyte: (2): Das Grenzgesetz fur die Elektrische Leiftfahrigkeit (On the theory of electrolytes 2: limiting law of electrical conductivity).* **Physik. Zeit.** ***24***, 305 (1923).

Coagulation+Diffusion

M. von Smoluchowski. *Drei Vortrage uber Diusion, Brownsche Molekularbewegung und Koagulation von Kolloidteilchen*. **Physik. Zeit.**, ***17***, p. 557-585 (1916).

M. von Smoluchowski. *Versuch eine mathematischen Theorie der Koagulationskinetik kolloidaler Losungen* **Z. Physik. Chem.** ***92***, 129-168 (1917).

Keller-Segel model of chemotaxis

E.F. Keller and L.A. Segel, *Initiation of slime mold aggregation viewed as an instability.* **J. Theoretical Biol**. ***26***, 399 (1970)

E.F. Keller and L.A. Segel *Model for chemotaxis*. **J. Theoretical Biol**, 225 (1971).

More general than the models considered here: reduces to class discussed here in limiting cases

Self-Aggregation (swarming) of insects

C. Topaz, A. Bertozzi and M. Lewis, ArXiv: q-bio PE/0504001 (2005).

Classical Debye-Huckel (etc) Equations

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\,(\rho \mathbf{u}) = D \Delta \rho \qquad \mathbf{u} = \mu \, \mathrm{grad} \Phi$$

$$\frac{\partial \Phi}{\partial t} + 0 = \Delta \Phi - \rho \; - \gamma \Phi$$

For particles of finite size, mobility can depend on density: at maximal density (1) mobility tends to zero

$$\mu = 1 - \rho$$

Model proposed

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\,(\rho \mathbf{u}) = D\Delta\overline{\rho} \qquad \mathbf{u} = \mu(\overline{\rho})\nabla\Phi$$

Potential $\Phi(x) = \int G(x - x')\rho(x')\mathrm{d}x' = (G * \rho)(x)$

Averaged Density $\overline{\rho}(x) = \int H(x - x')\rho(x')\mathrm{d}x' = (H * \rho)(x)$

We use $\mu(\overline{\rho}) = 1 - \overline{\rho}$ or $\mu(\overline{\rho}) = 1$

Previous work: $H(x) = \delta(x)$

$G(x)$ is inverse Laplacian or Helmholtz

Our work: *H*, *G* are nice functions

$$G(x) = e^{-|x|/\alpha} \qquad H(x) = \frac{1}{2\beta}e^{-|x|/\beta}$$

Blow-up and regularity for positive mobility

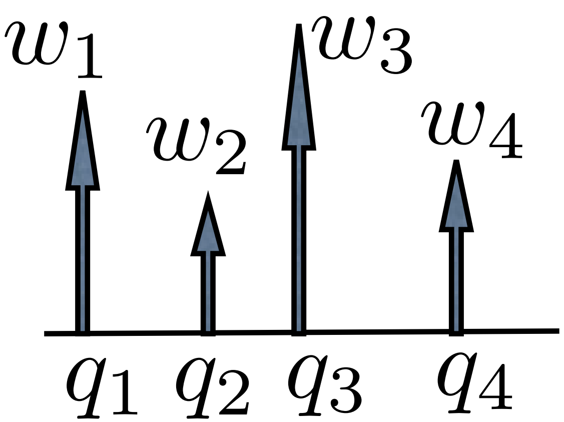
Classical case: $H(x) = \delta(x) \qquad G(x) = \Delta^{-1}$

One dimension: no blow-up, global bound in time for ρ in L^∞ and Φ in $W^{\sigma,p}$

T. Nagai *Adv. Math.Sci.Appl* **5**, 581 (1995); Hillen,Potapov *Math Meth. Appl. Sci* **27**, 1783 (2004):

Two or more dimensions - blow up Brenner *et al*, *Nonlinearity* ***12***, 1071 (1999)

