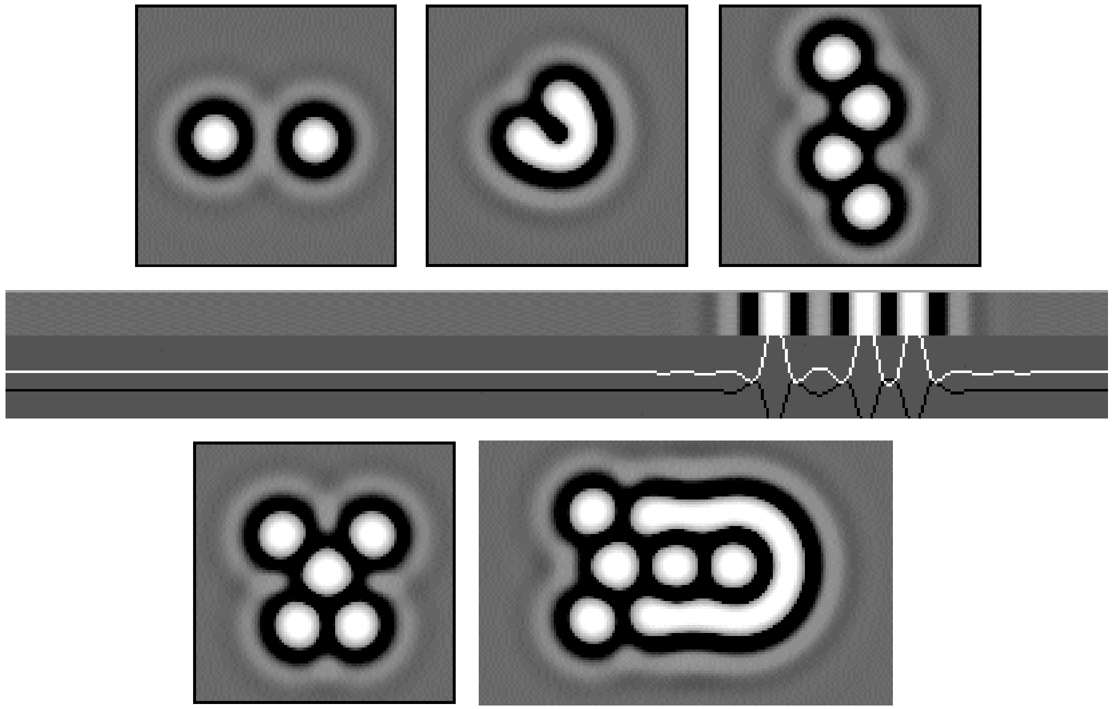
Stable moving patterns in the 1-D and 2-D Gray-Scott Reaction-Diffusion System



Robert Munafo

Rutgers Mathematical Physics Seminar Series

2010 Dec 9, 2 PM - Hill 705

Revised, 2010 Dec 12

Contents (outline of this talk)

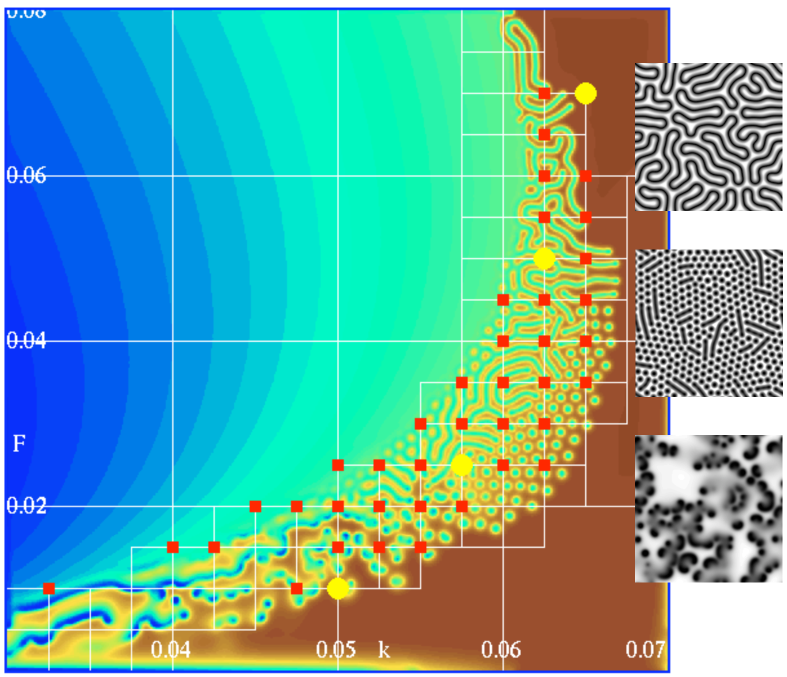
- Brief history, motivation and discovery
- Methods and testing
- New patterns and interactions (mostly video)
- Connections; Open questions
- Discussion

Brief History: Initial Motivation

- 1994: Looking for a problem to run on new hardware
- Supercomputer research led to Williams exhibit at Caltech (shown, left)
- Literature was easy to find; problem was appealing
- Exploring parameter space more closely

Xmorphia

Instructions: Click on the red squares for **images**, and on the yellow blobs for **movies**.



Morphogenesis from a Reaction-Diffusion System

Roy Williams
Concurrent Supercomputing Facilities
California Institute of Technology

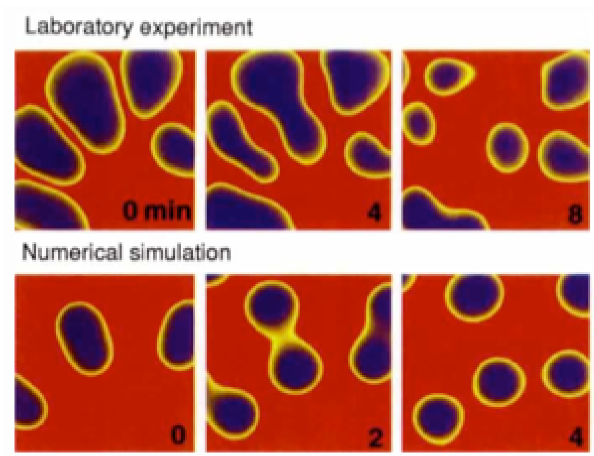
Roy Williams "Xmorphia" web exhibit (Caltech, 1994)

$$\frac{\partial U}{\partial t} = D_u \nabla^2 U - UV^2 + F(1-U)$$

$$\frac{\partial V}{\partial t} = D_v \nabla^2 V + UV^2 - (F+k)V$$

Pearson "Complex patterns in a simple system" (*Science* **261** 1993) (illust. next slide)

Lee et al. "Experimental observation of self-replicating spots in a reaction-diffusion system" (*Nature* **369** 1994)



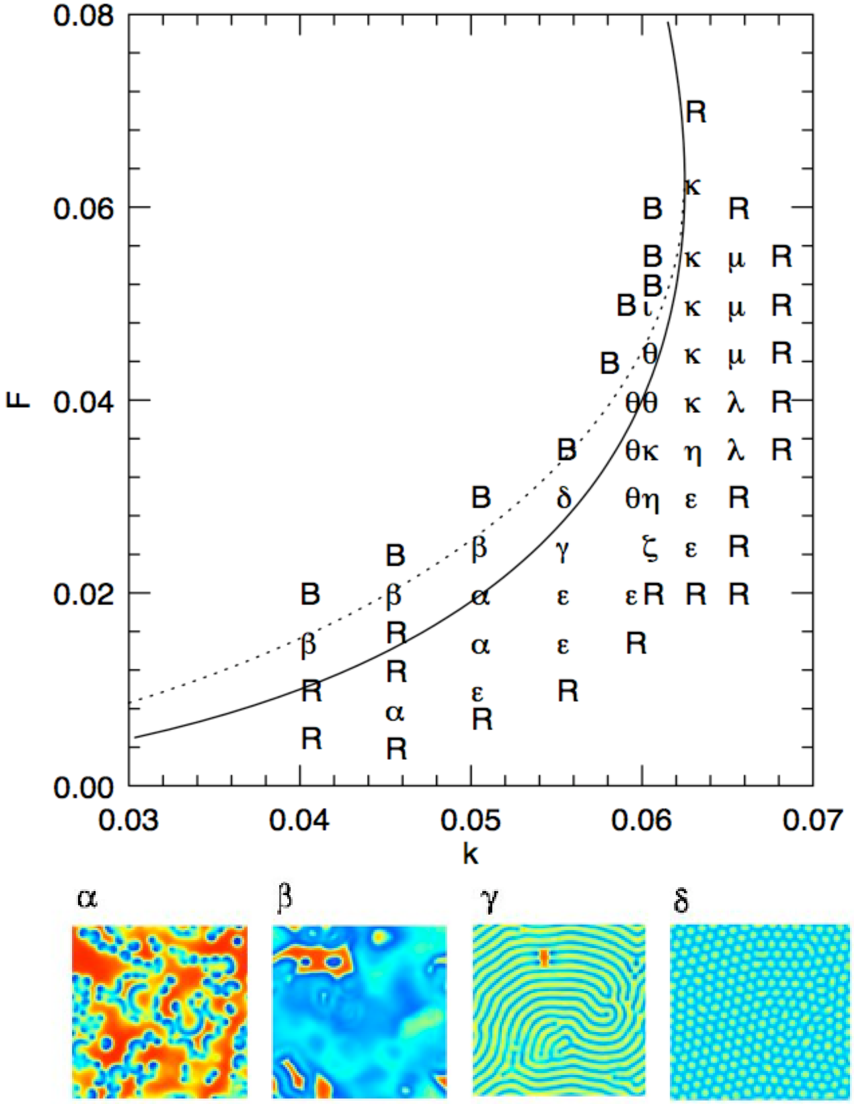
Ferrocyanide–iodate–sulphite reaction in gel reactor

