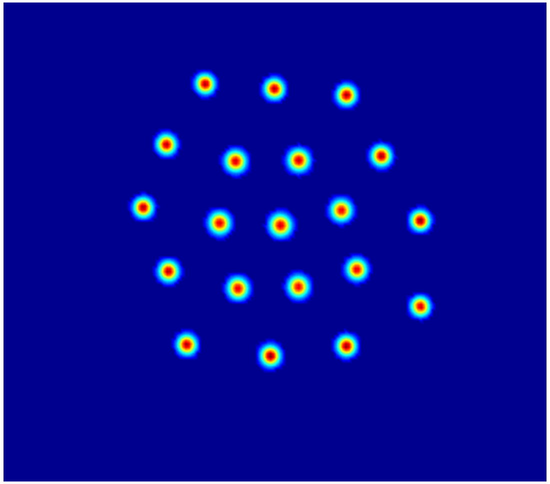
Pattern density distribution in PDE's



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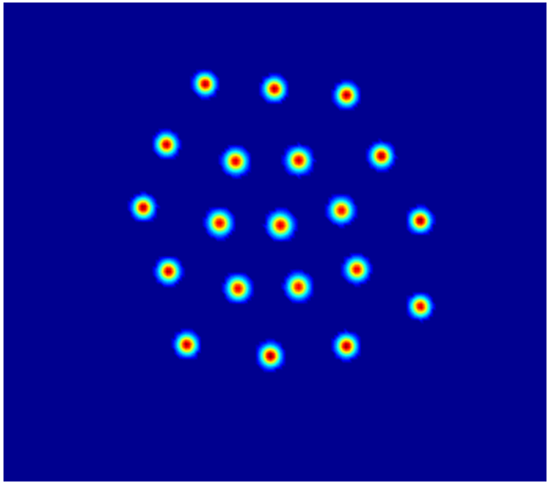
Spike lattices

- Solutions to many Reaction-Diffusion systems consist of spikes (or spots)

- Question: how are these spots distributed in the domain?

- Example: hexagonal spike clusters in Gierer-Meinhardt model with percursor:



- Philosophy: treat spikes as "points" in space, derive reduced ODE-algebraic system for evolution of N spikes; take the limit as $N \to \infty$

Warmup: single PDE with precursor

- Warmup problem: elliptic PDE (1d or 2d):

$$0 = \Delta u - u + u^2 + \varepsilon |x|^2 \tag{1}$$

  in either one or two dimensions.

- When $\varepsilon = 0$, the problem was extensively studied by many authors
  - [Gidas-Nirenberg, 1981] established uniqueness of a single radial spike on all of $\mathbb{R}^d$;
  - [Ni-Wei, 95; Gui-Wei, 97]: N spikes on a bounded domain satisfy a “ball-packing” problem: each spike location is furthest away from all other spikes.
  - No muti-spike steady state when $\varepsilon = 0$ (spikes repell each other...)

- Here, $\varepsilon |x|^2$ acts as a confinement well.

- Multi-spike solutions exist when $\varepsilon > 0$.

Step 1: reduced system for spike centers

- "Standard" asymptotic reduction, obtain ***algebraic system***

$$ax = -\nabla_{x_k} \left(\sum_{j \neq k} K(|x_j - x_k|) \right) \quad (2)$$

  - Here, $K(r)$ is Helmholtz Green's function: $K(r) = e^{-r}$ in 1D and $K(r) = K_0(r)$ (Bessel K0) in 2d.

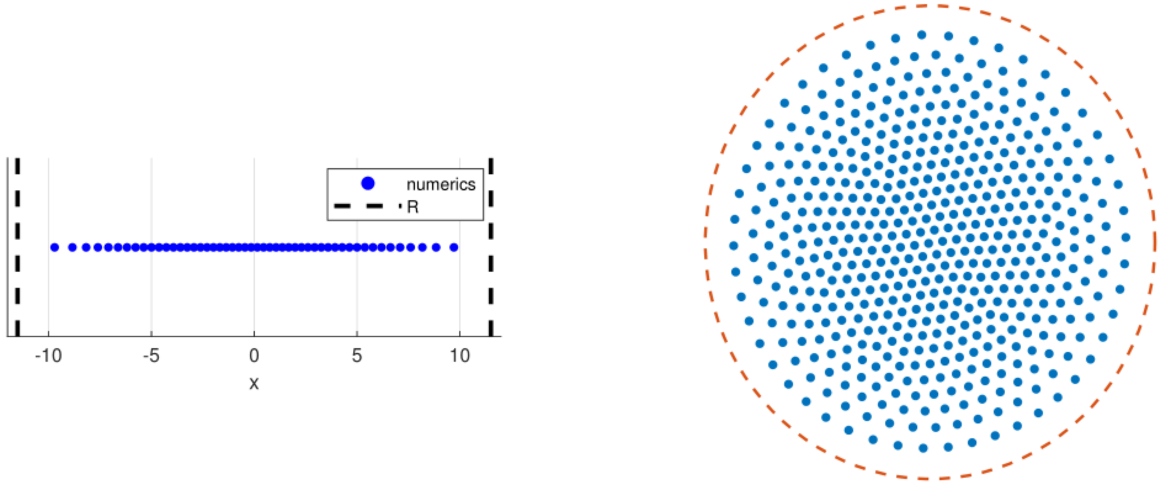
  - a is an $O(\varepsilon)$ constant.

- The sum is inter-spikes interacting through their tails; the term ax is due to trap confinement.

- To solve (2) we solve the related ODE whose steady state satisfies (2)

$$\frac{dx_k}{dt} = -ax_k + \sum_{j \neq k} K'(|x_j - x_k|) \frac{x_j - x_k}{|x_j - x_k|}, \quad k = 1 \ldots N. \quad (3)$$

- System (3) is one of the simplest swarming models [Bernoff+Topas, 2013]. It leads to compact swarms:



- The key to our computations is that the kernel $K(r)$ decays rapidly; ***its decay is sufficiently fast*** so that the summation can be expanded in Taylor series locally.

1D system: $\sum_{j \neq k} e^{-|x_k - x_j|} \frac{x_k - x_j}{|x_k - x_j|} \sim a x_k, \quad k = 1 \ldots N$

- Key observation: due to exponential decay, assume that the ***sum is dominated by nearby neighbours*** [similar to "Laplace integration"]. Then expand everything in ***Taylor series***, to two orders.
  - Parametrize: $x_k = x(s)$,where $k = s \in [1, N]$.
  - Define inter-spike distance,

$$u := \frac{dx}{ds} \approx x_{s+1} - x_s. \tag{4}$$

  - Expand to two orders:

$$x_{k+l} - x_k \sim lu + \frac{l^2}{2} u_x u;$$

$$\sum_{j \neq k} e^{-|x_k - x_j|} \operatorname{sign}(x_k - x_j) \sim u_x \sum_{l=1}^{\infty} u l^2 e^{-ul}$$

$$\sim u_x u \frac{e^{-u}(e^{-u} + 1)}{(1 - e^{-u})^3}$$

- Obtain the ODE for the inter-spike distance $u(x)$:

$$\frac{du}{dx} u \frac{e^{-u}(e^{-u}+1)}{(1-e^{-u})^3} \sim ax, \tag{5}$$

- Solution blows up at $x = \pm R$. Spike density is given by $\rho = 1/u$, so that

$$\int_{-R}^{R} \frac{1}{u} dx = N; \text{ where } u(\pm R) = \infty. \tag{6}$$

- Together, (5) and (6) fully determines $u(x)$.

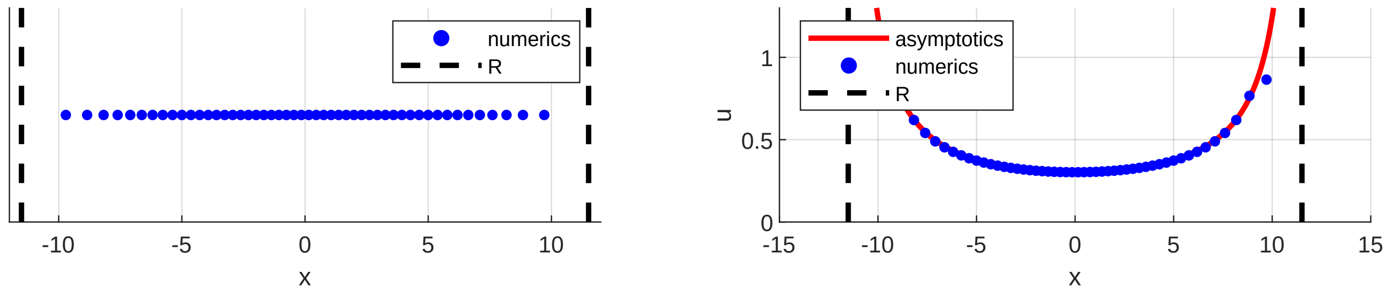


Figure 1: Comparison with numerics $a = 0.1$ and $N = 50$.

- Ode (5) has an implicit solution

$$\frac{1}{e^u - 1} + \frac{ue^u}{\left(e^u - 1\right)^2} = \frac{a}{2}\left(R^2 - x^2\right), \tag{7}$$

but integral in (6) does not appear to have an explicit form. So integrate (5, 6) numerically instead.

- Scaling analysis: if we double N, we can quarter a and retain the same spike density but on the domain double the size. So the solution is in the “spreading” regime, opposite of [Bernoff+Topaz 2013], [Fetecau-K-Huang, 2011]

2D cluster: $\sum_{j\neq k} K_0'\left(\left|x_k - x_j\right|\right)\frac{x_j - x_k}{|x_j - x_k|} = a x_k$

- Numerics indicate that this steady state has a hexagonal latttice structure.

- While the ***overall*** density is clearly non-uniform, the ***local*** structrue is still nearly hexagonal. So we ***assume:***

  (a) the lattice structure is nearly-hexagonal at every position x_k; (b) Locally, the lattice is a small conformal deformation of a perfect hexagonal lattice. (c) the steady state is nearly radially symmetric in the limit of large N.

- Define $u(x_k)$ to be the lattice spacing at x_k, that is, the distance from x_k to its closest neighbour:

$$u(x_k) = \min_{j\neq k} |x_j - x_k| .$$

  This allows to estimate:

$$\sum_{j\neq k} K_0'(|x_k - x_j|)\frac{x_k - x_j}{|x_k - x_j|} \sim u_r \phi_2(u)$$

  where

$$\phi_2(u) := \frac{1}{2}\sum\sum\left[-|l|\, K_0'(u\,|l|) + ul\,\mathrm{Re}(l) K_0(u\,|l|)\right]$$

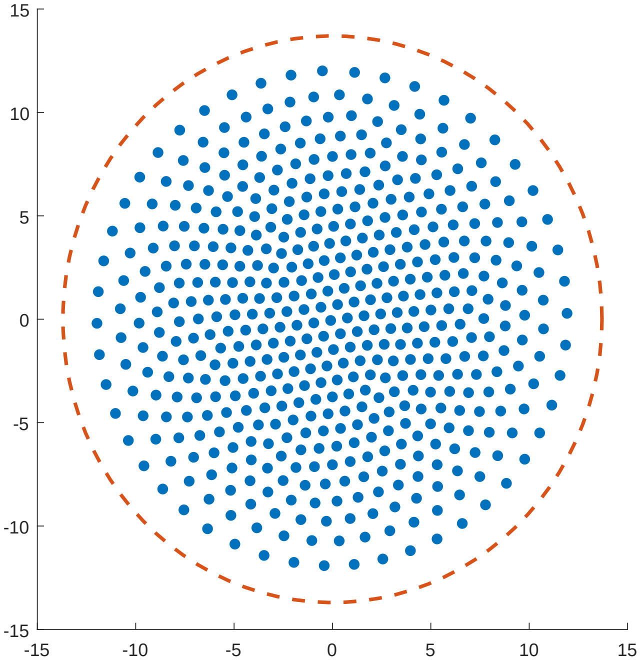
  where double sum is over lattice points: $l = l_1 + e^{i\pi/3} l_2, \ \ (l_1, l_2) \in \mathbb{Z}^2 \backslash \{0\}$

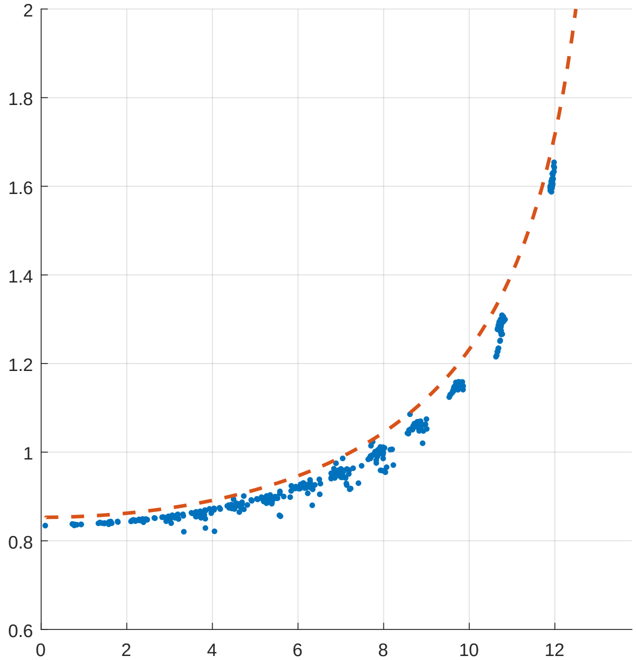
- Continuum limit becomes

$$\frac{du}{dr}\phi_2(u) = -ar \tag{8}$$

coupled to integral boundary condition for mass conservation:

$$N = \frac{2}{\sqrt{3}} \int_0^R \left(\frac{1}{u(r)}\right)^2 2\pi r dr \text{ where } u(R) = \infty \tag{9}$$





- Scaling analysis: if we double N, we can half a and retain the same spike density but on a domain that has twice the area (whose radius is $\sqrt{2}$ larger).