Are singularities bad? Look for



$$\rho(x,t) = \sum_{j=1}^{N} w_j(t)\delta(x - q_j(t))$$

$$\overline{\rho}(x,t) = \sum_{j=1}^{N} w_j(t)H(x - q_j(t))$$

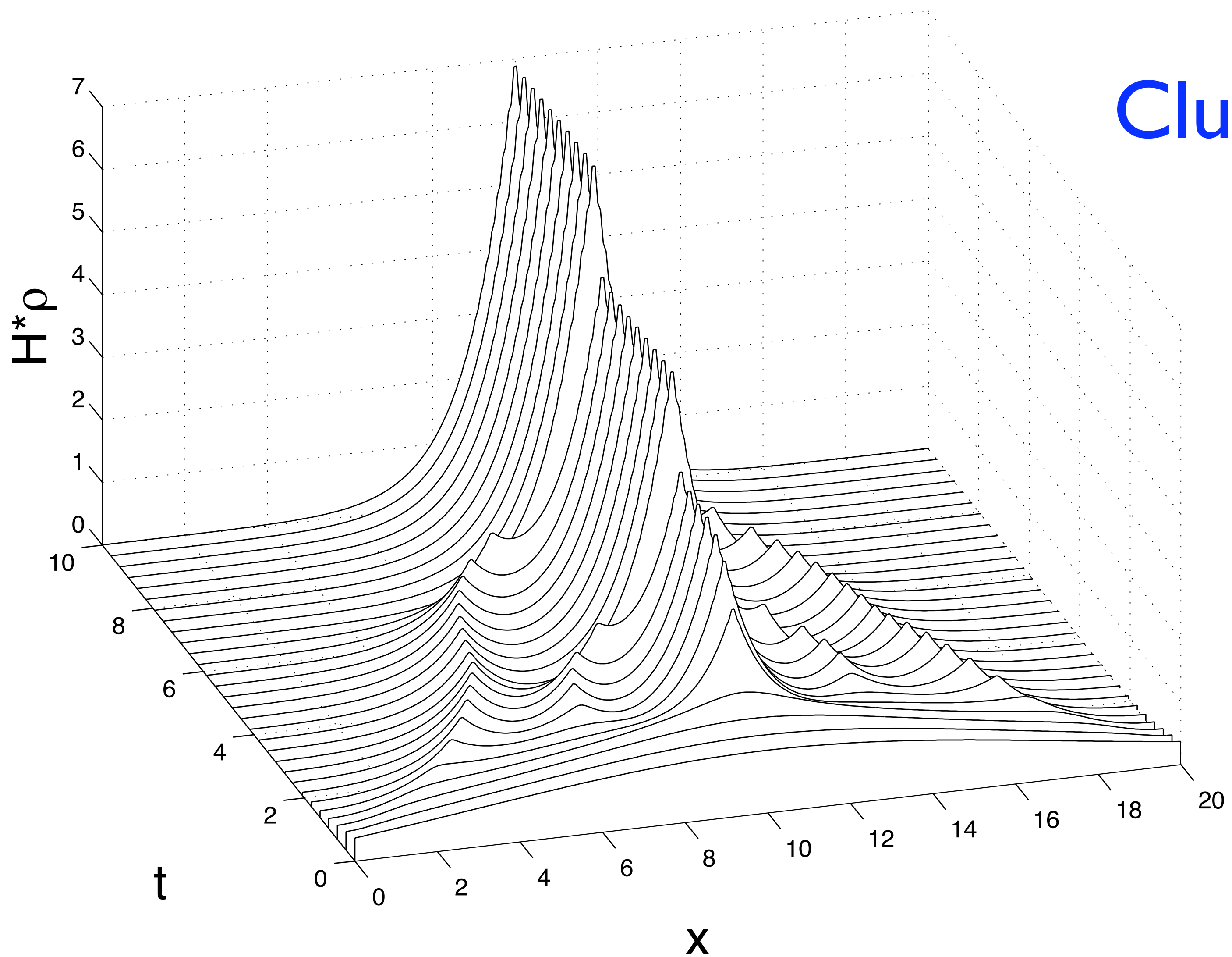
Clumpons!

A closed system of equations emerges

$$\dot{w}_i(t) = 0 \qquad \dot{q}_i(t) = -\sum_{j=1}^{N} w_j \mu(\overline{\rho}) G'(q_i - q_j)$$

Diffusion $D\Delta\overline{\rho}$ in our model does not prohibit formation of singularities, even in one dimension

Note: Energy remains finite on delta-functions



Clumpons!

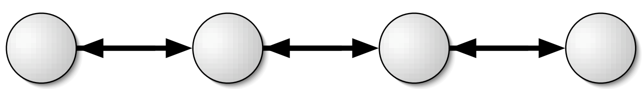
What are stationary solutions for $\mu(\overline{\rho}) = 1 - \overline{\rho}$?

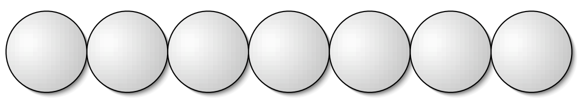
Particle velocity $\mathbf{u} = \mu(\overline{\rho})\nabla\Phi = 0$