($K_4Fe(CN)_6 \cdot 3H_2O$, $NaIO_3$, Na_2SO_3 , H_2SO_4 , NaOH , bromothymol blue)

$$\frac{\partial U}{\partial t} = D_U \nabla^2 U - UV^2 + A(U_0 - U)$$

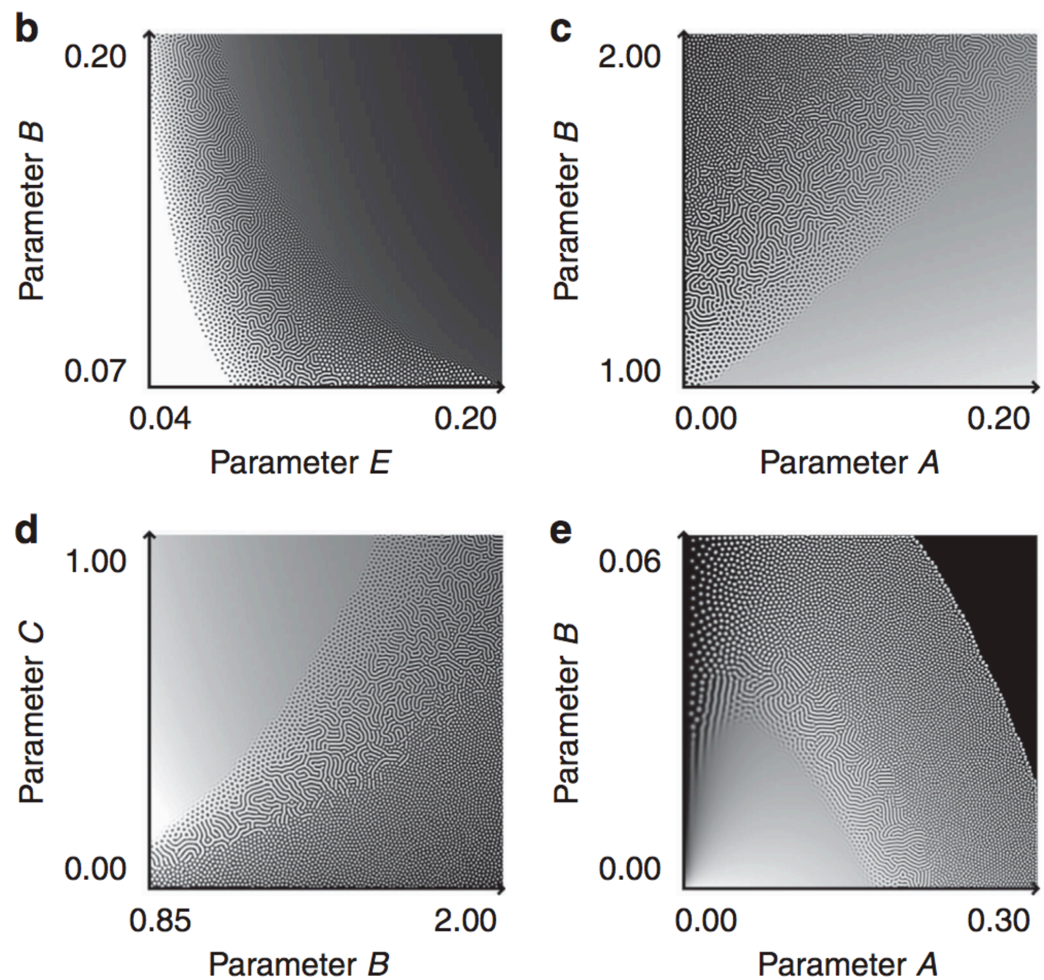
$$\frac{\partial V}{\partial t} = D_V \nabla^2 V + UV^2 + B(V_0 - V)$$

Brief Intro: Parameter Space



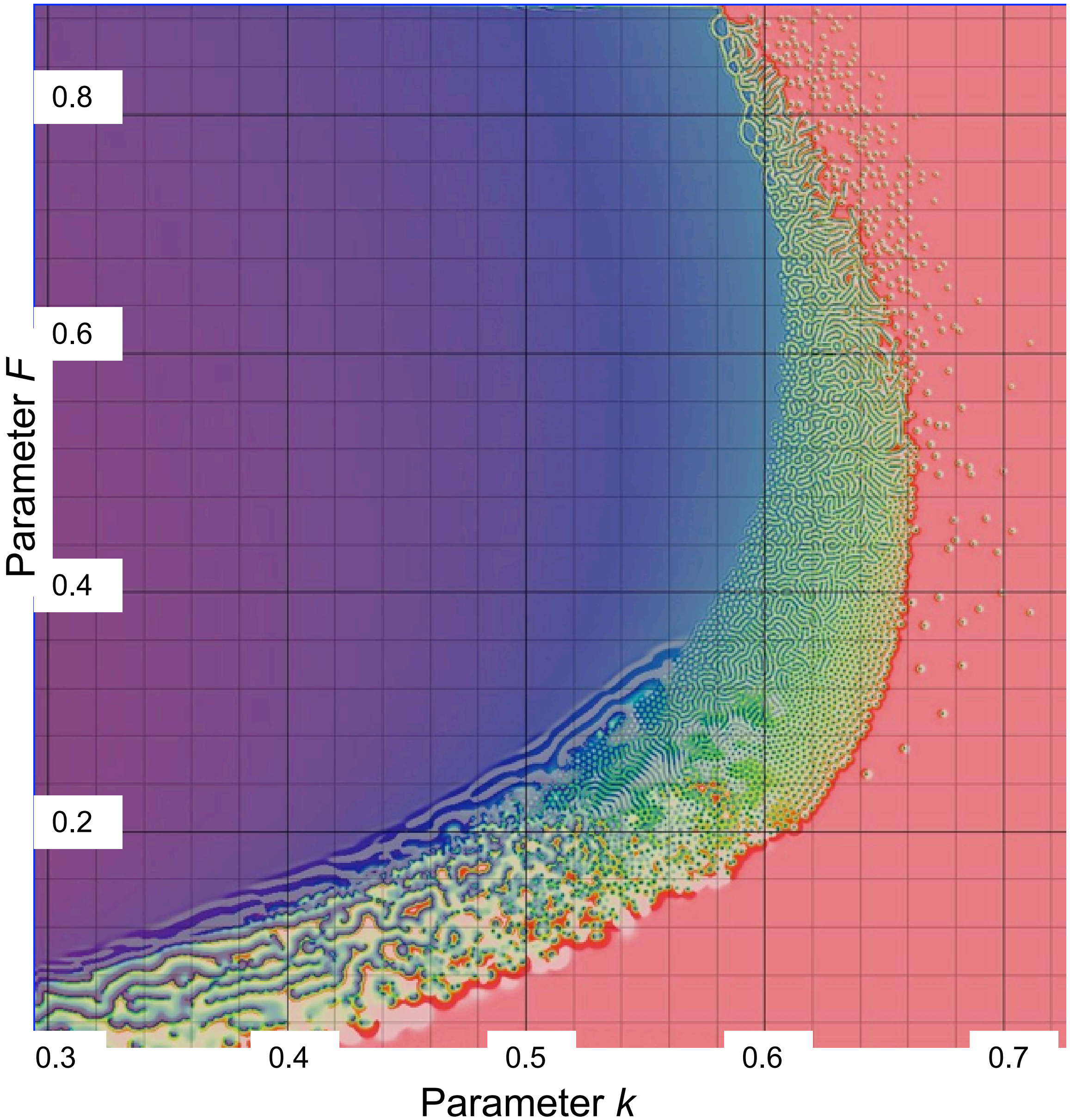
Parameter space and four pattern examples, from Pearson (ibid. 1993)