GM in 2d

GM model:

$$a_t = \varepsilon^2 \Delta a - \mu(x) a + \frac{a^2}{h}, \qquad 0 = \Delta h - h + \frac{a^2}{\varepsilon^2}, \quad x \in \mathbb{R}^2 \tag{10}$$

Reduced equations:

$$H_k \sim \mu_k H_k^2 \frac{\int w^2}{2\pi} \log \varepsilon^{-1} + \sum_{j \neq k} \mu_j H_j^2 K_0 \left(|x_k - x_j| \right) \frac{\int w^2}{2\pi} \tag{11}$$

$$0 = \frac{\nabla \mu_k}{\mu_k} \frac{1}{2} + \frac{1}{H_k} \sum_{j \neq k} \mu_j H_j^2 K_0' \left(|x_k - x_j| \right) \frac{x_k - x_j}{|x_k - x_j|} \frac{\int w^2}{2\pi} \tag{12}$$

Here, x_j is the location of j-th spike, $\mu_j = \mu\left(x_j\right)$ and $H_j \sim h(x_j)$.

As before, assume hexagonality and radial symmetry.

Continuum limit

Define $u(x_k) = \min_{j \neq k} |x_j - x_k|$. In the limit $N \to \infty$:

$$H(x) \sim \frac{\alpha}{(\log \varepsilon^{-1} + \phi_1(u(x)))} \frac{1}{\mu(x)};$$

$$u'(r) = \frac{\mu'(r)}{\mu(r)} \left[\frac{\left(\phi_3(u) + \left(\phi_1(u) + \log \varepsilon^{-1}\right)/2\right)\left(\log \varepsilon^{-1} + \phi_1(u)\right)}{\left(\left(\log \varepsilon^{-1} + \phi_1(u)\right)\phi_2(u) - 2\phi_1'(u)\,\phi_3(u)\right)} \right]$$

where

$$\phi_1(u) = \sum\sum K_0(u\,|l|)$$

$$\phi_2(u) = \frac{1}{2}\sum\sum \left[-|l|\,K_0'(u\,|l|) + ul\,\mathrm{Re}(l) K_0(u\,|l|)\right]$$

$$\phi_3(u) = u\sum\sum \mathrm{Re}(l)\,\frac{l}{|l|} K_0'(u\,|l|)\,,$$

$$\phi_1'(u) = \sum\sum |l|\,K_0'(u\,|l|)\,.$$

where double sum is over lattice points: $l = l_1 + e^{i\pi/3} l_2, \quad (l_1, l_2) \in \mathbb{Z}^2 \backslash \{0\}$; and,

$$N = \frac{2}{\sqrt{3}} \int_0^R \left(\frac{1}{u(r)}\right)^2 2\pi r\,dr; \qquad u(r) \to \infty \text{ as } r \to R^-. \tag{13}$$

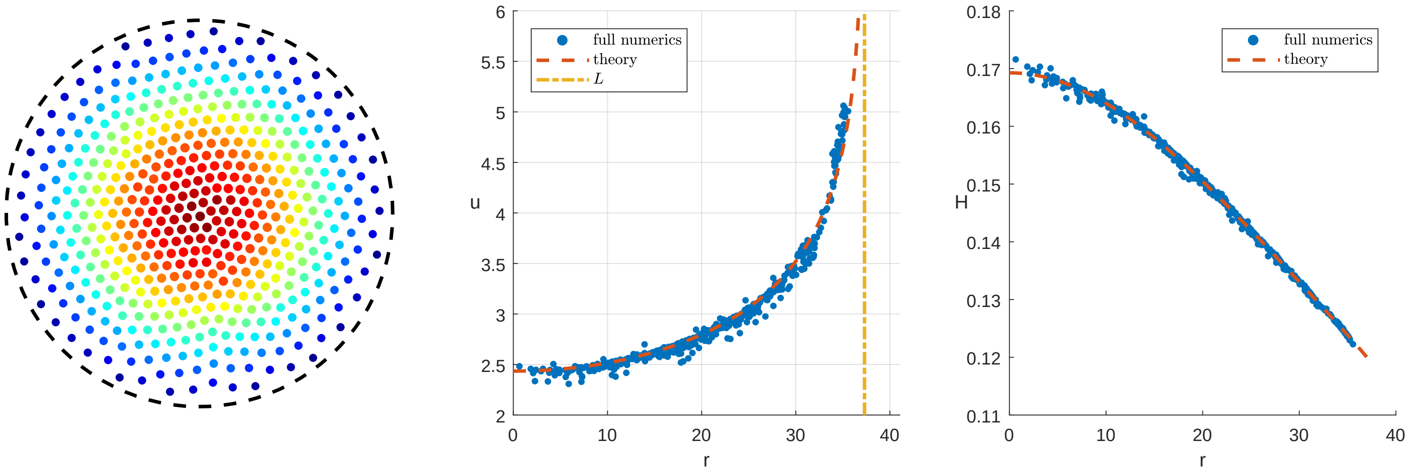
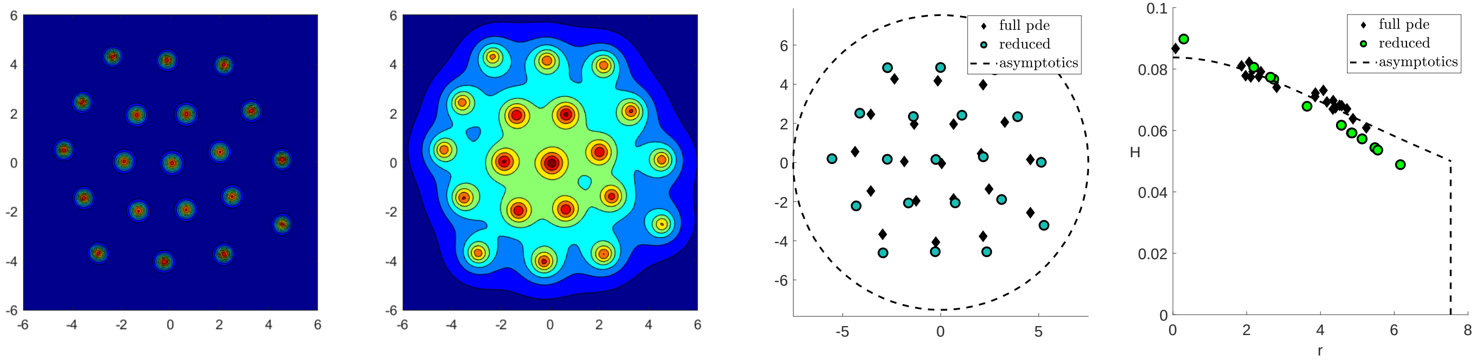


Figure 2: LEFT: Steady state for (34) with $N = 500$, $\mu(x) = 1 + 0.025x^2$ and $\varepsilon = 0.08$. Dots represent the steady state x_j; their size and colour are proportional to H_j. Dashed line represents the theoretical boundary of the steady state in the continuum limit $N \gg 1$. MIDDLE: scatter plot of the average distance $u(x_j)$ from a point to any of its neighbours, as a function of $|x_j|$. Solid curve is the analytical prediction of the continuum limit as given by (**??**). RIGHT: Scatter plot of the H_j as a function of $|x_j|$ and comparison to theory.



(a) (b) (c) (d)

Figure 3: Cluster steady-state solution to GM pde consisting of 20 spikes. Contour plot of a and h are shown in (a) and (b) respectively. Parameter values are $\varepsilon = 0.15$ and $\mu(x) = 1 + 0.02\,|x|^2$. Computational domain was taken to be $x \in (-15, 15)^2$; increasing the computational domain did not change spike locations. (c): Centers of spikes from the PDE simulation compared with centers generated by the reduced system. Dashed line denotes spike boundary computed asymptotically. (d): Spike height $h(x_j)$ versus $|x_j|$. Comparison between full numerical simulation, the reduced system (34) and theoretical prediction (**??**).

GM with precursor $\mu(x)$ in 1D

Equations:

$$a_t = \varepsilon^2 a_{xx} - \mu(x)\,a + a^2/h, \qquad 0 = Dh_{xx} - h + \frac{a^2}{\varepsilon} \tag{14}$$

Reduced dynamics: Assume that

$$D := \frac{d^2}{N^2}, \quad d = O(1), \quad N \gg 1 \text{ and } \varepsilon \ll 1/N.$$

Then

$$h(x_k,t) \sim v_k; \qquad a(x,t) \sim \sum_{j=1}^{N} v_j \mu(x_j)\,\frac{3}{2}\,\mathrm{sech}^2\left(\frac{x - x_j}{2\varepsilon\mu^{-1/2}(x_j)}\right),$$

$$\frac{d}{dt}x_k = -2\mu^{1/2}(x_k)\left(\frac{\langle v_x\rangle_k}{v_k} + \frac{5}{4}\frac{\mu'(x_k)}{\mu(x_k)}\right),$$

$$v_k = \sum_{j=1}^{N} S_j \frac{N}{2d} e^{-|x_k - x_j|\frac{N}{d}}, \quad \langle v_x\rangle_k = \sum_{j=1}^{N} S_j \frac{N^2}{2d^2} e^{-|x_k - x_j|\frac{N}{d}}\,\mathrm{sign}(x_j - x_k)$$

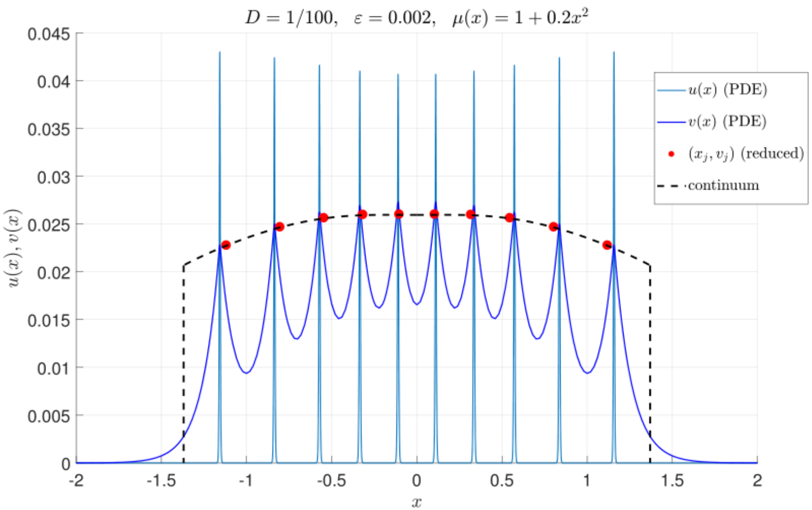
where $S_k = 6\mu^{3/2}(x_k)\,v_k^2$

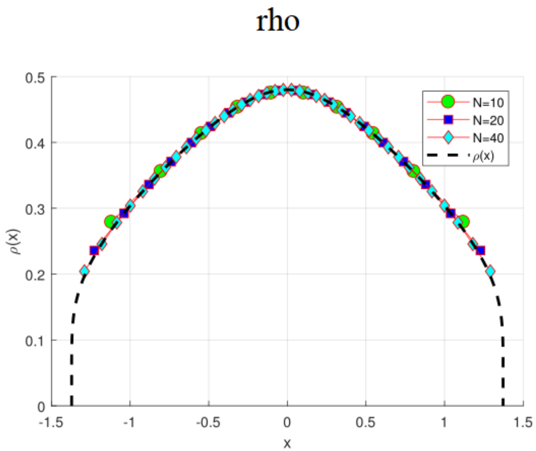
Mean-field limit

let $\rho(x_k) := \dfrac{d}{(x_{k+1} - x_k)\, N}$. then

$$\frac{d\rho}{dx} = \frac{\mu'(x)}{\mu(x)} \frac{3\rho^3 \sinh(1/\rho) - \frac{5}{2}\rho^2 \sinh^2(1/\rho)}{\cosh(1/\rho) - 3}; \quad \int_a^b \rho dx = d, \quad \rho(a) = \rho(b) = 0,$$