Two types of stationary solutions

$\Phi = \text{const}$

$\overline{\rho} = 1$





Equilibrium Solutions

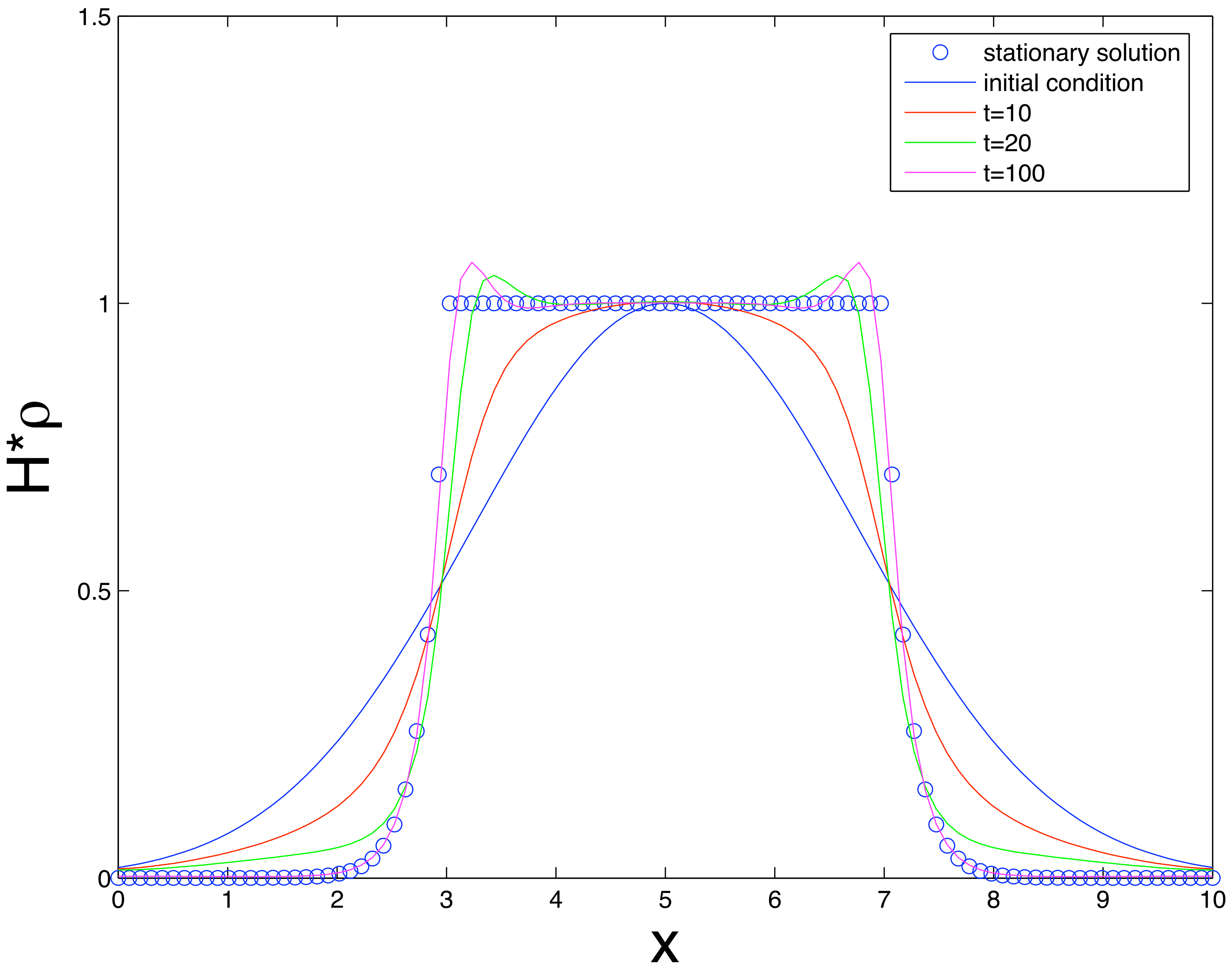
Jammed Solutions

Physically, we expect:

Unstable
(purely attractive force)

Stable

Full numerical simulation starting with Gaussian initial conditions



Analytical solutions in two dimensions

Look for jammed solution with compact support

$$\bar{\rho} = H * \rho = 1$$

Linear equation!

Analytical solutions for the case of inverse Helmholtz

An isolated patch with constant strength delta function at the boundary

2 D Helmholtz equation is separable in 4 cases (- cartesian)

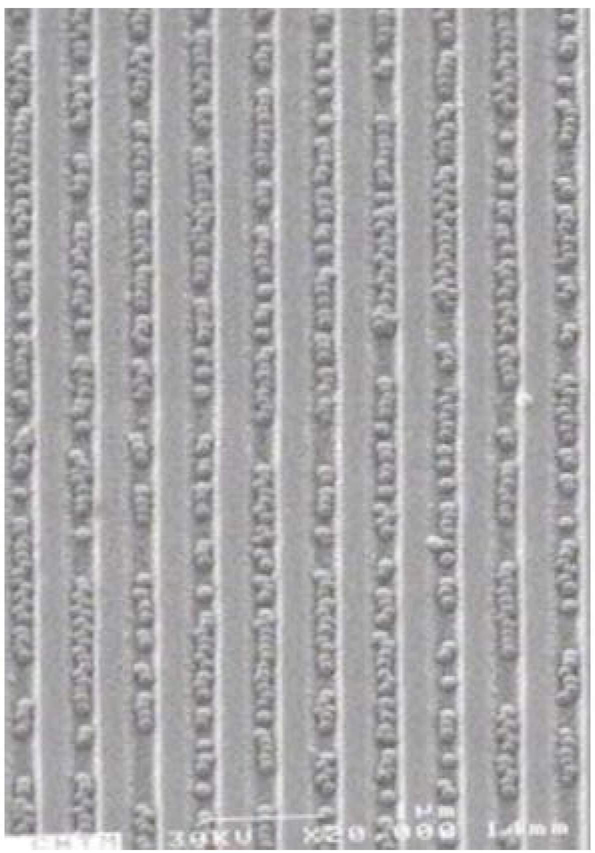
Polar coordinates	Circles	Bessel Functions
Elliptic Cylindrical	Ellipses	Modified Matthew Functions
Elliptic Cylindrical	Hyperbolae	Matthew Functions
Parabolic Cylindrical	Parabolae	Parabolic Cylinder Functions