Coloring imitates bromothymol blue pH indicator as in Lee et al. “Pattern formation by interacting chemical fronts” (*Science* **261** 1993): blue = low U; yellow = intermediate; red = high U



Parameter space visualizations for several reaction-diffusion models, from fig. 3, Miyazawa et al. “Blending of animal colour patterns by hybridization” (*Nature Comm.* **1(6)** 2010)

Brief History: 2009 Website Project



False color images: purple = lowest U, red = highest U, pastels = $\partial U/\partial t > 0$

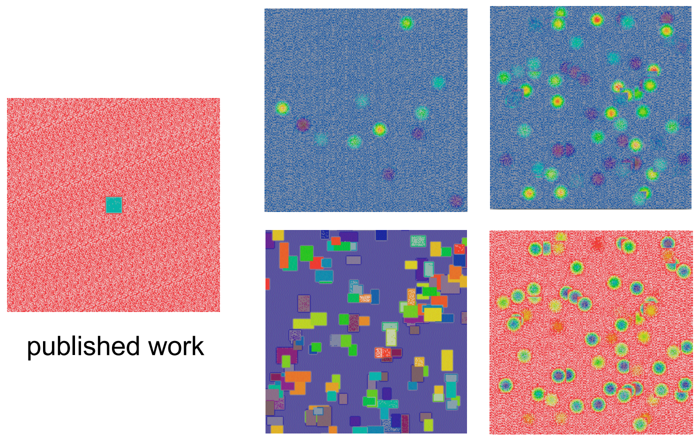
- Denser coverage; explore more extreme parameter values

  Pearson: 34 sites; $0.045<k<0.066$; $0.003<F<0.061$; all static

  Williams: 45 sites; $0.032<k<0.066$; $0.01<F<0.07$; 4 video

  Munafo: 150+ sites; $0.03<k<0.072$; $0.004<F<0.098$

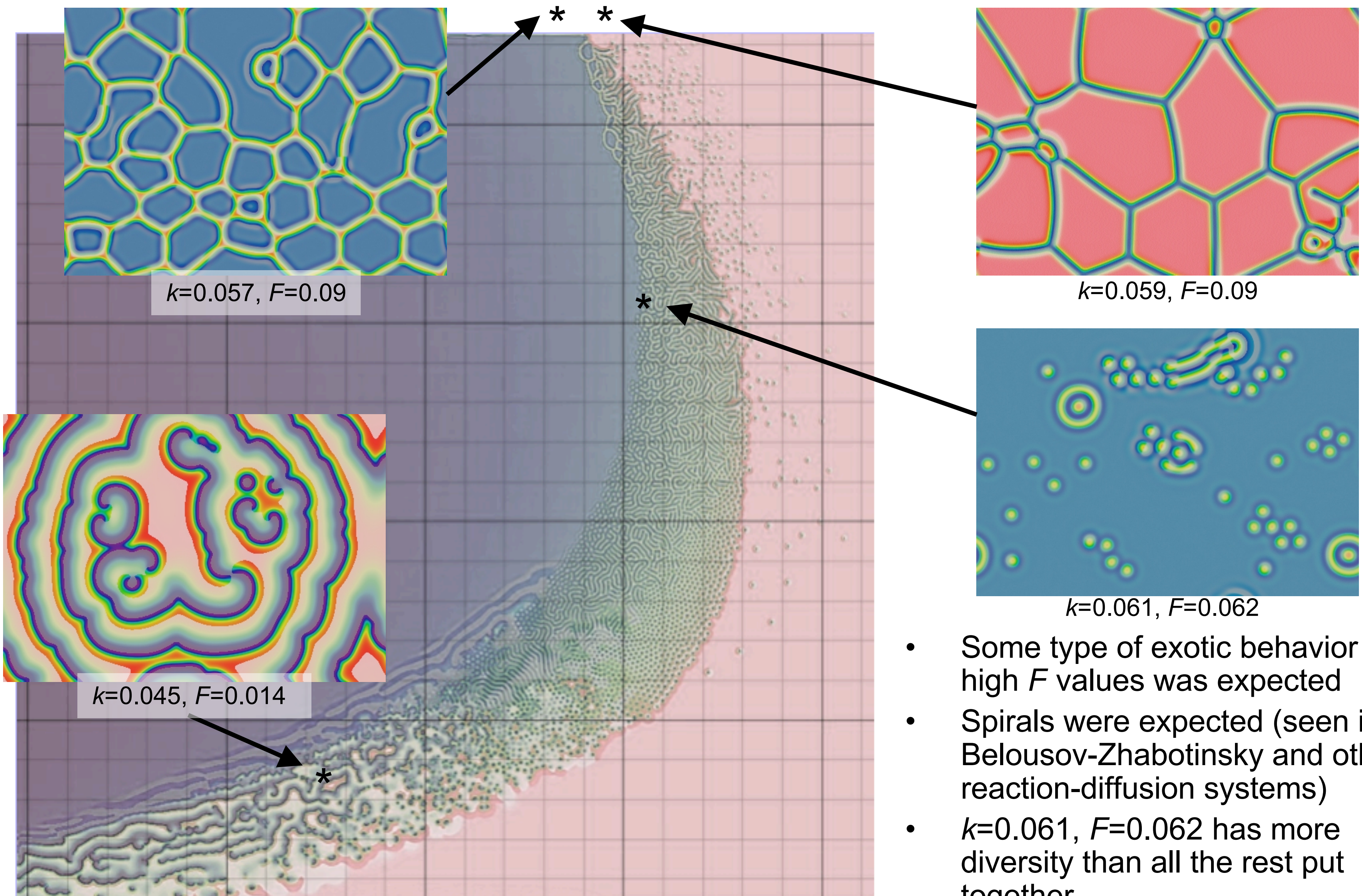
- Several types of starting patterns



published work

- Video for each (k,F) point
- Higher resolution and precision
- Coloring to show both U and $\partial U/\partial t$
- Describe and catalog all phenomena
- Run each pattern "to completion" no matter how long that takes

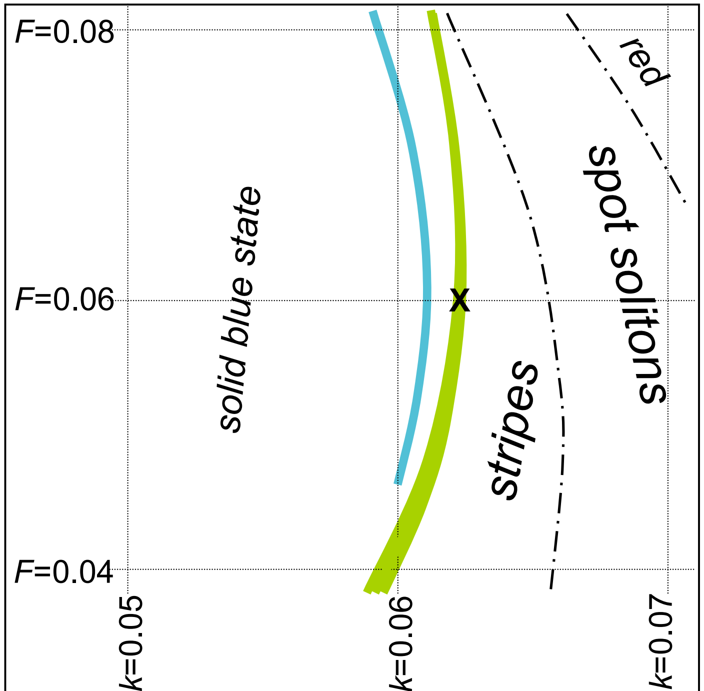
New pattern types (2009)



Munafo (2009) www.mrob.com/pub/comp/xmorphia

- Some type of exotic behavior at high *F* values was expected
- Spirals were expected (seen in Belousov-Zhabotinsky and other reaction-diffusion systems)
- *k*=0.061, *F*=0.062 has more diversity than all the rest put together
- Also found: mixed spots and stripes; variations in branching; etc.