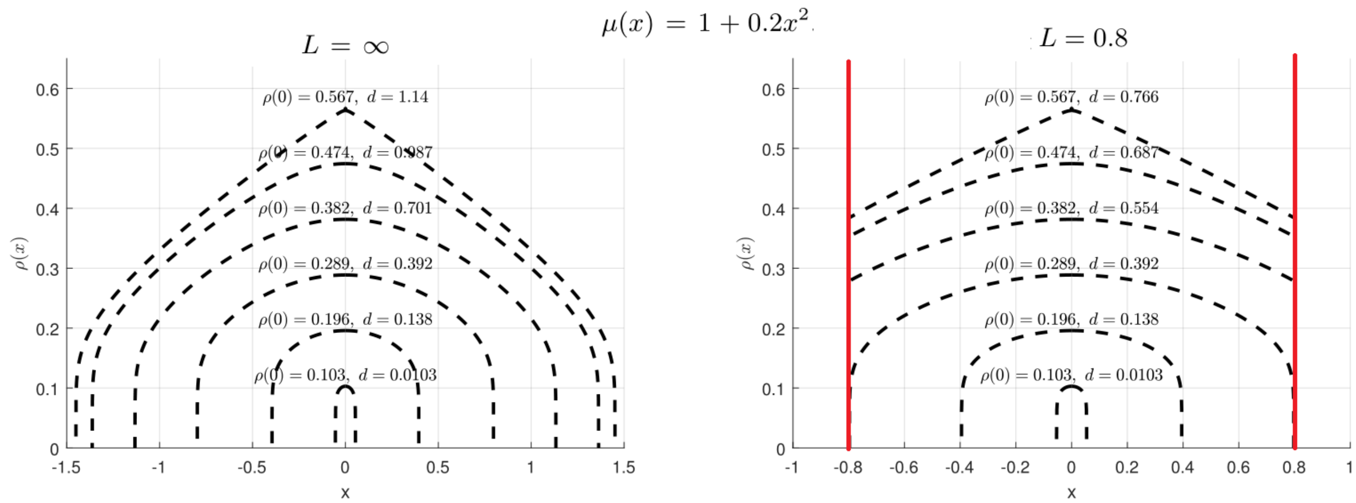
$$v_k \sim 12N \tanh\left(\frac{1}{2\rho(x_k)}\right) \mu^{-3/2}(x_k).$$





Existence of maximum density

$$\frac{d\rho}{dx} = \frac{\mu'(x)}{\mu(x)} \frac{3\rho^3 \sinh(1/\rho) - \frac{5}{2}\rho^2 \sinh^2(1/\rho)}{\boxed{\cosh(1/\rho) - 3}}; \qquad \int_a^b \rho dx = d, \quad \rho(a) = \rho(b) = 0$$



- Singularity when $\rho = \rho_{\max}$:

$$\rho_{\max} = \frac{1}{\operatorname{arccosh}(3)} \approx 0.5673$$

- **Main result:** Suppose that $\max_{x\in[a,b]} \rho(x) = \rho_{\max}$ and let $d_{\max} = \int_a^b \rho dx$. Then the spike cluster solution exists when $d < d_{\max}$ and disappears when $d > d_{\max}$.

- **Corollary 1**: for ***any*** choice of $\mu(x)$, we have:

$$\min |x_j - x_{j-1}| \geq \sqrt{D} \operatorname{arccos}(3). \tag{15}$$

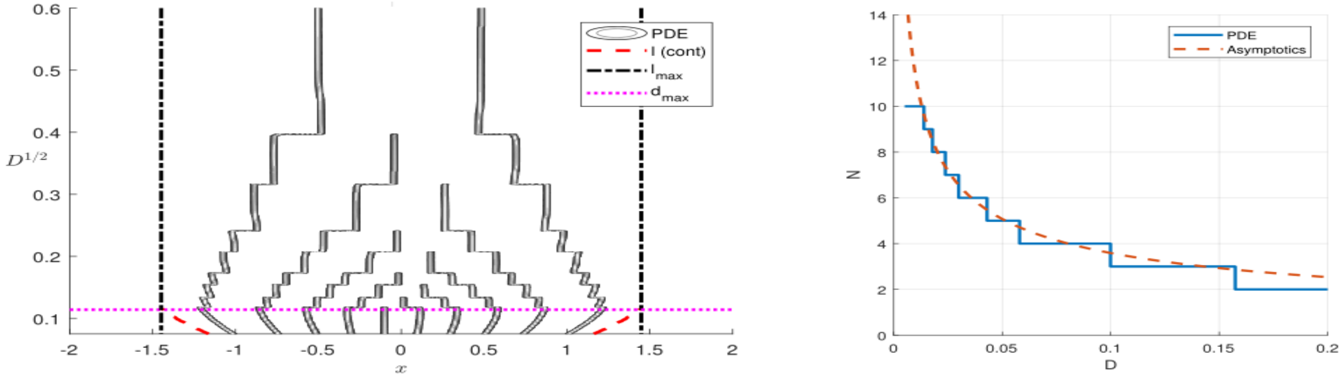
- **Corollary 2:** For ***constant*** $\mu(x)$, $|x_j - x_{j-1}| = 2L/N$ and (xxx) becomes

$$L/N \geq \sqrt{D}\frac{\operatorname{arccos}(3)}{2} = \log\left(1+\sqrt{2}\right)\sqrt{D}. \tag{16}$$

  This recovers (and generalizes) instability thresholds for N spikes derived by [Iron, Ward, Wei 2000].

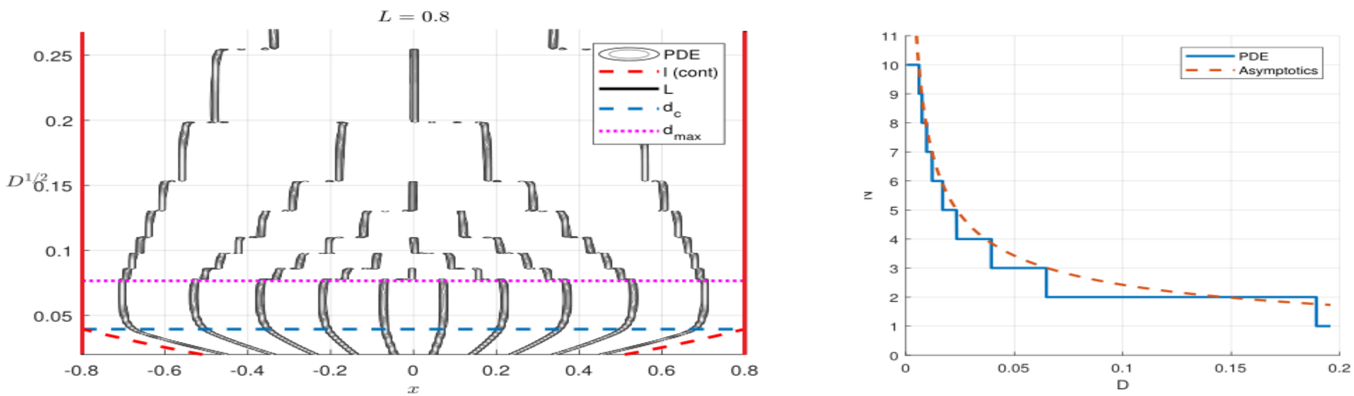
- **OPEN QUESTION: 2D instability thresholds...**

$L = \infty$



PDE
l (cont)
l_max
d_max
D^{1/2}
x
PDE
Asymptotics
N
D

$L = 0.8$



L = 0.8
PDE
l (cont)
L
d_c
d_max
D^{1/2}
x
PDE
Asymptotics
N
D

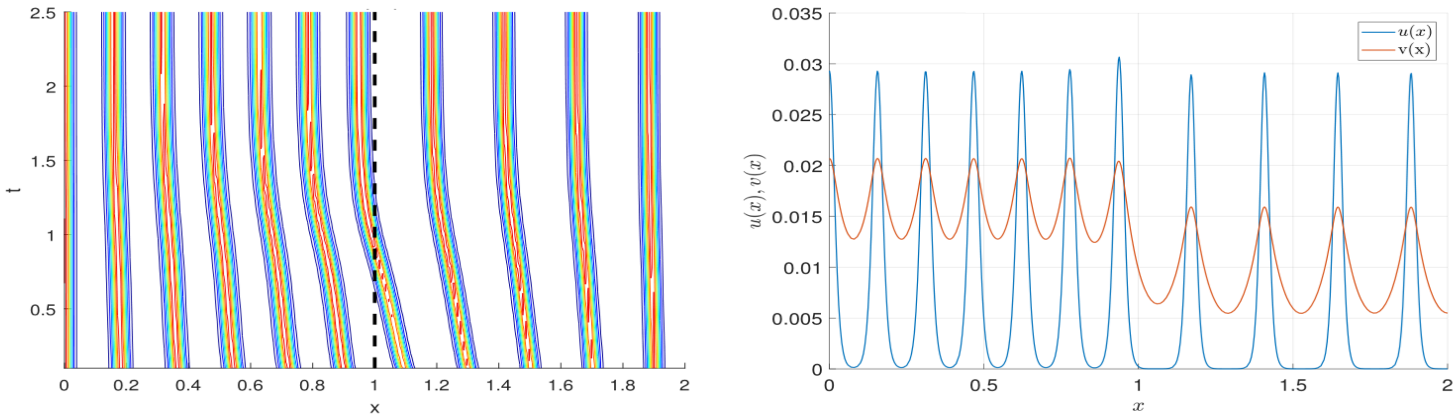
Piecewise constant precursor

$$\mu = \begin{cases} \mu_1, & 0 < x < l \\ \mu_2, & l < x < L \end{cases} \tag{17}$$

Then:

$$\rho(x) = \begin{cases} \rho_1, & 0 < x < l \\ \rho_2, & l < x < L \end{cases} \tag{18}$$

where $$\int_{\rho_2}^{\rho_1} \frac{\cosh(1/\rho) - 3}{\rho^2 \sinh(1/\rho)\left(3\rho - \frac{5}{2}\sinh(1/\rho)\right)} d\rho = \log\left(\frac{\mu_1}{\mu_2}\right). \tag{19}$$



$\mu_1 = 1, \mu_2 = 1.25, l = 1, L = 2$

Theory: 64% of spikes on the left, or 6.7 out of 10.5.
Numerics: 6.5 out of 10.5 on the left!

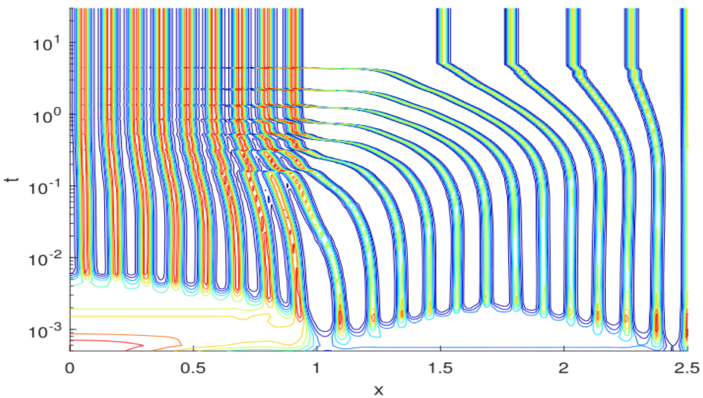
Cluster formation, piecewise constant

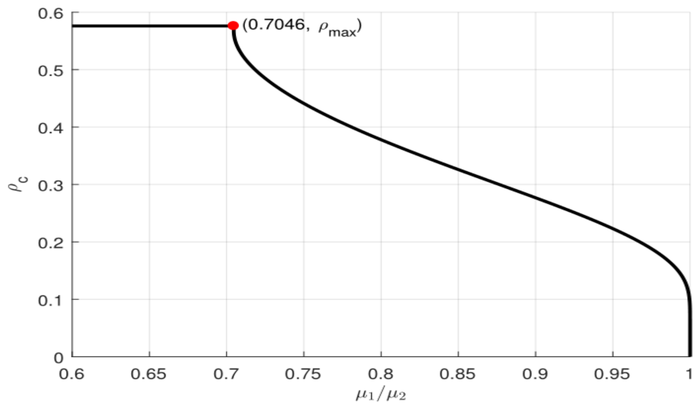
$$\int_{\rho_2}^{\rho_1} \frac{\cosh(1/\rho) - 3}{\rho^2 \sinh(1/\rho)\left(3\rho - \frac{5}{2}\sinh(1/\rho)\right)} d\rho = \log\left(\frac{\mu_1}{\mu_2}\right).$$

Since $\rho_1, \rho_2 \in [0, \rho_{\max}]$, we have:

$$\max(LHS) = \int_0^{\rho_{\max}} \frac{\cosh(1/\rho) - 3}{\rho^2 \sinh(1/\rho)\left(3\rho - \frac{5}{2}\sinh(1/\rho)\right)} d\rho = \log(0.7046)$$

Consequence: If $\mu_1/\mu_2 < 0.7046$ then $\rho_2 = 0$. Example:





$$\mu_1 = 1,\ \mu_2 = 2;$$

$$\mu_1/\mu_2 = 0.5 < 0.7046$$

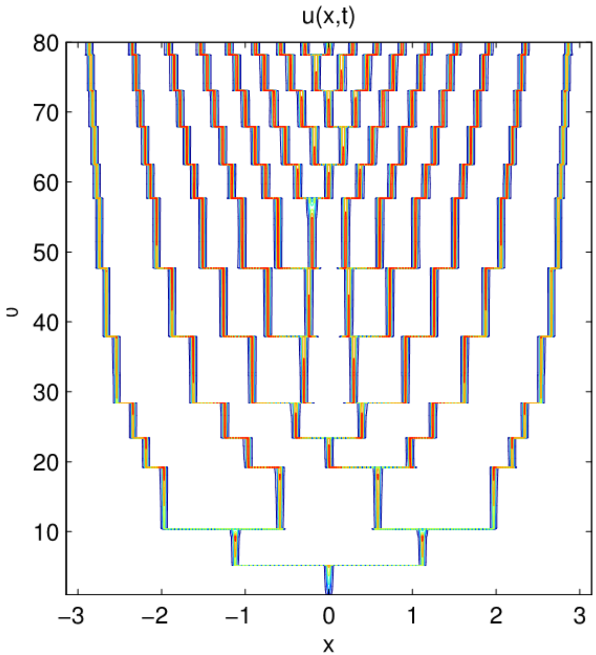
Schnakenberg (vegetation) model

$$\begin{cases} \varepsilon^2 u_t = \varepsilon^2 u_{xx} - u + u^2 v, \quad x \in (-L, L) \\ 0 = v_{xx} + a(x) - \dfrac{u^2 v}{\varepsilon}, \quad x \in (-L, L) \\ u_x = 0 = v_x \text{ at } x = \pm L \end{cases}$$