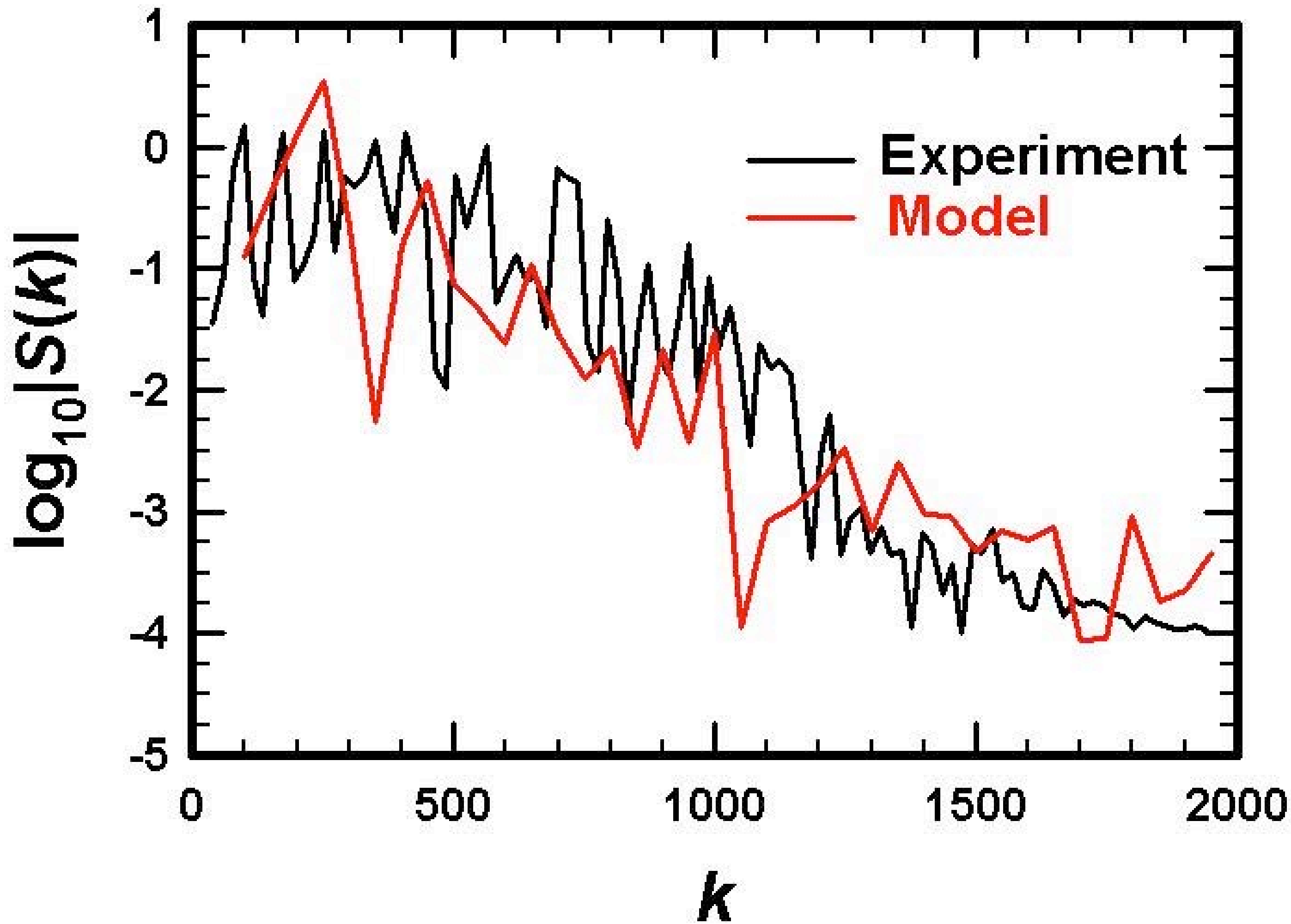
Density Spectrum: Simulation vs Experiment

$$\alpha = 1$$

$$\beta = 0.1$$

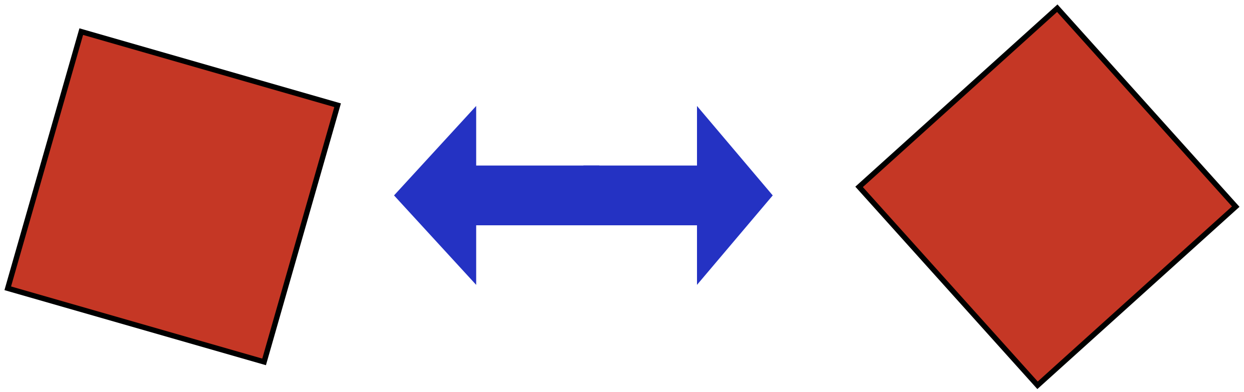
$$D = 0.01$$

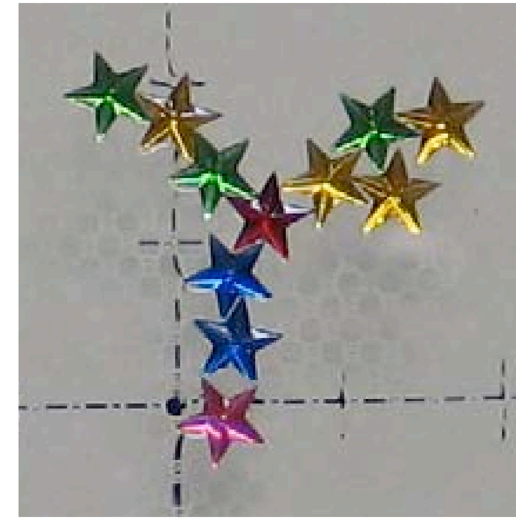




K. Mertens, V. P., D. Xia and S. Brueck, J. Applied Physics, ***98***, 094309 (2005).

Theoretical model II: Non-central interaction





Need to consider density (scalar)+ orientation (matrix in *SO(3)*)

Now consider an arbitrary geometric quantity $\kappa(\boldsymbol{x}, t)$
We want to define equation of motion, based on Darcy's law

velocity is proportional to force

so it reduces to Debye-Huckel equations when $\kappa(\boldsymbol{x}, t)$
is density (3-form).