Inherent Instability



Gray-Scott parameter values for Turing instability (green; width to scale) and stable moving patterns (blue; width exaggerated). The video is at **X**

k=0.062, *F*=0.06

Periodic boundary conditions; size 3.35w x 2.33h

Each second is 1102 **dtu**

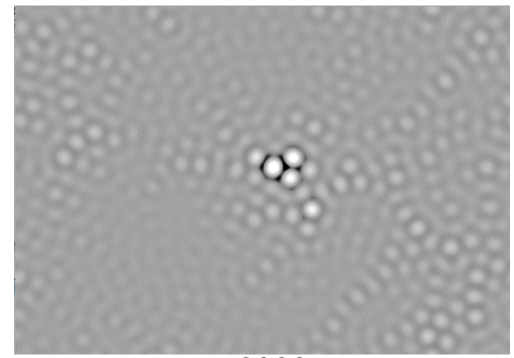
Initial pattern of low-level random noise (0.4559<*U*<0.4562; 0.2674<*V*<0.2676)

Final values: 0.35<*U*<0.90; 0.00<*V*<0.36 (approx.)

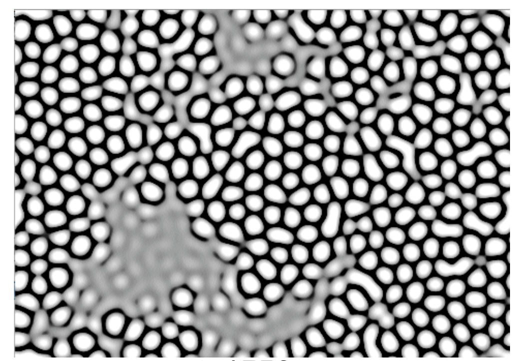
(Contrast-enhanced images; lighter = higher *U*)

Turing-F600-k620.mp4 -- youtube.com/v/kXDTqqgrYCg

t=3000



t=3900



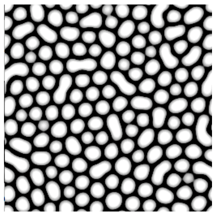
t=4550

• At many parameter values, patterns like this grow out of any inhomogeneity, no matter how small

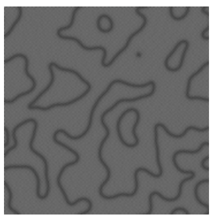
• This is not a consequence of numerical approximation error: proven by mathematical analysis. Dominant wavelength (spot size) depends on reaction dynamics and diffusion rate.

Turing “The chemical basis of morphogenesis” (*Phil. Trans. Royal Soc. London B* **237(641)** 1952)

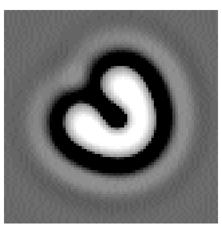
How can we trust these results?



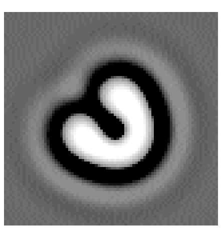
Turing instability



Numerical instability



Euler integration

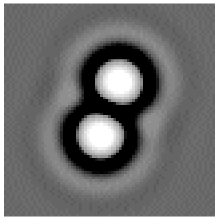


4th-order Runge-Kutta

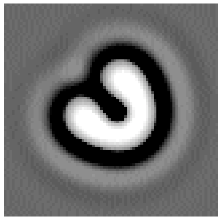
- Arbitrarily low-level noise can generate strong patterns
- Instabilities can exist in the ideal (exact) system, and can be introduced by the numerical method
- Complex patterns are already proven to be real
- These new patterns are far more extraordinary
- Mathematical proof/disproof probably impossible
- How much precision is necessary? Is any finite precision sufficient for proof?
- Is the standard precision “too accurate” to be relevant? The real world has known levels of quantization and randomness: “finite precision”
- Goals:
  - Eliminate suspicion of numerical error
  - Quantify the sensitivity of these pattern phenomena to precision, randomness, reaction parameters and other environmental conditions

Verification Examples

- Two stable moving phenomena
- One is clearly bogus, the other might be real



Two spots maintain the same distance while the pair rotates toward a 45° alignment



U-shaped pattern moves at about 1 **dlu** per 62,000 **dtu** (dimensionless units of length, time)

- Define something that is measurable
- Model the sources of error, e.g.:

measured value = true value + simulation error + measurement error

simulation error = *f*(stability, precision, grid spacing, ...)

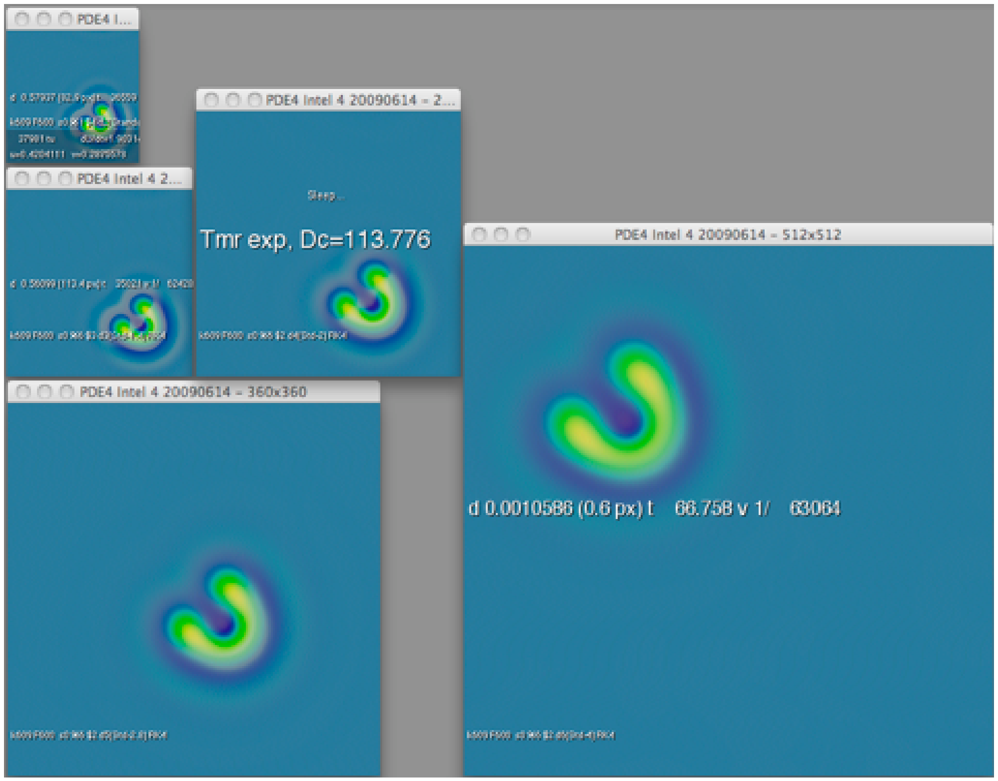
CFL (Courant-Friedrichs-Lewy 1928) stability criterion (for the Laplacian term):

$$C\ \Delta x^2/\Delta t$$

(A higher value means greater stability. Constant *C* depends on e.g. *k* and *F* for the Gray-Scott system)

- Progressively improve the simulation and look for a trend

Verification Procedure

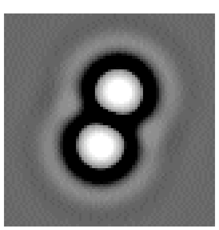


- Progressively improve Δx by $\sqrt{2}$
- Progressively improve CFL stability by $\sqrt{2}$
- Progressively improve Δt by needed amount ($2\sqrt{2}$)

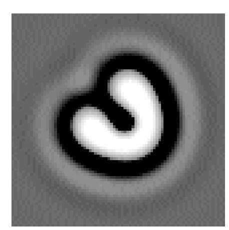
	Δx	Δt	$\Delta x^2/\Delta t$	pixels(typ.)
"std"	0.00699	0.5	9.78e-5	128x128
"s1.4"	0.00495	0.177	1.38e-4	180x180
"s2"	0.00350	0.0625	1.96e-4	256x256
"s2.8"	0.00247	0.0221	2.77e-4	360x360
"s4"	0.00175	0.00781	3.91e-4	512x512

(amount of calculation increases by $4\sqrt{2}$ each time: ratio of 1024 to 1 between "std" and "s4")

Expected Results:



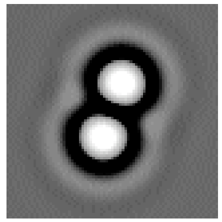
Movement is 100% spurious: measurements should tend towards zero



If real, velocity should clearly converge on a nonzero value

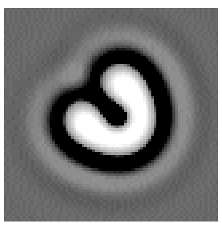
Verification Examples - Results

Suspect rotating 2-spot phenomenon



model	max dU/dt	cross-qtr. interval	relative velocity
std	8.97e-7	5.6e5	1.0
s1.4	4.57e-7	1.12e6	0.50
s2	2.31e-7	2.18e6	0.26
s2.8	1.158e-7	4.34e6	0.129
s4	5.80e-8	8.7e6	0.064

Velocity of U-shaped pattern



model	dist	pixels	time	velocity (meas.err)
std	0.55418	79.2	35076	1/63294(45)
s1.4	0.59863	121.1	37342	1/62379(64)
s2	0.57042	163.1	35456	1/62159(27)
s2.8	0.56947	230.3	35258	1/61913(44)
s4	0.56553	323.5	35009	1/61905(12)

Same tests using 4th order Runge-Kutta

model	dist	pixels	time	velocity	(meas.err)
std	0.57937	82.9	36559	1/63101	
s1.4	0.56053	113.4	35021	1/62479	same
s2	0.56351	161.2	35008	1/62124	as
s2.8	0.56517	228.6	35003	1/61934	above
s4	0.56574	323.6	35002	1/61870	

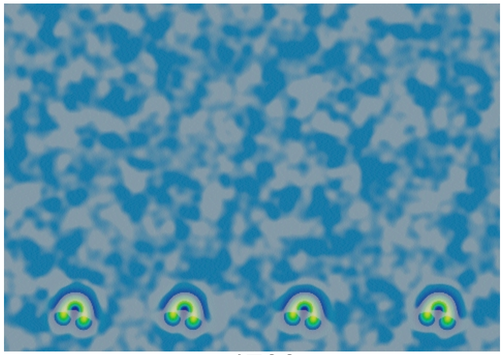
Limits on parameter *k* (when *F*=0.06) for stability of U-shaped pattern

model	minimum	maximum
std	0.0608833	0.0609829
s1.4	0.0608796	0.0609831
s2	0.0608777	0.0609831
s2.8	0.0608767	0.0609830
s4	0.0608762	*did not test*

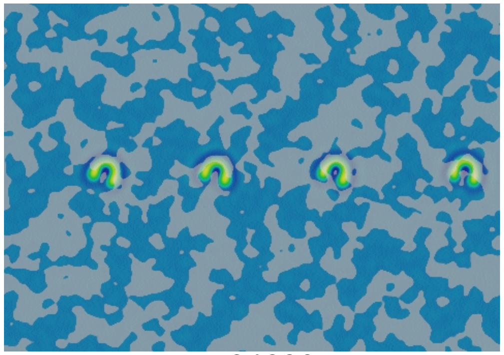
measurement error in all values is +-1 in the last digit

- Two-spot pattern movement is bogus
- Moving U-shaped pattern is real; Runge-Kutta gives little if any benefit
- Asymptotic trends in values and in measurement errors, as expected

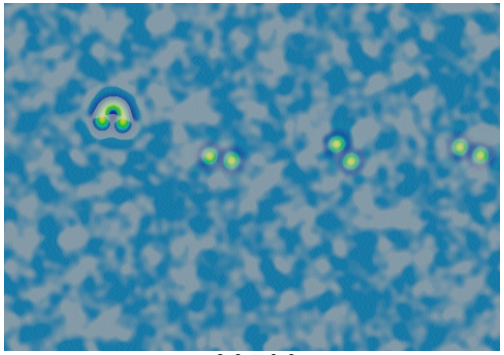
Immunity to Noise



t=4700



t=64680



t=88500

k=0.0609, *F*=0.06

Periodic boundary conditions; size 3.35w x 2.33h   1 second ≈ 1100 **dtu**

4 U-shaped patterns traveling "up"

Systematic noise perturbation applied once per 73.5 **dtu**

Amplitude of each noise event starts at 0.001 and doubles every 11,000 **dtu** (10 seconds in this movie)

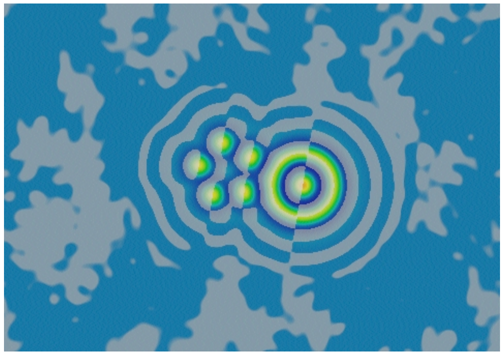
At noise level 0.064, three patterns are destroyed; noise amplitude is then diminished to initial level

(False-color: yellow = high *U*; pastel = positive $\partial U/\partial t$)

U-noise-immunity.mp4 -- youtube.com/v/_sir7yMLvIo

- Pattern continues to move in the presence of noise, and generally behaves as expected of a real phenomenon
- Similar tests (e.g. more frequent noise events each of lower amplitude) give similar results

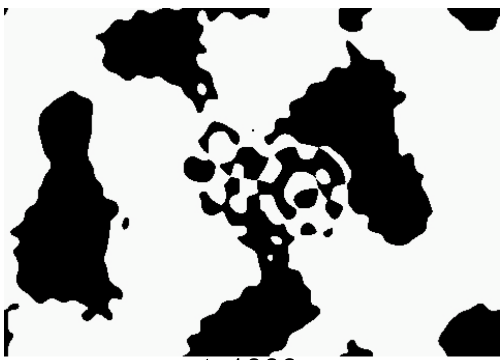
Symmetry-based Instability Tests



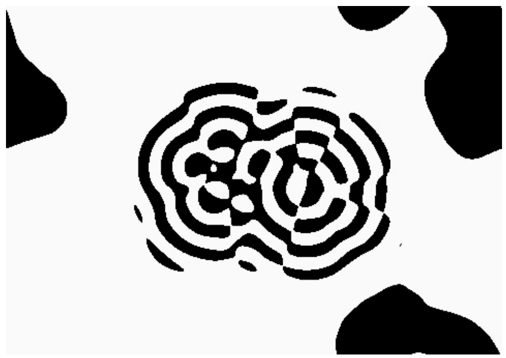
k=0.0609, *F*=0.06 — Periodic boundary conditions; size 2.36w x 1.65h — Manually constructed initial pattern based on parts of naturally-evolved systems — 1 second = 265 **dtu**

Two sets of three noise events; noise event amplitudes are 10^{-5}, 0.001 and 0.1; pattern allowed to recover after each event

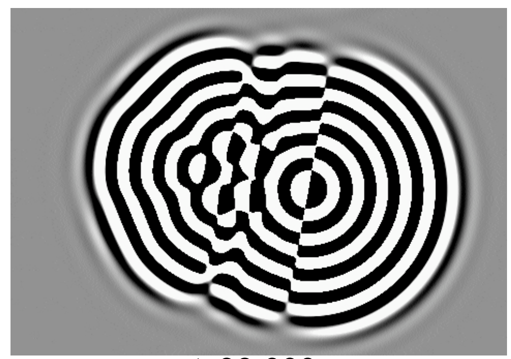
Coloring (left image) same as before — Coloring (images below): white = positive $\partial U/\partial t$, black = negative $\partial U/\partial t$, shades of gray when magnitude of $\partial U/\partial t$ is less than about 5×10^{-13}



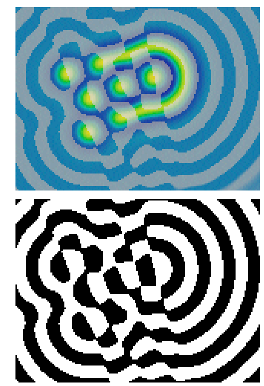
t=1000



t=2850



t=38,000



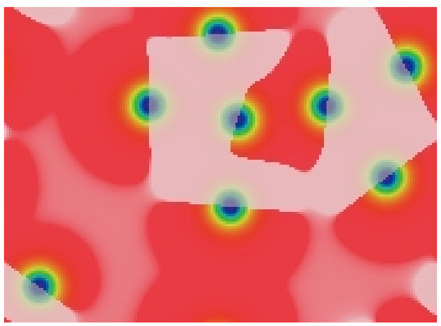
A pattern with an instability that this test does not help reveal

Daedalus-stability.mp4 -- youtube.com/v/fWfsMVEeP5k

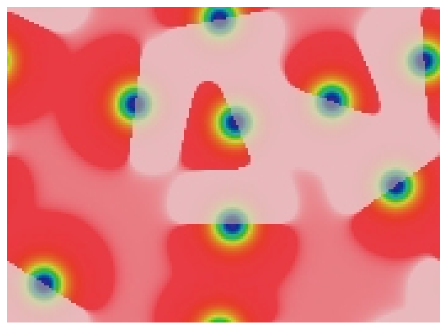
- Rotating and moving patterns have rotational or bilateral (resp.) symmetry which persists if the pattern is stable.
- Instability and/or a return to symmetry are easier to observe in the derivative
- Test static and linear-moving patterns at different angles to reveal influence by grid effects
- Other tests include shifting parts of a pattern, applying noise to only part of a pattern, etc.
- Such tests can reveal instability more quickly but do not prove stability.