- This model is among the simplest prototypical reaction-diffusion models.
- Fast-diffusing water v is consumed by a slowly diffusing vegetation u, which decays with time.
- Water precipitation has ***space-dependent feed rate*** $a(x)$.
- This model is also a limiting case of the Klausmeyer model of vegetation (where u represents plant density, v represents water concentration in soil, $a(x)$ is the precipitation rate, and v_{xx} is replaced by $v_{xx} + cv_x - dv$) as well as the Gray-Scott model (where v_{xx} is replaced by $v_{xx} - dv$).
- ***GOAL:*** compute the effect of ***space-dependent*** $a(x)$ on spike distribution and stability thresholds

Numerical experiment 1: increasing $a(x)$

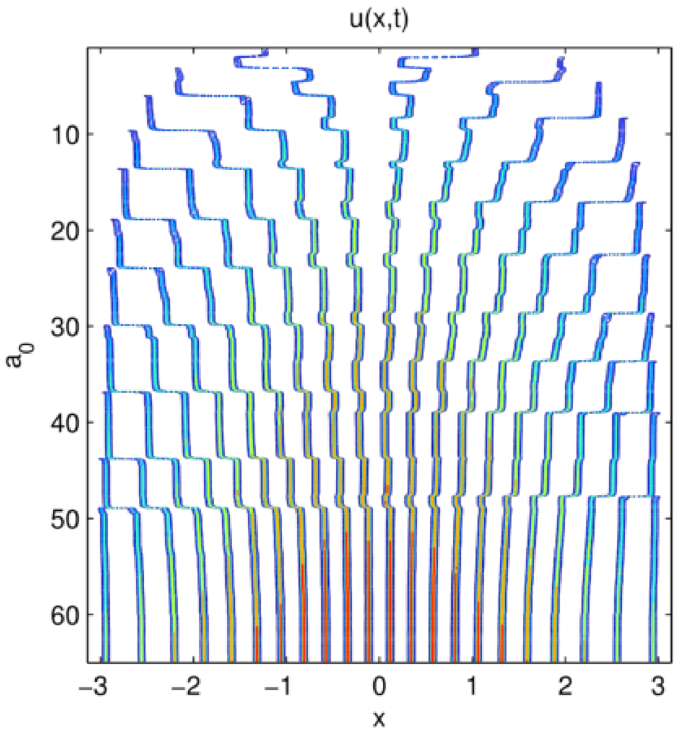
- $a(x) = a_0\,(1 + 0.5\cos(x))$, $L = \pi$.
- Start with $a_0 = 2$ and very gradually decrease a_0

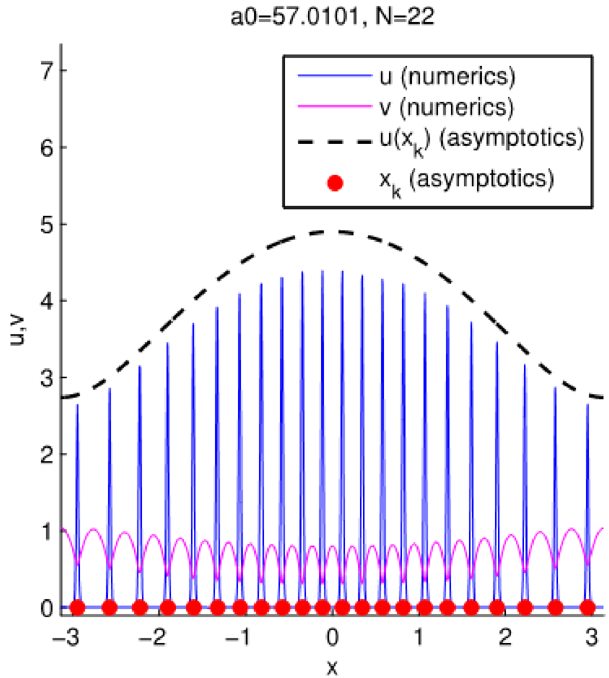


- Movie: increase

Numerical experiment 2: decreasing $a(x)$

- $a(x) = a_0\,(1 + 0.5\cos(x))$, $L = \pi$.
- Start with $a_0 = 80$ and very gradually decrease a_0





- Movie: decrease

Reduction to interacting particle system

Proposition. Consider the Schankenberg system with N fixed and with $\varepsilon \to 0$. Suppose that

$$a(x) = a_0 A(x)$$

Assume that $A(x)$ is even on interval $[-L, L]$. Define $P(x)$ and b by

$$P''(x) = A(x) \text{ with } P'(0) = 0; \quad b := 6N^3/a_0^2. \tag{20}$$

Assume $\varepsilon N \ll 1$. The dynamics of N spikes are asymptotically described by ODE system

$$\frac{dx_k}{dt}\frac{S_k}{18N} = \frac{1}{N}\sum_{\substack{j=1\ldots N \\ j\neq k}} \frac{S_j}{2}\frac{x_k - x_j}{|x_k - x_j|} - P'(x_k) \tag{21}$$

subject to $N+1$ albegraic constraints

$$\frac{b}{N^2}\frac{1}{S_k} = \frac{1}{N}\sum_{j=1}^{N} S_j \frac{|x_k - x_j|}{2} - P(x_k) + c, \quad k = 1\ldots N; \tag{22}$$

$$\frac{1}{N}\sum_{j=1}^{N} S_j = \int_{-L}^{L} A(x)dx. \tag{23}$$

Near x_k, the quasi-steady state is approximated by

$$u \sim \operatorname{sech}^2\left(\frac{x - x_k}{2\varepsilon}\right)\frac{S_k}{4N}, \quad v(x_k) \sim \frac{6N}{S_k}. \tag{24}$$

Steady state

$$0 = \frac{1}{N} \sum_{j \neq k} \frac{S_j}{2} \frac{x_k - x_j}{|x_k - x_j|} - P'(x_k)$$

$$\frac{b}{N^2} \frac{1}{S_k} = \frac{1}{N} \sum_{j=1}^{N} S_j \frac{|x_k - x_j|}{2} - P(x_k) + c$$

$$\frac{1}{N} \sum_{j=1}^{N} S_j = 2P'(L).$$

Continuum limit

- Spike locations x_j define ***density distribution*** $\rho(x)$.
  - Formally, take

$$\rho(x) = \frac{1}{N} \sum \delta(x - x_j)$$

  - More precisely, define $\rho(x)$ using

$$x_j := x(j) \text{ where } x(j) : [1, N] \to [-L, L];$$
$$\frac{dx}{dj} = \frac{1}{N\rho(x)}$$

- Spike "heights" define ***height distribution***: $S_j = S(x_j)$

- Leading order approximations:

$$\begin{cases} \dfrac{b}{N^2} \dfrac{1}{S_k} = \dfrac{1}{N} \displaystyle\sum_{j=1}^{N} S_j \dfrac{|x_k - x_j|}{2} - P(x_k) \\ 0 = \dfrac{1}{N} \displaystyle\sum_{j \neq k} \dfrac{S_j}{2} \dfrac{x_k - x_j}{|x_k - x_j|} - P'(x_k) \end{cases} \to \begin{cases} \displaystyle\int |x - y| \dfrac{S(y)}{2} \rho(y) dy \approx P(x) \\ \displaystyle\int \dfrac{x - y}{|x - y|} \dfrac{S(y)}{2} \rho(y) dy \approx P'(x) \end{cases}$$

- Problem the second equation is just the derivative of the first!

$$\frac{d}{dx}\left(\int |x-y|\,\frac{S(y)}{2}\rho(y)dy\right) = \int \frac{x-y}{|x-y|}\frac{S(y)}{2}\rho(y)dy$$

- However, note that $\frac{d^2}{dx^2}\left(\frac{|x-y|}{2}\right) = \delta(x-y)$ so that

$$\frac{d^2}{dx^2}\left(\int |x-y|\,\frac{S(y)}{2}\rho(y)dy \sim P(x)\right)$$
$$\int \delta(x-y)S(y)\rho(y)dy \sim P''(x) = A(x)$$
$$S(x)\rho(x) \sim A(x)$$

- Need to ***estimate the difference between continuum and discrete!***

Key ingredient:

- The ***Euler-Maclaurin formula***

$$\sum_{j=1}^{N} f(j) = \int_{1}^{N} f(j)dj + \frac{1}{2}\left(f(1) + f(N)\right) + \frac{1}{12}\left(f'(N) - f'(1)\right) + O(f''')$$

- to get next-order terms:

$$\frac{1}{N}\sum_{j\neq k} S_j \frac{1}{2}\frac{x_k - x_j}{|x_k - x_j|} = \int_{-L}^{L} S\left(y\right)\rho(y)\frac{1}{2}\frac{x_k - y}{|x_k - y|}dy + \frac{1}{N^2}\left(\frac{1}{12}\frac{S'(x_k)}{\rho\left(x_k\right)}\right) + O(N^{-4}).$$

$$\frac{1}{N}\sum_{j\neq k} S_j \frac{|x_k - x_j|}{2} = \int_{-L}^{L} S\left(y\right)\rho(y)\frac{|x_k - y|}{2}dy + \frac{1}{N^2}\left(-\frac{1}{12}\frac{S(x_k)}{\rho\left(x_k\right)} + C_0\right) + O(N^{-4}).$$

Expand $S(x) = S_0(x) + \frac{1}{N^2}S_1(x) + \ldots$. End result is

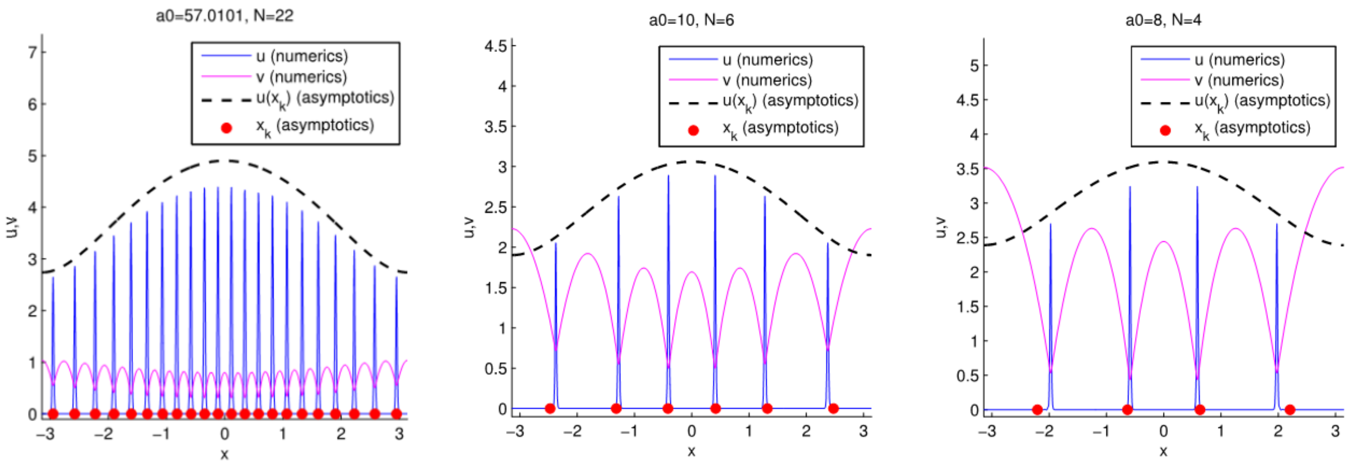
$$\rho' = \frac{2S_0'}{S_0}\rho - 12b\frac{S_0'}{S_0^3}\rho^2, \text{ subject to } S_0\rho = A, \int_{-L}^{L}\rho(y)dy = 1 \qquad (25)$$

- General solution is

$$\frac{A^2}{\rho^3} + 12b \log\left(\rho/A\right) = C \text{ subject to } \int_{-L}^{L} \rho(x)dx = 1, \quad S = A/\rho. \tag{26}$$

- This describes the steady state!

- Example $a(x) = a_0 \left(1 + 0.5 \cos x\right)$



Large feed rate: self-replication

- If $a_0 \gg 1$ then $A^2/\rho^3 \sim C$, $S\rho = A$, so that

$$\rho \sim c_0 A^{2/3}(x), \quad S \sim c_0^{-1} A^{1/3}(x), \quad c_0 = \int_{-L}^{L} A^{2/3}(x)dx.$$

- ***Self-replication*** is initiated when S_j becomes “too large”.