But what is Darcy's law for an arbitrary geometric quantity?
How do we express it for, say, 1-form densities, 2-forms, density+orientation *etc?*

Mathematical Digression: Diamond and Gradient

Define a *pairing* $\langle \cdot\, ,\ \cdot \rangle$ (for *dual* things that can be multiplied and integrated, like scalars and 3-forms).

Then, define a *diamond* operator $b \diamond a$ for dual objects *a* and *b* (it takes two dual objects and produces 1-form density): for any vector field η

$$\langle b \diamond a\, ,\ \eta \rangle \equiv - \langle b\, ,\ \pounds_\eta\, a \rangle$$

Diamond operator is antisymmetric: $\langle\, b \diamond a + a \diamond b\, ,\ \eta \rangle = 0$

Explicit examples of diamond operator - RHS multiplied by $\cdot\, d\boldsymbol{x} \otimes d^3x$

f	is a scalar	$f \diamond \dfrac{\delta E}{\delta f} = \dfrac{\delta E}{\delta f} \nabla f$
$\mathbf{A} \cdot d\boldsymbol{x}$	is a one-form	$\mathbf{A} \diamond \dfrac{\delta E}{\delta \mathbf{A}} = \dfrac{\delta E}{\delta \mathbf{A}} \times \operatorname{curl} \mathbf{A} - \mathbf{A} \operatorname{div} \dfrac{\delta E}{\delta \mathbf{A}}$
$\mathbf{B} \cdot d\boldsymbol{S}$	is a two-form	$\mathbf{B} \diamond \dfrac{\delta E}{\delta \mathbf{B}} = \mathbf{B} \times \operatorname{curl} \dfrac{\delta E}{\delta \mathbf{B}} - \dfrac{\delta E}{\delta \mathbf{B}} \operatorname{div} \mathbf{B}$
$D\, d^3x$	is a three-form	$D \diamond \dfrac{\delta E}{\delta D} = -D \nabla \dfrac{\delta E}{\delta D}$

Let us also define operators relating of lowering and raising indices (no metric)

$$\left(\mathbf{A} \cdot d\mathbf{x} \otimes d^3x\right)^\sharp = \mathbf{A} \cdot \frac{\partial}{\partial \mathbf{x}} \qquad \left(\mathbf{B} \cdot \frac{\partial}{\partial \mathbf{x}}\right)^\flat = \mathbf{B} \cdot d\mathbf{x} \otimes d^3x$$

Motivating the answer

Density $\rho \mathrm{d}^n x$ (n-form) → Arbitrary Geometric Quantity κ

$$\frac{\partial \rho}{\partial t} = -\mathrm{div}\,(\rho u)$$

$$\frac{\partial \rho}{\partial t} = -\pounds_u \rho \quad \rightarrow \quad \frac{\partial \kappa}{\partial t} = -\pounds_u \kappa$$

Darcy's velocity → Mobility μ is of the same type as κ

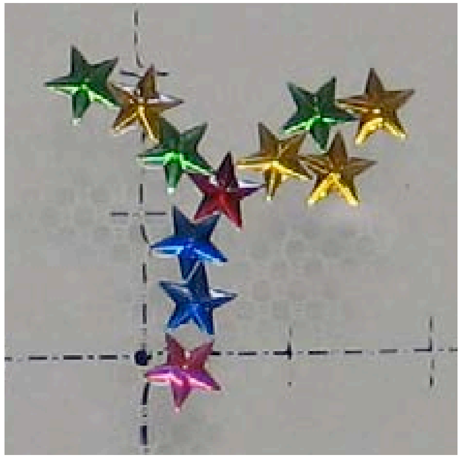
$$u = \left(\mu \nabla \frac{\delta E}{\delta \rho}\right)^\sharp \quad \rightarrow \quad u = \left(\mu \diamond \frac{\delta E}{\delta \kappa}\right)^\sharp$$