Logarithmic Timebase, Long Duration

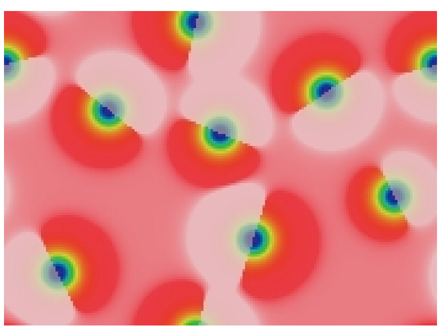
- Some phenomena appear asymptotic to stability but actually keep moving forever
- Running a simulation for as long as possible (currently >10^8 time units) and viewing the results at an exponentially accelerating speed can reveal some of these phenomena
- Repulsion of solitons in 1-D (pictured, lower-right) has been studied mathematically for high ratios D_U/D_V (Doelman et al. “Slowly modulated two-pulse solutions...”, *SIAM Jrl. on Appl. Math.* **61(3)** 2000) with the result: (speed of movement) = Ae^{-Bt} for positive constants A,B
- There are many other phenomena in Gray-Scott systems that slow at similar rates



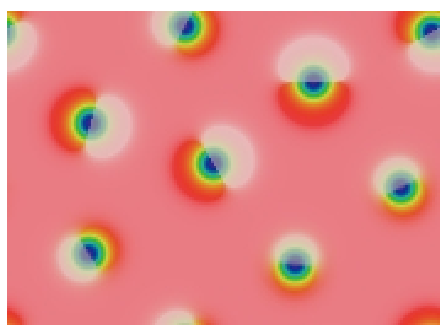
t=78,125



t=1,250,000

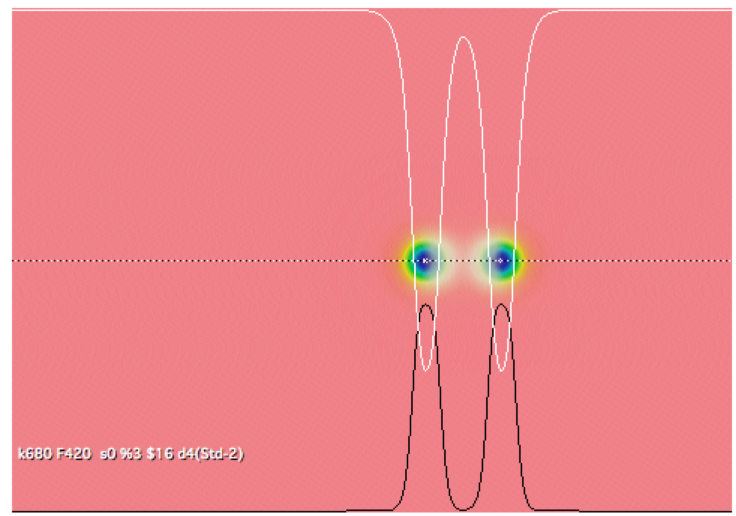


$t=2\times10^7$

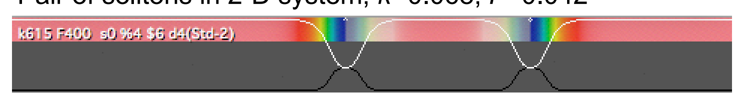


$t=3.2\times10^8$

Eight solitons in a 2-D system, k=0.067, F=0.046

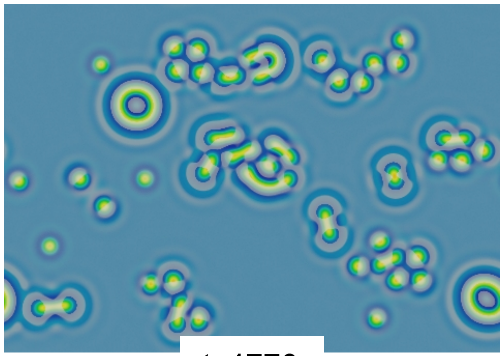


Pair of solitons in 2-D system, k=0.068, F=0.042

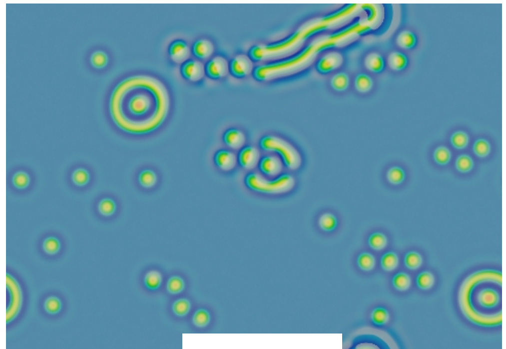


Pair of solitons in 1-D system, k=0.0615, F=0.04

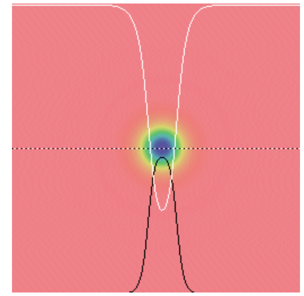
Discovery – Great Diversity



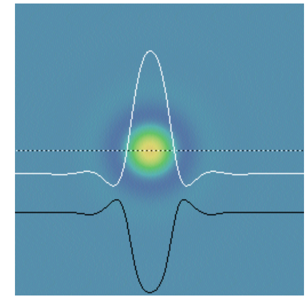
t=4770



t=47700



Ordinary spot soliton
(*k*=0.067, *F*=0.062)



“negative soliton”
(*k*=0.061, *F*=0.062)

White curve = *U*; Black curve = *V*; dotted line shows cross-section taken

k=0.061, *F*=0.062   Periodic boundary conditions; size 3.35w x 2.33h

1 second ≈ 1190 **dtu**

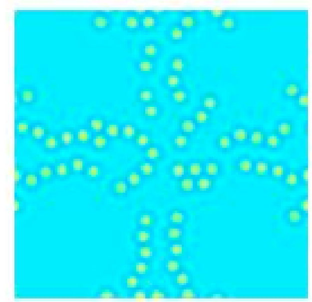
Initial pattern of a few randomly placed spots of relatively high *U* on a “blue” background (secondary homogeneous state, approx. *U*=0.420, *V*=0.293)

(False-color: yellow = high *U*; pastel = positive $\partial U/\partial t$)

Original-F620-k610-fr159.mp4 -- youtube.com/v/wFtXwFfrwWk

- Part of routine scan for website exhibit project
- “Negative solitons” (hereafter called “negatons”) exhibit attraction and multi-spot binding
- Several types of patterns in one system
- The “target” pattern is not stable at these parameter values, but **is** stable at the nearby parameters *k*=0.0609, *F*=0.06

ι

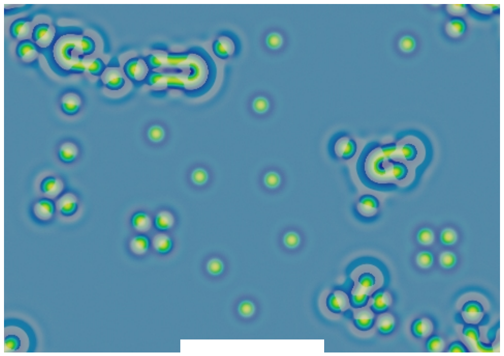


“negative solitons” in Pearson (ibid. 1993)

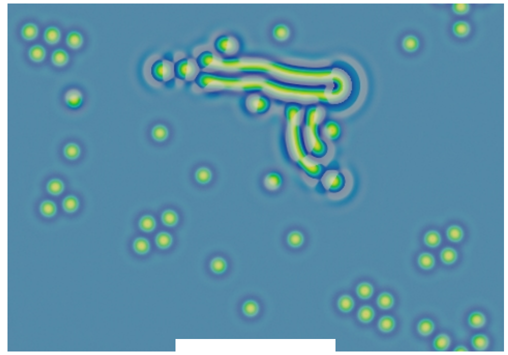
“Pattern ι is time independent and was observed for only a single parameter value.”