Main result. Suppose that $a(x) = a_0 A(x)$ and define

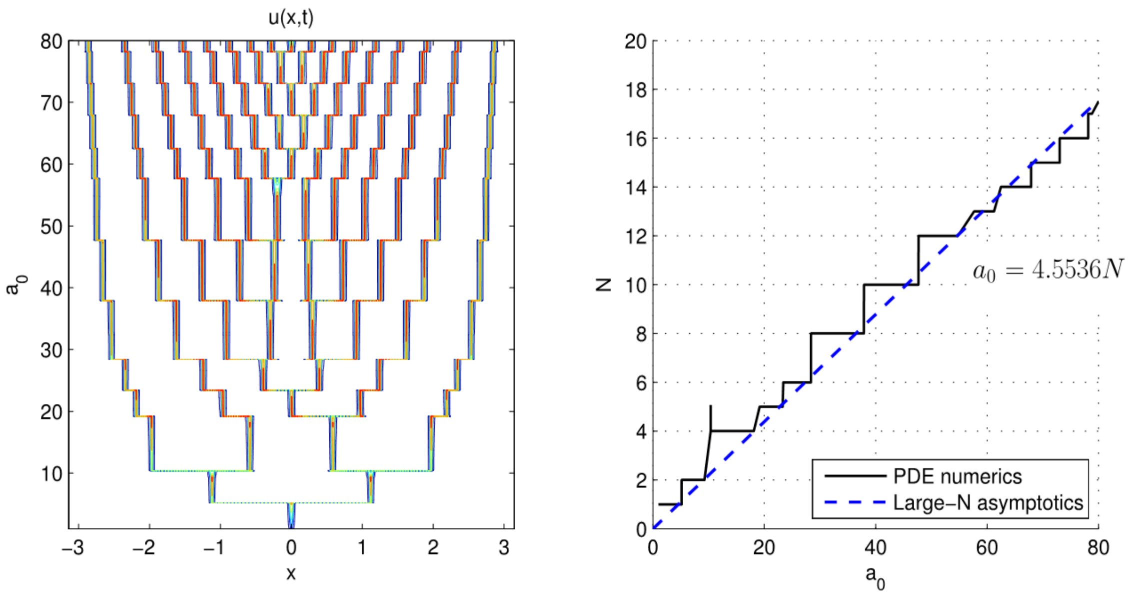
$$\beta := \frac{2.70}{\max A^{1/3}(x_j) \left(\int_{-L}^{L} A^{2/3}(x)dx \right)}.$$

Then N spikes undergo self-replication if a_0 is increased past

$$a_{0c} := \beta N \varepsilon^{-1/2}.$$

Example

$A = 1 + 0.5\cos x$, $\varepsilon = 0.07$, then $\beta = 0.3809$, $a_{0c} = 4.5536N$. (when $A = 1$, $\beta = 0.430$)



Small feed rate: coarsening

Solution does not exist if a_0 is too small.

Main stability result. Suppose $a(x) = a_0 A(x)$. Let α_c be the solution to the following problem:

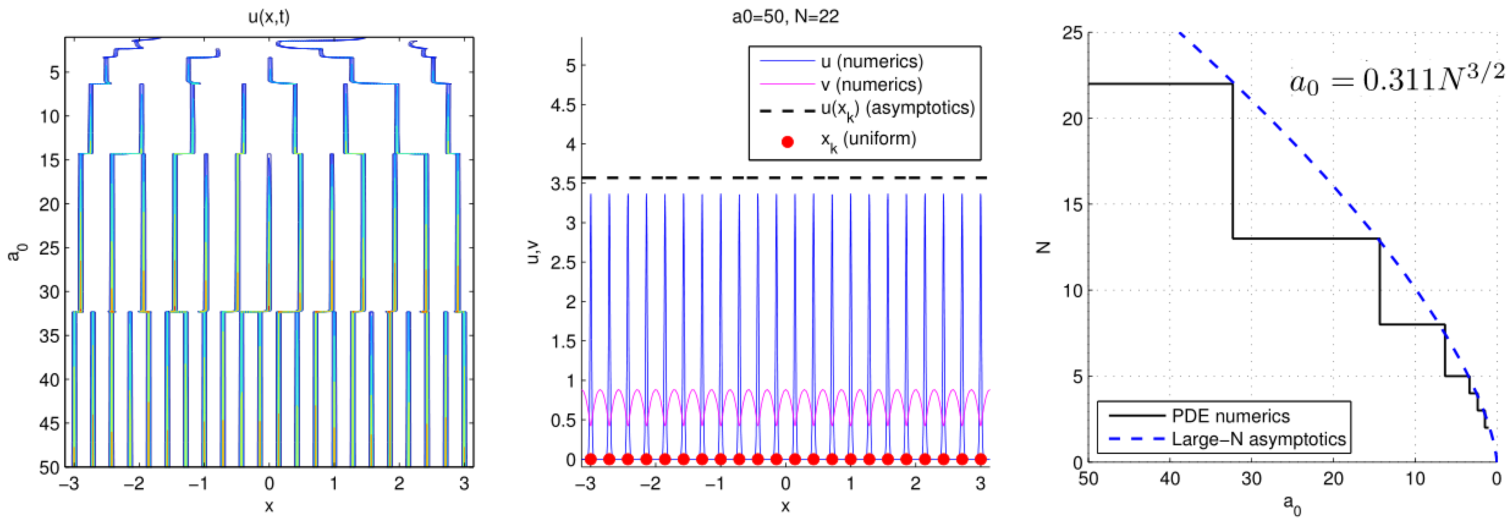
$$\frac{A^2(x)}{\rho^3(x)} + \frac{72}{\alpha_c} \log\left(\frac{\rho(x)}{A(x)}\right) = \frac{24}{\alpha_c}\left(1 - \log\left(\frac{24}{\alpha_c} A_{\min}\right)\right), \quad \int_{-L}^{L} \rho(x) = 1. \tag{27}$$

where $A_{\min} = \min_{x\in[-L,L]} A(x)$. Then N spikes are stable if $a_0 < \alpha N^{3/2}$ and are unstable if $a_0 > \alpha_c N^{3/2}$.

If $A(x) = 1$ then $\alpha_c = \sqrt{3} L^{-3/2}$.

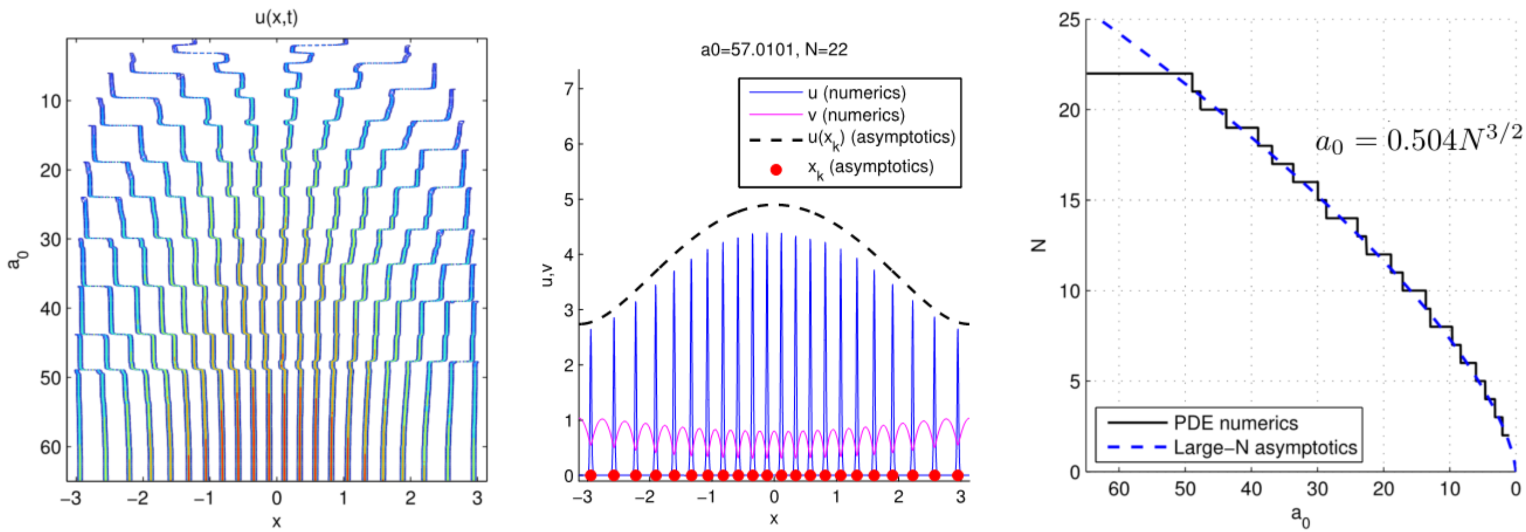
Example

$a(x) = a_0$ with $L = \pi$. Then $\alpha_c = 0.3111$. Start with $a_0 = 70$ and $N = 22$ and very gradually decrease a_0



Example

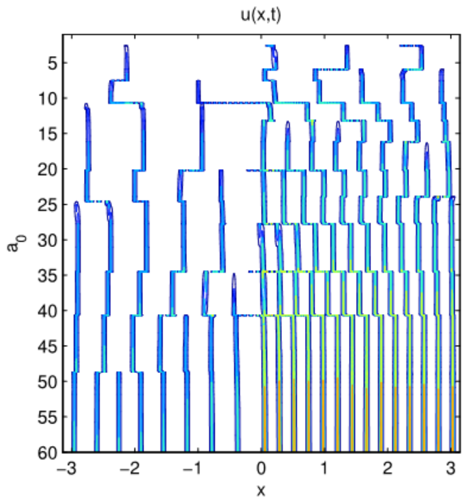
$a(x) = a_0\,(1 + 0.5\cos(x))$ with $L = \pi$. Then $\alpha_c = 0.504$. Start with $a_0 = 70$ and $N = 22$ and very gradually decrease a_0

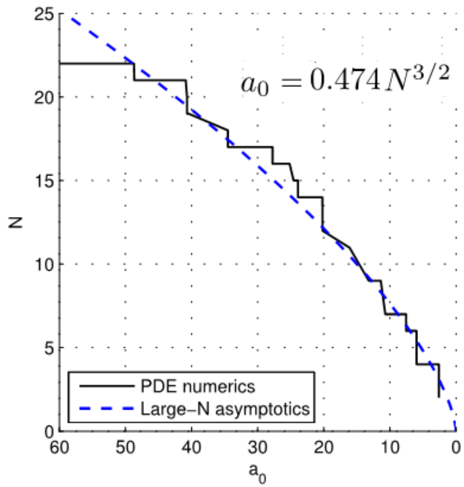


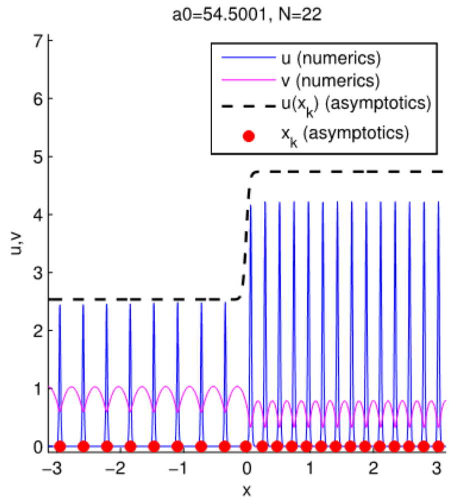
Example

$$a(x) = a_0 \begin{cases} 0.5, & x < 0 \\ 1.5, & x > 0 \end{cases}$$

with $L = \pi$. Then $\alpha_c = 0.474$. Start with $a_0 = 70$ and $N = 22$ and very gradually decrease a_0:







Grand conclusion

Suppose that $a(x) = a_0 A(x)$. Suppose that

$$N\varepsilon \ll 1.$$

Then N spikes are stable provided that

$$N_{\min} < N < N_{\max}$$

where

$$N_{\min} \equiv a_0 \frac{\varepsilon^{1/2}}{\beta}; \quad N_{\max} \equiv \left(\frac{a_0}{\alpha_c}\right)^{2/3}$$

Alternatively, N spikes are stable when

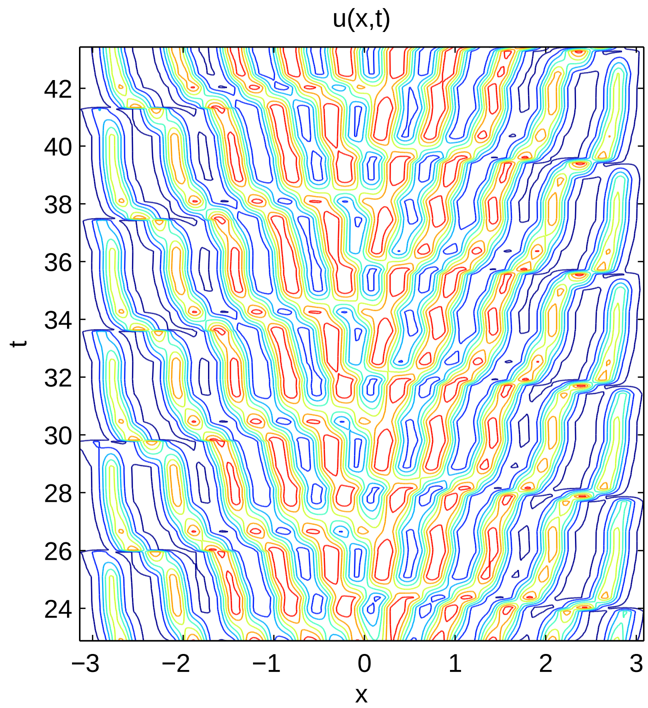
$$a_{0,\text{coarse}} < a_0 < a_{0,\text{split}}$$

where

$$a_{0,\text{coarse}} = \alpha_c N^{3/2}; \qquad a_{0,\text{split}} = \beta N \varepsilon^{-1/2}.$$

When $A = 1$ then $\beta = 1.35/L,\ \alpha_c = \sqrt{3} L^{-3/2}$.