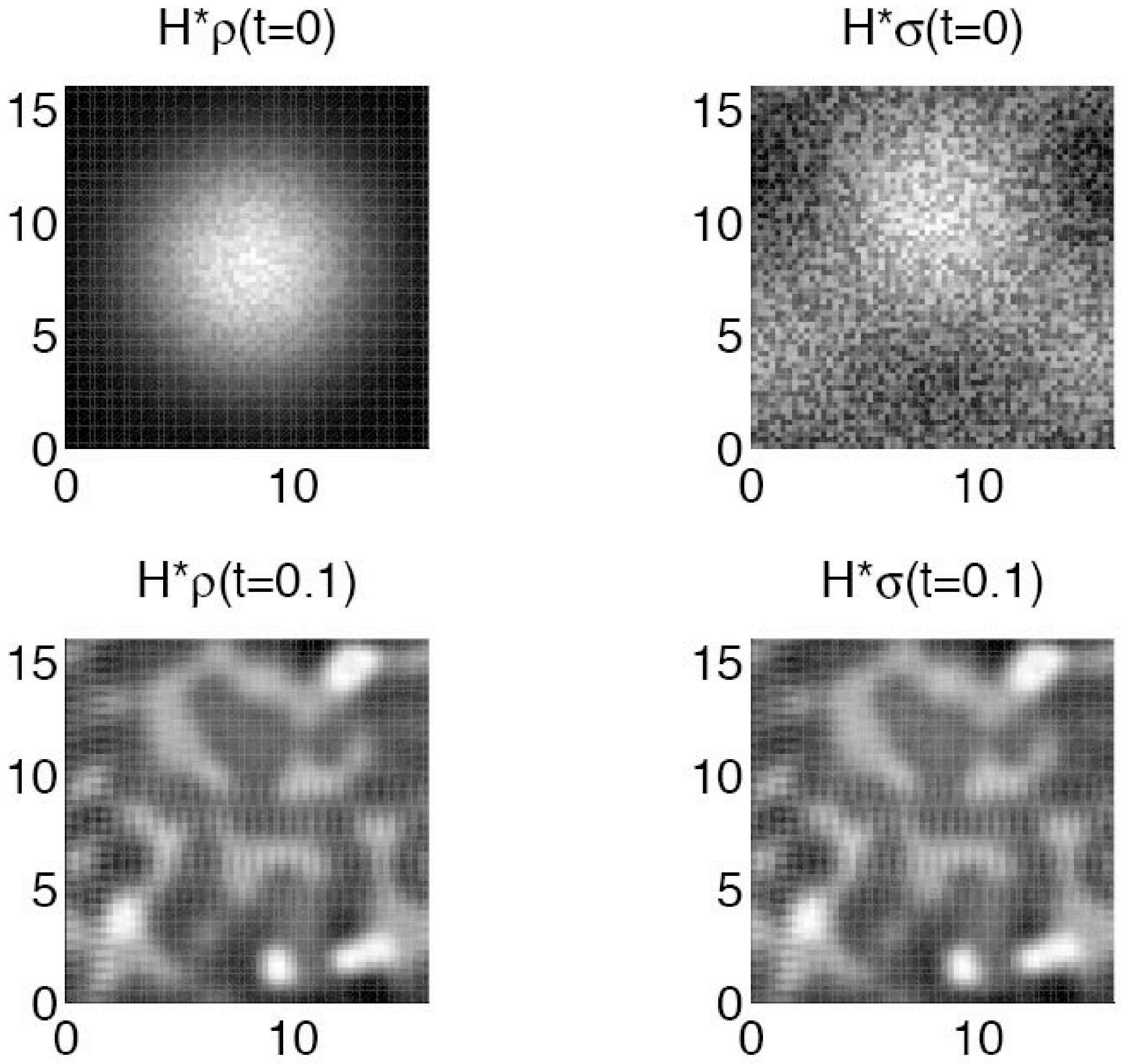
Final answer must be

$$\frac{\partial \kappa}{\partial t} = -\pounds_{(\mu \diamond \frac{\delta E}{\delta \kappa})^\sharp} \kappa$$

Simulation of Geometric Order Parameter (GOP) equation for orientation

2D simulation
Initial conditions are given by an isolated patch with random orientation





Theorem [Energy dissipation]: *Energy E is evolving according to*

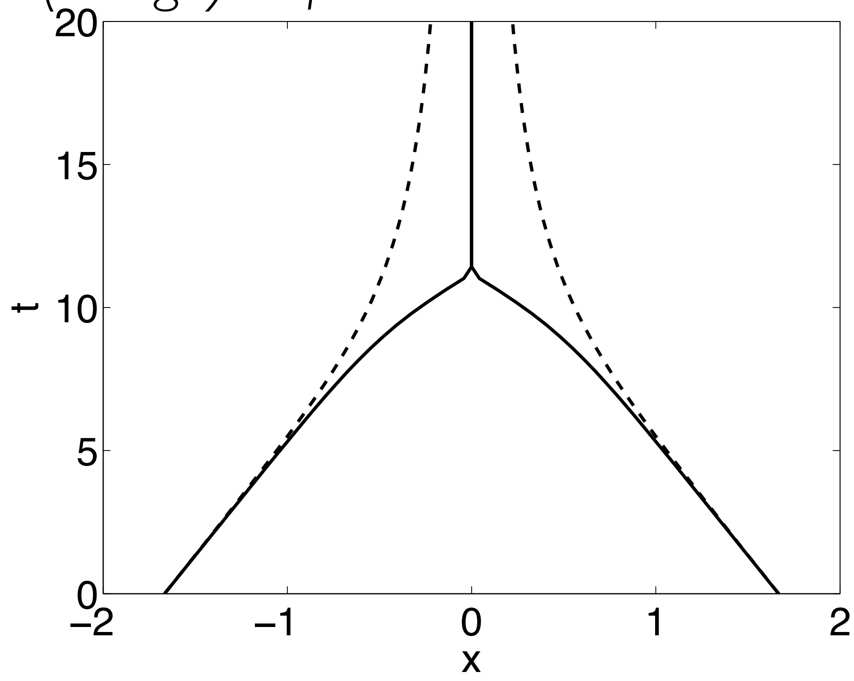
$$\frac{dE}{dt} = -\left\langle \left(\kappa \diamond \frac{\delta E}{\delta \kappa}\right), \left(\mu[\kappa] \diamond \frac{\delta E}{\delta \kappa}\right)^{\sharp} \right\rangle$$