(parameters unpublished, probably *k*=0.06, *F*=0.05)

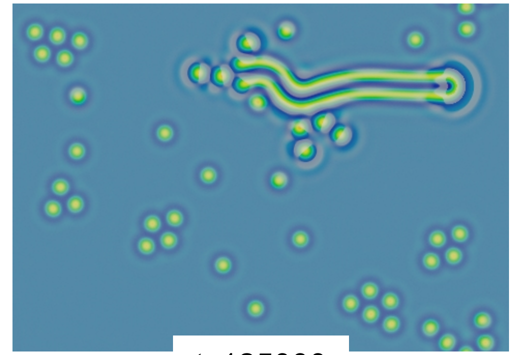
Discovery – Moving U Pattern



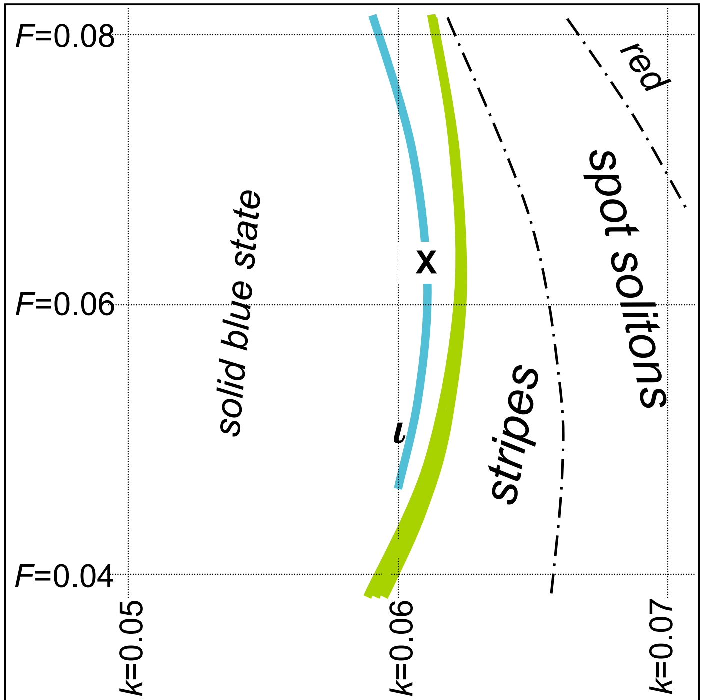
t=8860



t=74200



t=125000



This video is at **X**; Pearson's type *ι* is shown

k=0.0609, *F*=0.062

Periodic boundary conditions; size 3.35w x 2.33h

1 second ≈ 3900 **dtu**

Initial pattern and coloring same as before

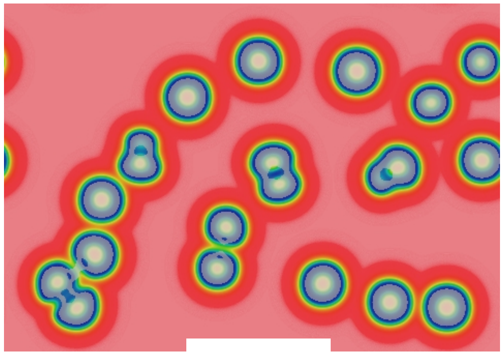
U-discovery-F620-k609-fr521.mp4 -- youtube.com/v/xGMuuPYhLiQ

Original coloring -- youtube.com/v/ypYFUGiR51c

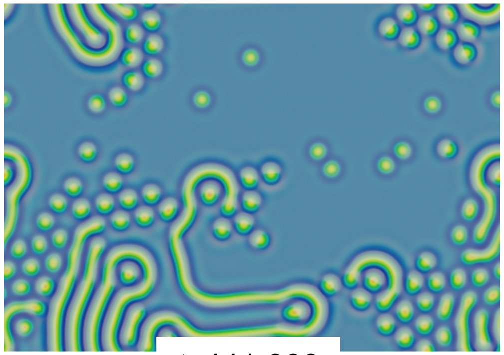
- Moving "U" visible to right of center, short-lived (hits two negatons)
- More unexpected negaton behavior: being "dragged" by other features

Long Duration Test

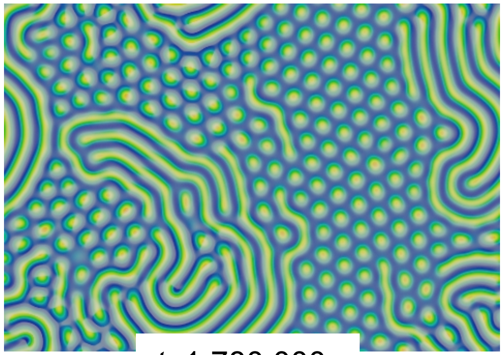
Different Behaviors at Multiple Time Scales



t=2500



t=441,000



t=1,780,000

k=0.0609, *F*=0.062 Periodic boundary conditions; size 3.35w x 2.33h

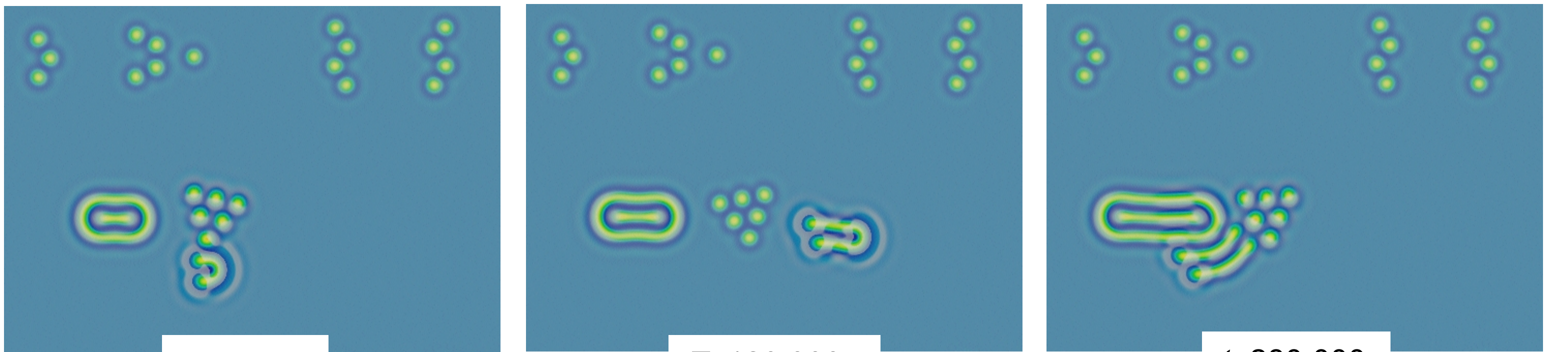
Initial pattern of spots (randomly chosen U<1, V>0) on solid red (U=1, V=0) background; coloring same as before

Video uses accelerating time-lapse: simulation speed doubles every 6.7 seconds

Exponential-time-lapse.mp4 -- youtube.com/v/-k98XOu7pC8

- First 30,000 **dtu** (40 seconds): blue spots grow to fill the space (a very common Gray-Scott behavior)
- Up to 1.25 million **dtu** (75 seconds): complex behavior, double-spaced stripes, solitary negatons, etc. until all empty space is filled
- Up to 6 million **dtu** (90 seconds): chaotic oscillation of parallel stripes growing, shrinking and twisting; gradually producing more spots
- Sudden onset of stability: All chaotic motion ends (whole system drifts very slowly)

Complex Interactions



t=60,000 *T*=120,000 *t*=280,000

k=0.0609, *F*=0.06

Periodic boundary conditions; size 3.35w x 2.33h

Each second is 10,000 **dtu**

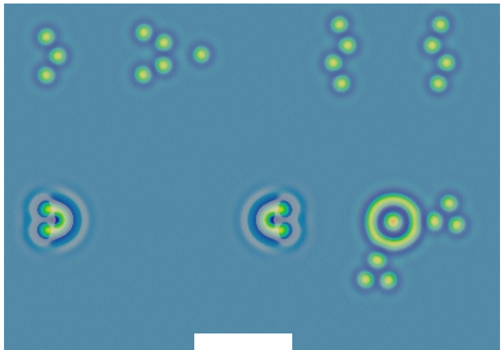
Manually constructed initial pattern based on parts of naturally-evolved systems