Creation-destruction loop



- $a(x) = 20\,(1 + 0.5\cos x)\,,\ \varepsilon = 0.05,\ \ x \in [-\pi, \pi]$
- Self-replication near the center; coarsening near the boundaries
- Creation-destruction feedback loop
- Movie: chaos

Vortex lattices in Bose Einstein Condensates

Observation of Vortex Lattices in Bose-Einstein Condensates

20 APRIL 2001 VOL 292 SCIENCE

J. R. Abo-Shaeer, C. Raman, J. M. Vogels, W. Ketterle

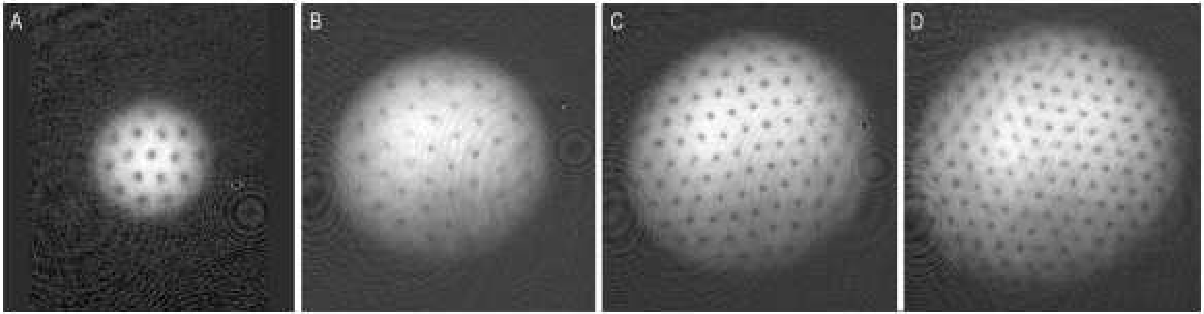


Fig. 1. Observation of vortex lattices. The examples shown contain approximately (**A**) 16, (**B**) 32, (**C**) 80, and (**D**) 130 vortices. The vortices have "crystallized" in a triangular pattern. The diameter of the cloud in (D) was 1 mm after ballistic expansion, which represents a magnification of 20. Slight asymmetries in the density distribution were due to absorption of the optical pumping light.

- Model: Gross-Pitaevskii Equation with rotation, anisotropic trap ***and small damping***

$$(\gamma - \kappa i) w_t = \Delta w + \frac{1}{\varepsilon^2}\left(V(x) - |w|^2\right) w + i\Omega\left(x_2 w_{x_1} - x_1 w_{x_2}\right) \qquad (28)$$

$$V(x) = 1 - x_1^2 - b^2 x_2^2 \qquad (29)$$

- Describes the quasi-2D condensate wavefunction $w(x, y, t)$ in the presence of rotation ($i\Omega$); inhomogeneous anisotropic trap $(b \neq 1)$

- Well-established BEC model [Pitaevskii&Stringari, 2003; Pethick&Smith2002; Kevrekidis,Frantzeskakis&Carretero, 2008]

- Generally speaking, vortices appear as Ω is increased.

- ***Small damping*** $\gamma \approx O(10^{-3})$ is used to to account for the role of finite temperature induced fluctuations in the BEC dynamics [Pitaevskii, 1958].
  - Without dissipation ($\gamma = 0$), all stable eigenvalues are purely imaginary (neutral modes). Adding small amout of dissipation “kicks” eigenvalues off the imaginary axis and leads to vortex crystals.

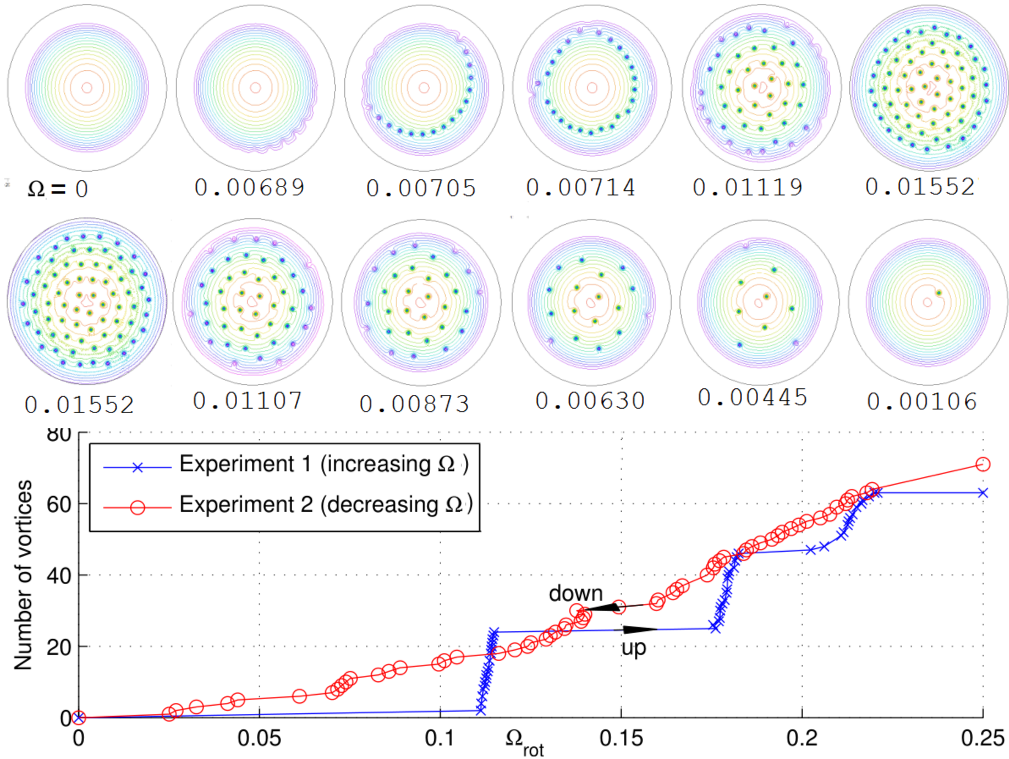
- More recently, thermal (non-zero) temperature effects were shown to play an important role in vortex dynamics and [e.g. Jackson,et.al, 2009; Allen et.al. 2013; Middlekamp et.al, 2010 and others]

Motivating example

$$(\gamma - \kappa i) w_t = \Delta w + \frac{1}{\varepsilon^2}\left(V(x) - |w|^2\right) w + i\Omega\left(x_2 w_{x_1} - x_1 w_{x_2}\right) \tag{30}$$

$$V(x) = 1 - x_1^2 - b^2 x_2^2 \tag{31}$$

- $\varepsilon = 0.0109$; $\gamma \gg 1, b = 1$. Start with zero rotation $\Omega = 0$ and ***gradually increase*** Ω.
- Then ***gradually decrease*** Ω back to zero. Movies: up,down



- Question: ***Can we predict*** how many vortices form as a function of dynamics?

GPE Vortex dynamics [Xie+Kevrekidis+K, submitted]

Overdamped limit $(\gamma \to \infty)$:

$$w_t = \Delta w + \frac{1}{\varepsilon^2}\left(V(x) - |w|^2\right) w + i\Omega\left(x_2 w_{x_1} - x_1 w_{x_2}\right) \tag{32}$$

$$V(x) = 1 - x_1^2 - b^2 x_2^2 \tag{33}$$

- Vortex dynamics are approximated by ODE's for their centers
- We follow ***direct method*** of [Weinan E, PhysD1994] to obtain

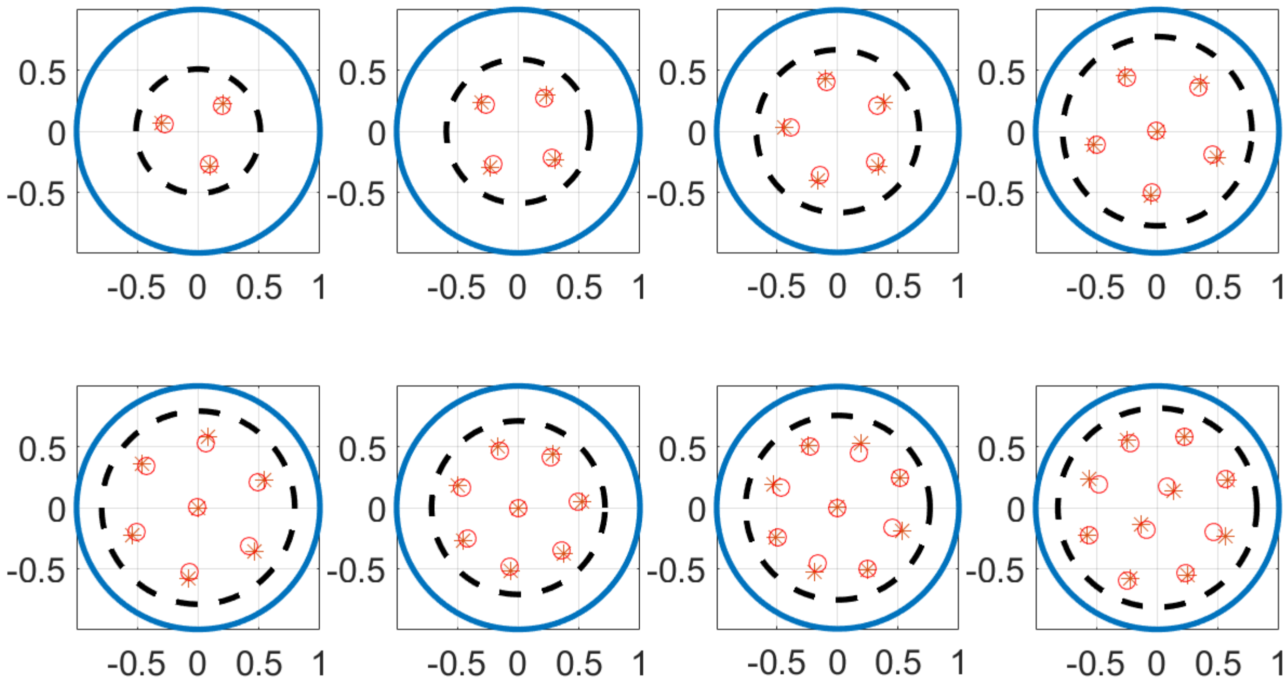
$$\xi_{jt} = \left(-\frac{2\Omega\nu}{1+b^2} + \frac{2}{V(\xi_j)}\right)\begin{pmatrix} 1 & 0 \\ 0 & b^2 \end{pmatrix}\xi_j + 2\nu \sum_{k\neq j} \frac{(\xi_j - \xi_k)}{|\xi_j - \xi_k|^2}\frac{V(\xi_j)}{V(\xi_k)}. \tag{34}$$

where

$$\nu = 1/\log\left(1/\varepsilon\right). \tag{35}$$

- The term $\frac{V(\xi_j)}{V(\xi_k)}$ is ***novel***. Previous works [e.g. Colliander,Jerrard, IMRN1998; Yan-Carretero-Frantzeskakis-Kevrekidis-Proukakis,PRA2014] used "classical" vortex-to-vortex interaction is $\sum_{k\neq j}\frac{(\xi_j-\xi_k)}{|\xi_j-\xi_k|^2}$, corresponding to homogeneous trap $(V = const.)$
- $\frac{V(\xi_j)}{V(\xi_k)}$ is especially felt away from trap center (e.g. when N is large).