Theorem [Existence of singular solutions-necessary conditions]: *The weak form of the GOP equation contains only values and first derivatives of the arbitrary function so singular solutions may exist*

$$\left\langle \frac{\partial \kappa}{\partial t}, \phi \right\rangle = \left\langle -\pounds_{(\mu \diamond \frac{\delta E}{\delta \kappa})^{\sharp}} \kappa, \phi \right\rangle = \left\langle \kappa \diamond \phi, (\mu \diamond \frac{\delta E}{\delta \kappa})^{\sharp} \right\rangle = \left\langle \kappa, \pounds_{(\mu \diamond \frac{\delta E}{\delta \kappa})^{\sharp}} \phi \right\rangle$$

Theorem [Collapse of singular solutions]: *There exist initial conditions for scalar equation for which singular solutions collapse (merge) in finite time*

Simulation of two singular solutions with opposite amplitudes collapsing in finite time.
(Solid -theory, dashed-simulation)



Metric formulation

For an arbitrary functional *F*,

$$\frac{dF[\kappa]}{dt} = \Big\langle \frac{\partial\kappa}{\partial t}\,,\,\frac{\delta F}{\delta\kappa}\Big\rangle \;=\; \Big\langle -\pounds_{(\mu[\kappa]\diamond\frac{\delta E}{\delta\kappa})^\sharp}\kappa\,,\,\frac{\delta F}{\delta\kappa}\Big\rangle$$

$$= \;-\Big\langle\Big(\mu[\kappa]\diamond\frac{\delta E}{\delta\kappa}\Big),\,\Big(\kappa\diamond\frac{\delta F}{\delta\kappa}\Big)^\sharp\Big\rangle =: \{\{\,E\,,\,F\,\}\}[\kappa]$$

defines *Metric Tensor* for any two functionals *F* and *E* and (as we see below) *Double Bracket (bracket of a bracket)*

Double Bracket comes from *Darcy's law* (force proportional to velocity) so it is a way to introduce dissipation in a physical system - *Lie-Darcy's dissipation*

Advantages:

1) Preserves coadjoint motion (modifying velocity) if added to inertia in the Euler-Poincare form

2) Allows singular solutions if mobility is nonlocal function

Connection to previous work

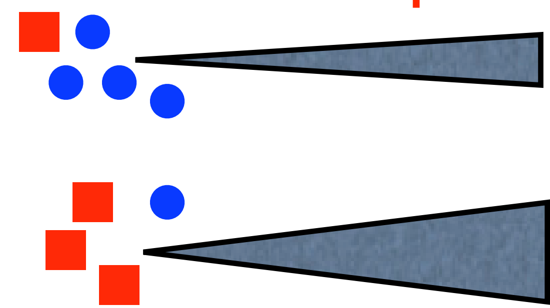
Double Bracket dissipation introduced before:

Bloch, Brockett, Ratiu, *Comm. Math. Phys*, ***147***, *57-74 (1992)*
Bloch, Krishnaprasad, Marsden, Ratiu, *Comm. Math. Phys*, ***175***, *1-42 (1996)*;
Bloch, Brockett and Crouch, *Comm. Math. Phys*, ***187***, *357-373 (1996)*

Motivation: Dissipation in Euler equations and list sorting
Brockett, *Linear Algebra and Applications*, ***122***,*761-777 (1989)*
Vallis, Carnevale and Young, *J. Fluid Mech*, ***207***, *133-152 (1989)*

Why not apply double bracket ideas to kinetic equations as a dissipation model?

Motivation: Mass-spectrometer using Atomic Force Microscope



Oscillating AFM tip creates particle dynamics

Possibility of separating particles (molecules) based on dynamical properties- Important to know dissipation

With Takashi Hikihara (Kyoto University, Engineering)

Mathematically:

Introducing dissipation into Vlasov's equation for f(p,q,t)

(D.D.Holm, V.Putkaradze and C.Tronci, C.R.Acad.Sci Paris, to appear (2007))

For any two functionals *E* and *F* define ({ , } is the Lie-Poisson bracket

$$\{\{\, E \,,\, F \,\}\} = -\left\langle \left\{ \mu[f] \,, \frac{\delta E}{\delta f} \right\} , \left\{ f \,, \frac{\delta F}{\delta f} \right\} \right\rangle = \left\langle \left\{ f, \left\{ \mu[f] \,, \frac{\delta E}{\delta f} \right\} \right\} , \frac{\delta F}{\delta f} \right\rangle$$

Then for arbitrary functional *F* dissipative dynamics is

$$\frac{dF}{dt} = \{\{\, E \,,\, F \,\}\}$$

A. Kaufman, *Phys Lett A*, ***100***, *419-422* (1984), P. Morrisson, *Phys Lett A*, ***100***, *419-422* (1984) - general double bracket form

H. Kandrup, *Astrophys. J.* ***380*** *511-514* (1991); $\mu[f] = \alpha f$

Dissipative Vlasov equation for particles with orientation

Suppose g is the space dual to the Lie algebra *so(3)* (or more general)
Define a bracket as in Gibbons, Holm and Kuppershmidt,
Phys. Lett A, ***90***, *281-283 (1982)*;
ibid, *Phys. D*, ***6,*** *179-194 (1982/3)*.

$$\{f,h\}_1 := \{f,h\} + \left\langle g, \left[\frac{\partial f}{\partial g}, \frac{\partial h}{\partial g}\right]\right\rangle$$

Taking moments & applying cold plasma closure yields *chromohydrodynamics*

The dissipative Vlasov equation is

$$\frac{\partial f}{\partial t} = \left\{ f, \left\{ \mu[f], \frac{\delta E}{\partial f} \right\}_1 \right\}_1$$

Equations of motion:
Moments - Define

$$\rho = \int f \, \mathrm{d}g \, \mathrm{d}p \qquad G = \int g \, f \, \mathrm{d}g \, \mathrm{d}p$$

$$\mu_\rho = \int \mu[f] \, \mathrm{d}g \, \mathrm{d}p \qquad \mu_G = \int g \, \mu[f] \, \mathrm{d}g \, \mathrm{d}p$$

Assume linearity in *g*; Integrate with respect to *p* and *g*
Neglect all moments involving product *pg*
Truncate terms with moments (in *p*) higher than one
We obtain, at zeroth order -

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial q}\left(\rho \, \mu[\rho] \, \frac{\partial}{\partial q} \frac{\delta E}{\delta \rho} \right)$$

Evolution equations for density and orientation

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial q}\left(\rho\left(\mu_\rho \frac{\partial}{\partial q}\frac{\delta E}{\delta \rho} + \left\langle \mu_G, \frac{\partial}{\partial q}\frac{\delta E}{\delta G}\right\rangle\right)\right)$$

$$\frac{\partial G}{\partial t} = \frac{\partial}{\partial q}\left(G\left(\mu_\rho \frac{\partial}{\partial q}\frac{\delta E}{\delta \rho} + \left\langle \mu_G, \frac{\partial}{\partial q}\frac{\delta E}{\delta G}\right\rangle\right)\right) + \mathrm{ad}^*_{\left(\mathrm{ad}^*_{\frac{\delta E}{\delta G}}\mu_G\right)^\sharp} G$$

Very cute

Diffusion

Lie-Darcy

Example: rod-like particles on a line - so(3) algebra

$G = \mathbf{m}(x)$, and $\mathrm{ad}^*_{\mathbf{v}}\mathbf{w} = -\mathbf{v}\times\mathbf{w}$ so

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(\rho\left(\mu_\rho \frac{\partial}{\partial x}\frac{\delta E}{\delta \rho} + \boldsymbol{\mu}_{\mathbf{m}} \cdot \frac{\partial}{\partial x}\frac{\delta E}{\delta \mathbf{m}}\right)\right)$$

$$\frac{\partial \mathbf{m}}{\partial t} = \frac{\partial}{\partial x}\left(\mathbf{m}\left(\mu_\rho \frac{\partial}{\partial x}\frac{\delta E}{\delta \rho} + \boldsymbol{\mu}_{\mathbf{m}} \cdot \frac{\partial}{\partial x}\frac{\delta E}{\delta \mathbf{m}}\right)\right) + \mathbf{m}\times\boldsymbol{\mu}_{\mathbf{m}}\times\frac{\delta E}{\delta \mathbf{m}}$$

Gilbert dissipation for Landau-Lifschitz equation

Connection to Smoluchowski's equation

Do not integrate with respect to *g* (only moments in *p*) $A_n(q,g) := \int p^n \, f(q,p,g)\, dp\,.$

Use *cold plasma* approximation $A_2 = \frac{A_1^2}{A_0}$

$$\frac{\partial A_0}{\partial t} = \frac{\partial}{\partial q}\Big(A_0 \mathcal{F}_{01}\Big) + \frac{\partial}{\partial g}\cdot\left(A_0\,\frac{\partial}{\partial g}\cdot(\widehat{g}\;\lambda_0) \;-\; A_1\,\frac{\partial}{\partial g}\cdot\widehat{g}\,\mathcal{F}_{01}\right)$$

$$\frac{\partial A_1}{\partial t} = \frac{\partial}{\partial q}\Big(A_1 \mathcal{F}_{01}\Big) - A_0\,\frac{\partial \lambda_1}{\partial q} + A_1\,\frac{\partial}{\partial q}\mathcal{F}_{01} + \frac{\partial}{\partial g}\cdot\left(A_1\,\frac{\partial}{\partial g}\cdot(\widehat{g}\;\lambda_0\,) \;-\; \frac{A_1^2}{A_0}\,\frac{\partial}{\partial g}\cdot\,(\widehat{g}\,\mathcal{F}_{01})\right)$$

Our variables *g* are on Lie Algebra - not Lie group (2-sphere)
Compare with e.g. P. Constantin, *Comm. Math. Sci*, ***3***, *531-544* (2005)

$$\frac{\partial A_0}{\partial t} = \partial_{\rm g}\left[\partial_{\rm g} A_0 - A_0 \partial_{\rm g}\left(G * A_0\right)\right]$$

Certain similarities are apparent but our tensors $\widehat{g}$ are antisymmetric, so equations look different

Summary

1)We derived new equations for self-organizations of oriented particles from general conservation principles
2) We suggested a dissipative Vlasov equation with the dissipation preserving weak solutions
3) We derived a new dissipative equations for momenta - Lie-Darcy dissipation
4) We suggested a kinetic origin of Gilbert dissipation in Landau-Lifshitz equations

Future work

1) Study the appearance and dynamics of the generalized solutions to the new dissipative kinetic equations
2) Study singular solutions in the new Lie-Darcy dissipative equations
3) Applications to self-organization and protein dynamics