Direct comparison: full PDE vs. ODE, isotropic case



Isotropic trap ($V(x) = 1 - |x|^2$) large N limit

ODE becomes

$$\xi_{j\tau} = \left(-\nu\Omega + \frac{2}{1-|\xi_j|^2}\right)\xi_j + 2\nu \sum_{k\neq j} \frac{\xi_k - \xi_j}{|\xi_k - \xi_j|^2} \frac{1-|\xi_j|^2}{1-|\xi_k|^2}. \tag{36}$$

- Coarse-grain by defining the particle density to be

$$\rho(x) = \sum \delta(x - \xi_k). \tag{37}$$

- Continuum limit $N \to \infty$ becomes

$$\rho_\tau(x,\tau) + \nabla_x \cdot (v(x)\rho(x,\tau)) = 0, \tag{38}$$

$$v(x) = \left(-\nu\Omega + \frac{2}{1-|x|^2}\right)x + 2\nu(1-|x|^2)\int_{R^2} \frac{x-y}{|x-y|^2}\frac{1}{1-|y|^2}\rho(y)dy, \tag{39}$$

$$\int \rho = N. \tag{40}$$

- Assume that the density is ***radial*** and has support a :

- Using key identity $\int_{R^2} \frac{x-y}{|x-y|^2} g(|y|)dy = x\frac{2\pi}{r^2}\int_0^r g(s)sds$,yields

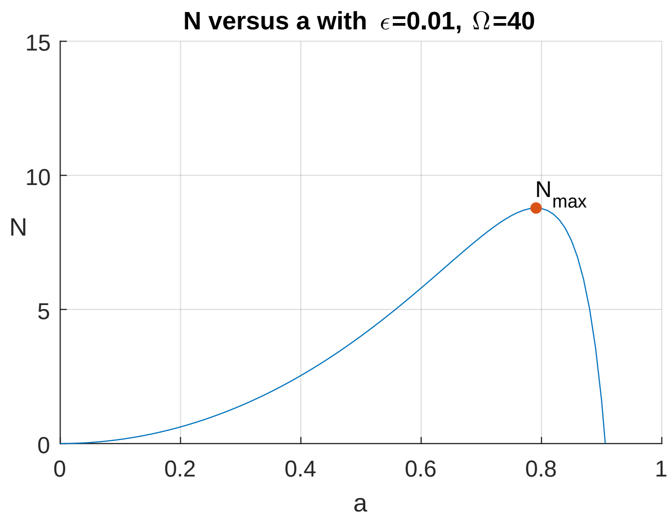
$$v(x) = \left(-\nu\Omega + \frac{2}{1-r^2} + \frac{4\pi\nu(1-r^2)}{r^2}\int_0^r \frac{1}{1-s^2}\rho(s)sds\right)x. \tag{41}$$

- Inside the support $r < a$, we set $v = 0$. Upon differentiating with respect to r we obtain

$$\rho(r) = \frac{1}{4\pi\nu}\left(-\frac{2\Omega\nu r}{(1-r^2)} - \frac{4}{1-r^2} + \frac{8}{(1-r^2)^2}\right), \quad r < a \tag{42}$$

- Radius a is determined using the constraint $\int_0^a \rho(s)sds = \frac{N}{2\pi}$, which yields

$$N = \frac{1}{\nu}\left(\left(-1 - \frac{1}{2}\Omega\nu\right)\ln(1-a^2) + 2 - 2(1-a^2)^{-1}\right) \tag{43}$$



- The curve $a \to N(a)$ attains the maximum $a = \frac{\sqrt{\Omega\nu - 2}}{\sqrt{\Omega\nu + 2}}$ with

$$\boxed{N_{\max} = \frac{1}{\nu}\left\{(\Omega\nu + 2)\left(\frac{1}{2}\ln(\Omega\nu + 2) - \ln(2) - \frac{1}{2}\right) + 2\right\}.} \qquad (44)$$

This is the key formula for explicit upper bound on the number of vortices as a function of rotation rate Ω!

Direct comparison: particle system vs. density

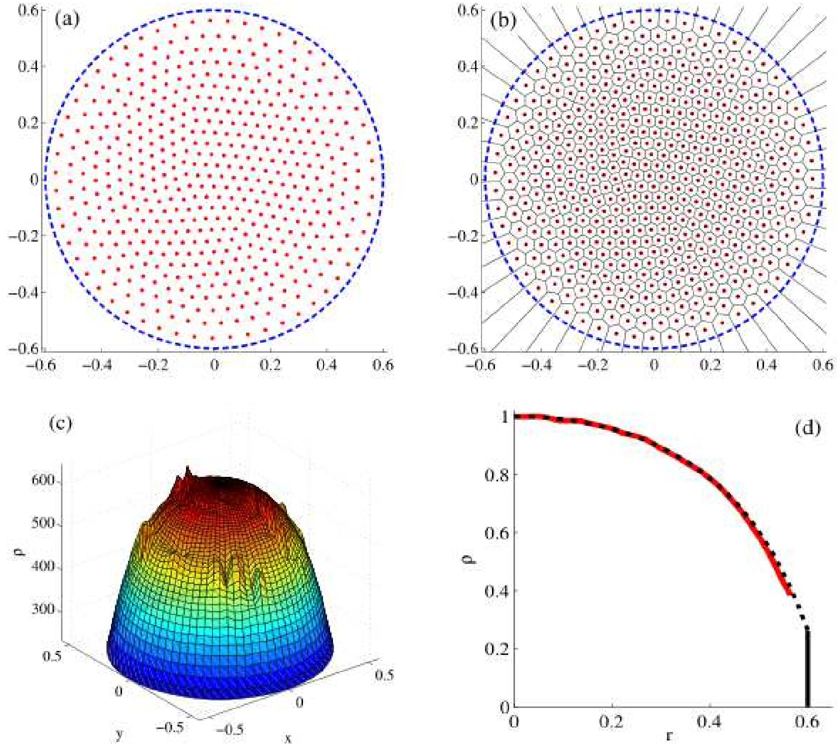


Figure 1. (a) Stable equilibrium of Eq. (2.4) with $f(r)$ as in Eq. (2.2). Parameter values are $N = 500, \omega = 2.95139, a = 1$ and $c = 0.001$. The dashed circle is the asymptotic boundary whose radius $R = 0.6$ is the smaller solution to Eq. (4.9). (b) Voronoi diagram used to compute the two-dimensional density distribution. (c) The corresponding density distribution ρ obtained by setting $\rho(x_j) = 1/\text{area}_j$ and extrapolating, where area_j is the area of the Voronoi cell that contains x_j. (d) Average of $\rho(|x|)/\rho(0)$ as a function of $r = |x|$. Solid curve corresponds to the numerical computation. The dashed curve is the formula (4.10). The vertical line is the boundary $r = R$.

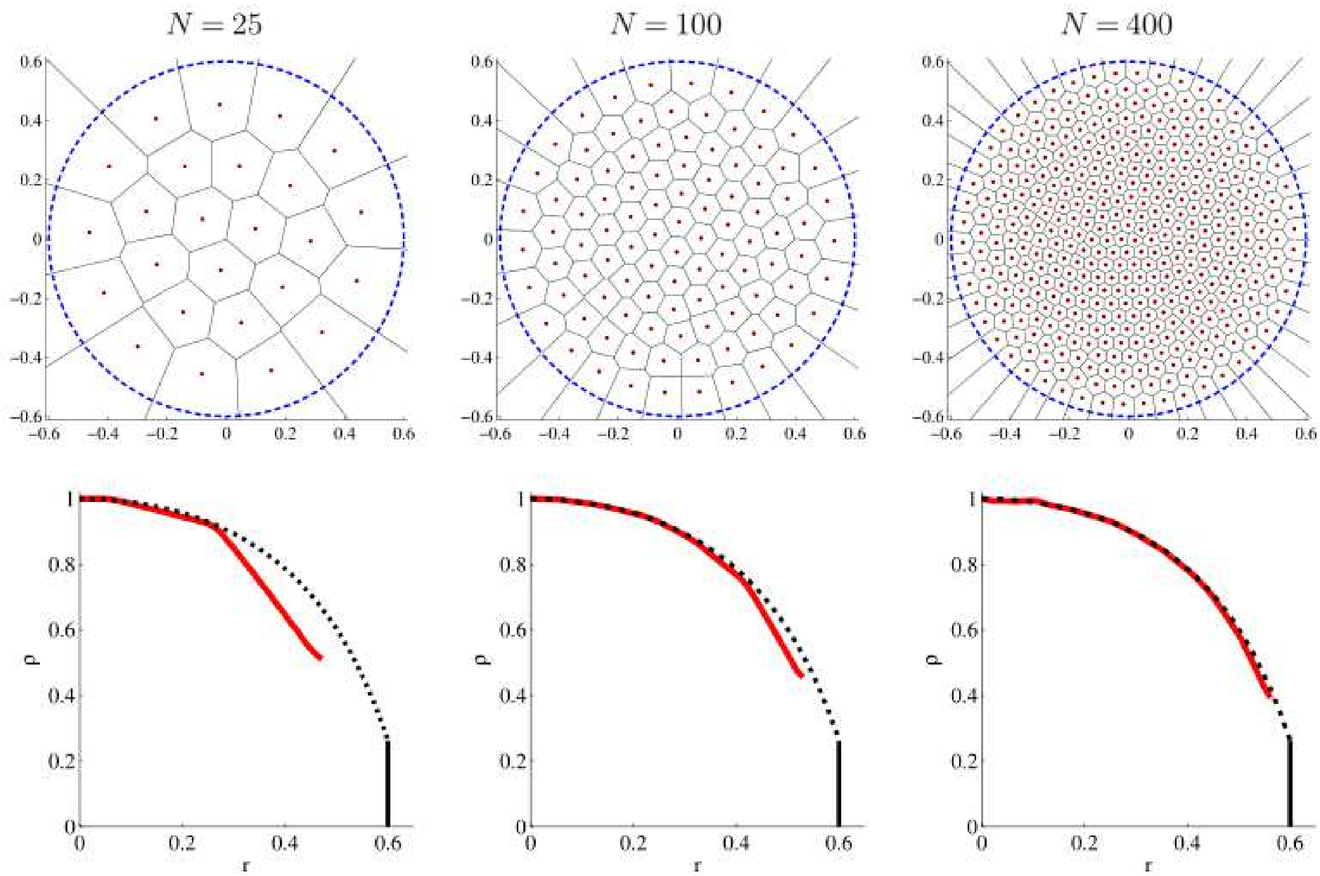
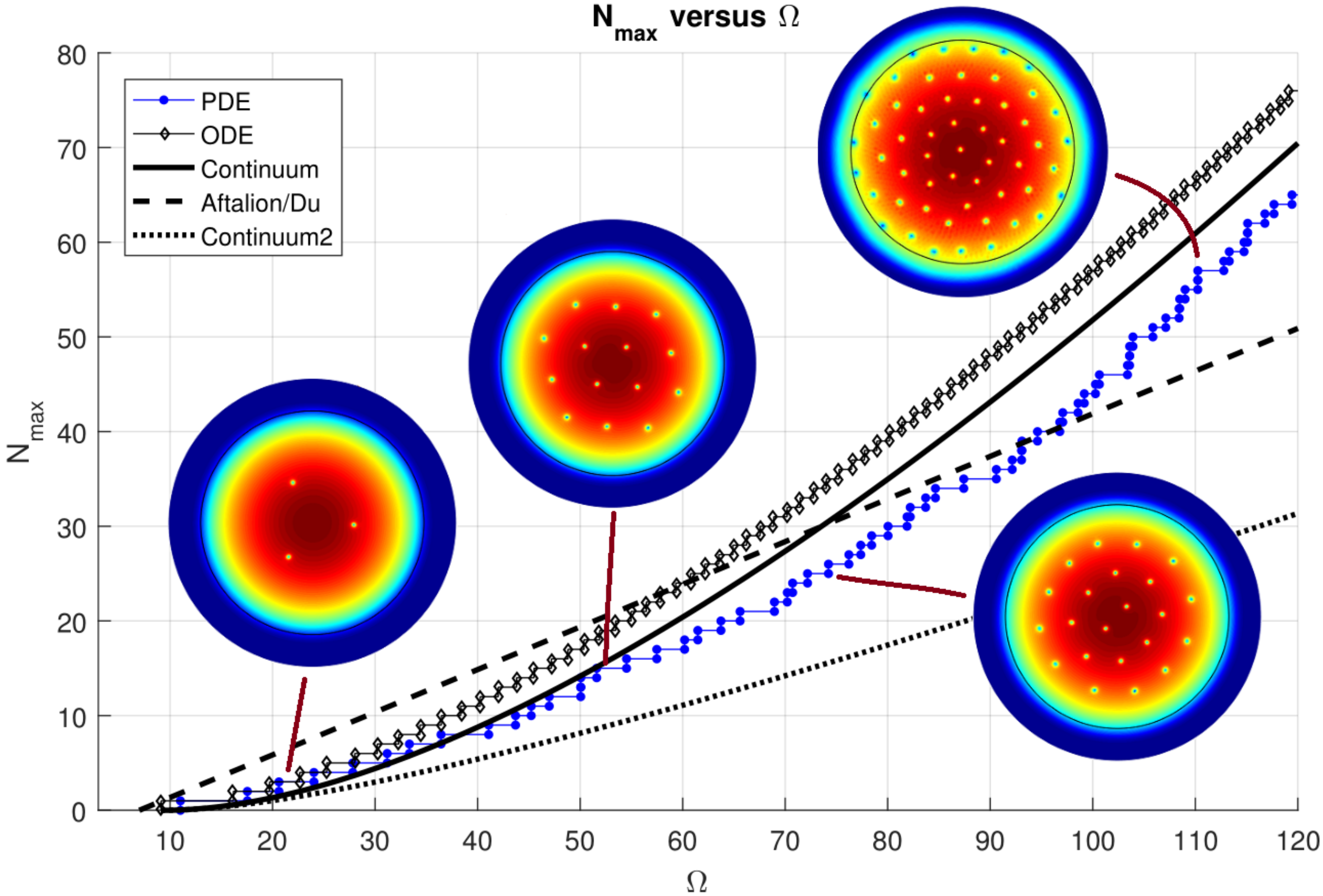


Figure 2. Top row: stable equilibrium of Eq. (2.4) with $f(r)$ as in Eq. (2.2), with N as shown in the title and with $c = 0.5/N$, $\omega = 2.95139$, $a = 1$. The dashed circle is the asymptotic boundary whose radius $R = 0.6$ is the smaller solution to Eq. (4.9). Bottom row: average of $\rho\,(|x|)/\rho(0)$ as a function of $r = |x|$. Solid curve corresponds to the numerical computation. Dashed curve is the formula (4.10). Vertical line is the boundary $r = R$.

Direct comparison: $N_{\max}$



Minimum N, isotropic case

- Vortices emerge near the ***trap boundary*** as the rotation rate Ω is increased

- [Anglin, PRL2001; Carretero-Kevrekidis-K,PhysD2015]: In the case of an isotropic trap, a zero-vortex state becomes unstable as Ω increases past $\underline{\Omega} = 2.561\varepsilon^{-2/3}$

- Approximate N vortices by a single vortex of degree N at the origin. Then similar computation yields $\underline{\Omega} = 2.53\varepsilon^{-2/3} + 2N$.

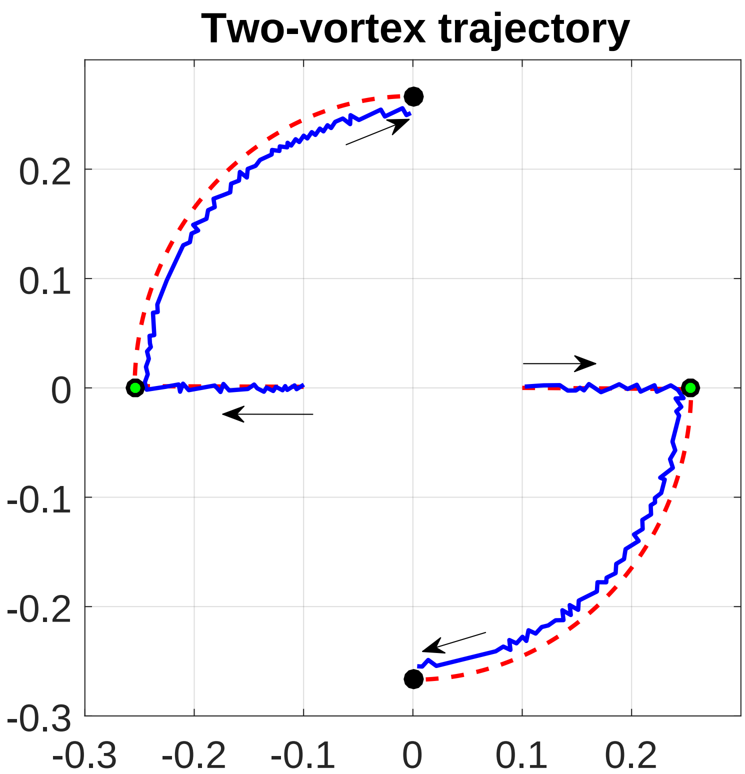
- Solving for N, this in turn yields the formula

$$N_{\min} = \frac{\Omega}{2} - 1.28\varepsilon^{-2/3}.$$

with $N_{\min} < N < N_{\max}$.

Anisotropy ($b \neq 1$) with two vortices

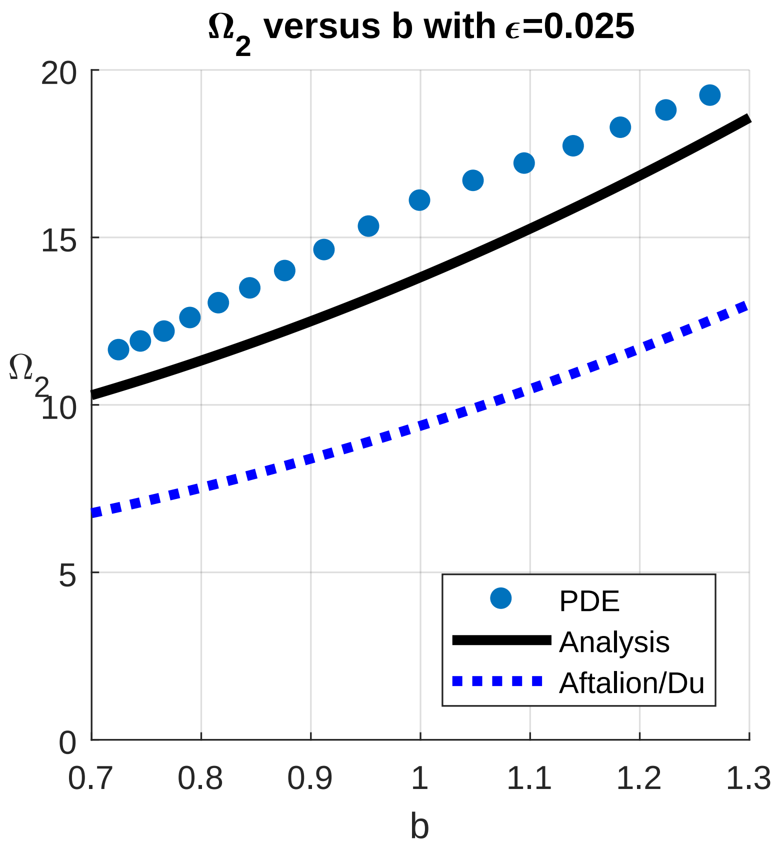
- Two vortices will align along the longer axis of the parabolic trap $x^2 + b^2y^2 = 1$.
  - x-axis if $b > 1$ and y-axis if $b < 1$
  - Example: $b = 0.9535$



- Fold as Ω is decreased below

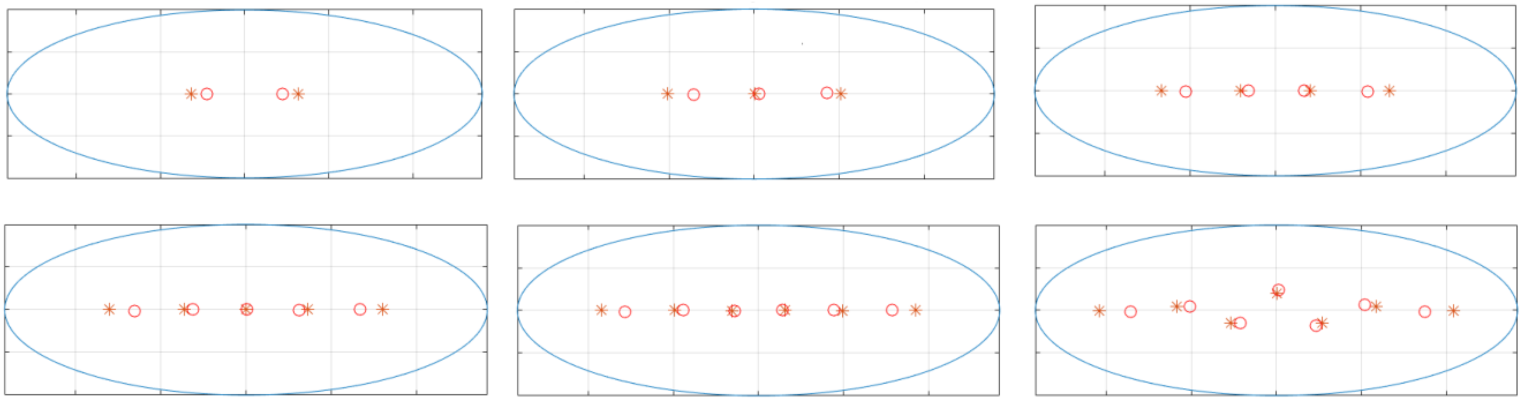
$$\Omega_2 = \frac{1}{\nu}\frac{1+b^2}{2}\left(\sqrt{2}+\sqrt{\nu}\right)^2 .$$

  - Two-vortex configuration disappears as Ω is decreased below Ω_2.



High-anisotropy regime

- For high anisotropy (large b), multipe vortices align themselves along the long axis



- Suppose $b \gg 1$ and all vortices are aligned along the x-axis. The steady state is

$$0 = \left(-\hat{\Omega} + \frac{1}{1-x_j^2}\right) x_j + \nu \sum_{k \neq j} \frac{1}{x_j - x_k} \frac{1-x_j^2}{1-x_k^2}, \qquad \hat{\Omega} := \nu \frac{\Omega}{1+b^2}. \tag{45}$$

- Continuum limit:

$$0 = \left(-\hat{\Omega} + \frac{1}{1-x^2}\right) z + \nu \fint_{-a}^{a} \frac{1}{y-x} \frac{1-x^2}{1-y^2} \rho(y)\,dy \tag{46}$$

where a is lattice “radius”, and subject to mass constraint:

$$\int_{-a}^{a} \rho(x)\,dx = N \tag{47}$$

- To solve (46): use Chebychev polynomials! They satisfy:

$$\fint_{-1}^{1} \frac{\sqrt{1-y^2}U_{n-1}(x)}{y-x}dy = -\pi T_n(x), \quad \fint_{-1}^{1} \frac{T_{n(x)}}{(y-x)\sqrt{1-y^2}}dy = \pi U_{n-1}(x) \tag{48}$$

The solution is given by

$$\rho(x) = -\frac{1}{\pi}\sum_{i=1}^{\infty} c_i U_{i-1}(\frac{x}{a}) \left(1-x^2\right) \sqrt{1-\frac{x^2}{a^2}}. \tag{49}$$

where

$$c_i = \frac{2}{\pi}\int_{-1}^{1} \left(-\hat{\Omega} + \frac{1}{1-a^2y^2}\right) \frac{ay}{\nu\left(1-a^2y^2\right)} T_i(y) \frac{1}{\sqrt{1-y^2}}dy. \tag{50}$$

and

$$N = \frac{1}{\nu}\left(\frac{\hat{\Omega}a^2}{2\sqrt{1-a^2}} - \frac{(a^2-2)^2}{\nu(1-a^2)^{\frac{3}{2}}} + 1\right). \tag{51}$$

The function $a \to N(a)$ has a unique maximum at $a^2 = 2\left(\hat{\Omega}-1\right)/(2\hat{\Omega}+1)$, given by

$$\boxed{N_{\mathrm{max,1d}} = \frac{1}{\nu}\left(1 + 3^{-3/2}(\hat{\Omega}-4)\sqrt{1+2\hat{\Omega}}\right)} \tag{52}$$

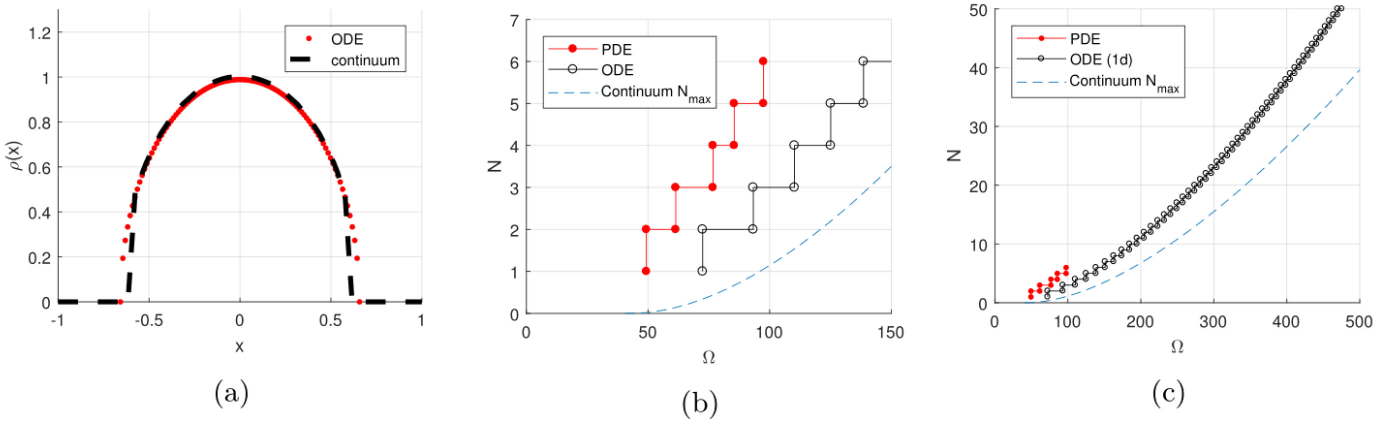


Figure 6: (a) Steady state density of the ODE system (63), compared with the continuum limit (66). Here, $N = 40$ and $\hat{\Omega} = 10.8$ (b) Maximal admissable number of vortices for the full PDE simulation of (1) versus the ODE system (2), versus the versus continuum formula (67). Both PDE and ODE simulations are fully two-dimensional. Parameters are $\gamma = 1, \kappa = 0, \varepsilon = 0.0088$, $b = 2.83$ and Ω is slowly decreasing according to the formula $\Omega = 150 - 10^{-4}t$. (c) Comparison of the ODE (63) and continuum limit formula (67) with ODE motion restricted to the x-axis, for larger number of vortices. Same parameters as in (b), except that $\Omega = 500 - 10^{-4}t$.

Further research

- For anisotropic trap, creation and destruction may happen at different points of the boundary, potentially leading to complex creation-destruction loops: Movie

- Papers discussed (available from my website)
  - S. Xie, P. Kevrekidis and T.. Kolokolnikov, Multi-vortex crystal lattices in Bose-Einstein Condensates with a rotating trap, ***Proceedings of the Royal Society A (2017), 474, 20170553.***

  - T. Kolokolnikov, P.G. Kevrekidis, and R. Carretero-Gonzales, A Tale of Two Distributions: From Few To Many Vortices In Quasi-Two-Dimensional Bose-Einstein Condensates. ***Proceedings of the Royal Society A (2014), 470, 20140048.***

Conclusions

Reduced dynamics of PDE's lead to new swarming systems which sometimes require new techniques

Techniques in swarming lead to new insights for PDE systems.

Good open problem: do stability of 2D GM clusters.