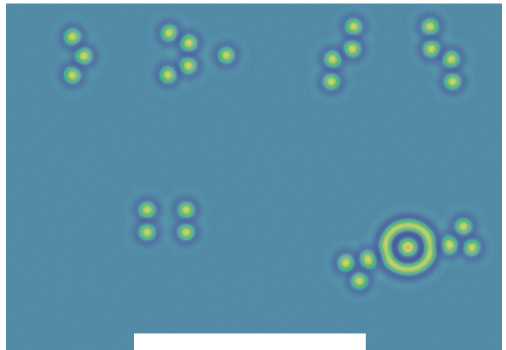
Coloring same as before

complex-interactions-1.mp4 -- youtube.com/v/hgTBOf7gg8E

- U-shape can influence other objects and survive (although it generally does not)
- The clusters of negatons along the top move and rotate, very slowly

Slow Movement, Rotation


t=0


T=1,500,000


T=7,000,000

k=0.0609, *F*=0.06

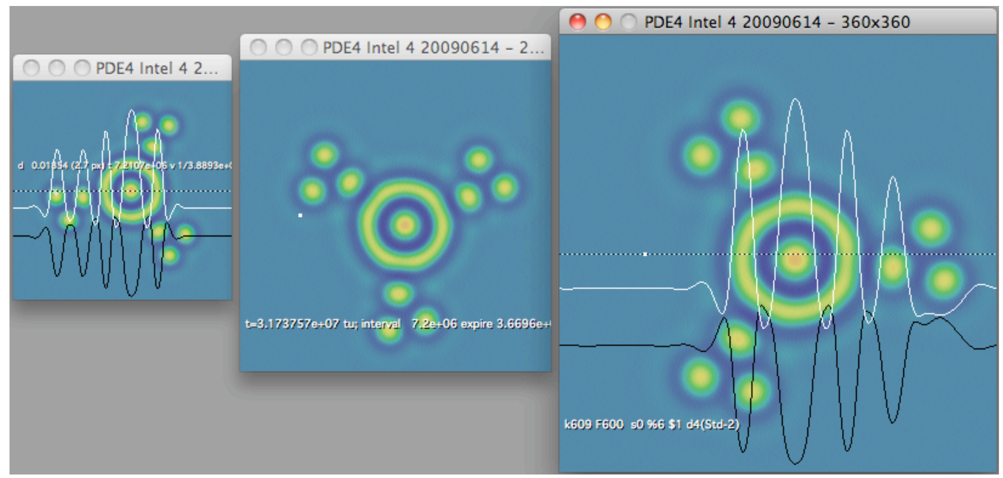
Periodic boundary conditions; size 3.35w x 2.33h

Each second is 100,000 **dtu**

Manually constructed initial pattern based on parts of naturally-evolved systems

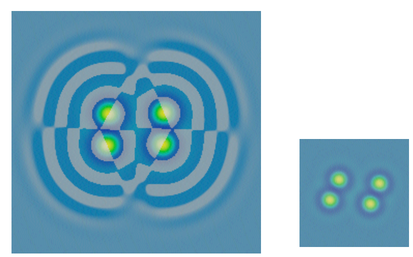
Coloring same as before

slow movers and rotaters.mp4 -- youtube.com/v/PB3lPMhwIo0

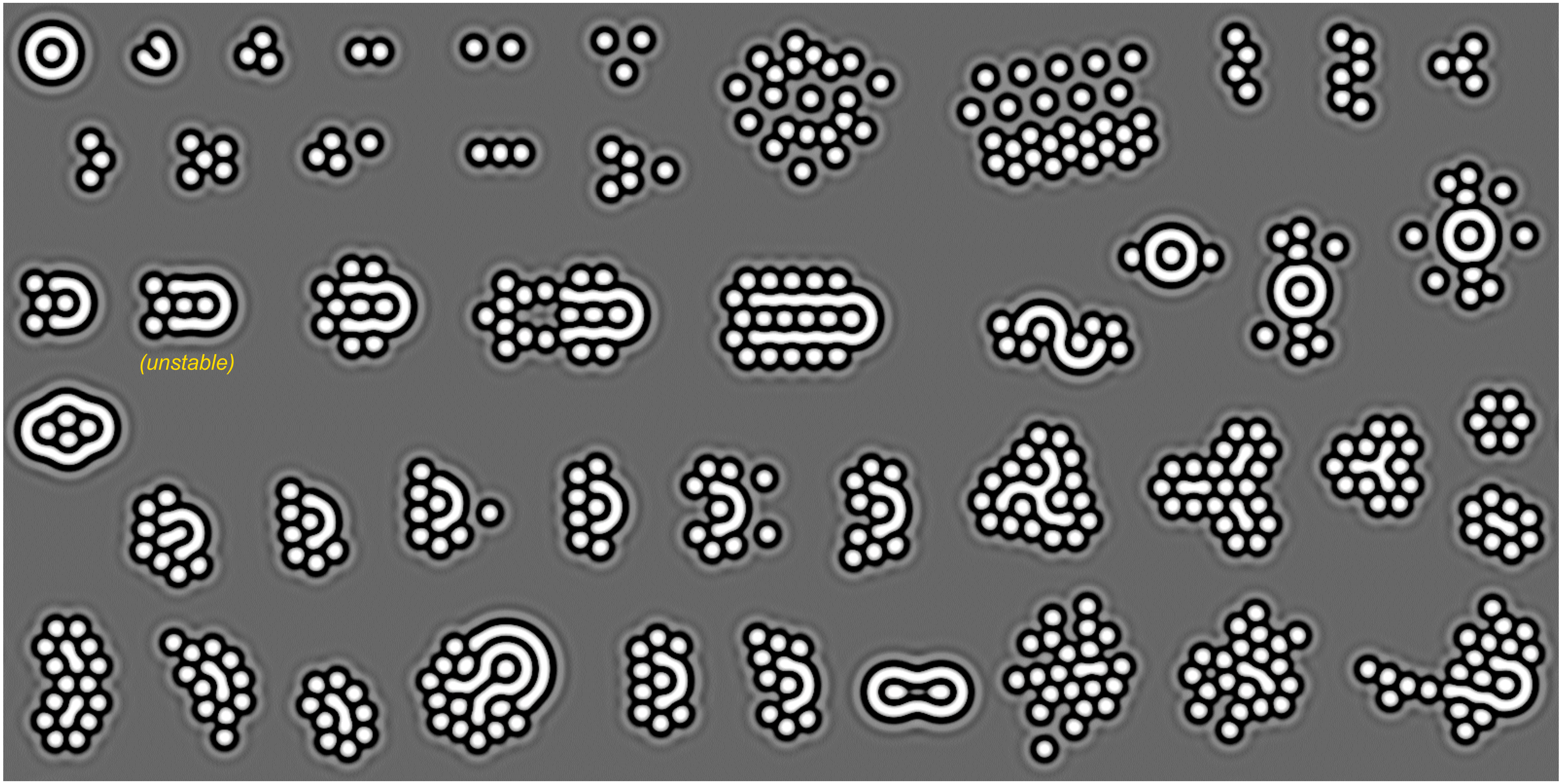


Stability analysis of another slow-rotating pattern

- There are many very slow patterns; a few of the more common are shown here
- The “target” (negaton with annulus) is a common product of spotlike initial patterns, and adjacent negatons typically make it move or rotate
- The 4 negatons left by the collision of two U patterns are in an unstable equilibrium


Stability testing of 4-negaton pattern; stable form shown at right

A Gray-Scott Pattern Bestiary



- Almost everything that keeps its shape moves indefinitely
- In general, a pattern will:
  - move in a straight line, if is has (only) bilateral symmetry
  - rotate, if it has (only) rotational symmetry
  - move on a curved path, if it has no symmetry at all
- Lone negatons are frequently “captured” and/or “pushed” by a moving pattern

k=0.0609, F=0.06   Contrast-enhanced grayscale, lighter = higher U

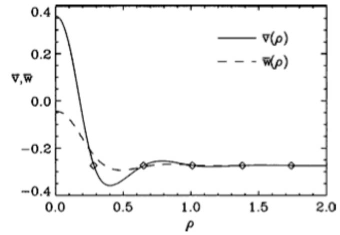
Most patterns were manually constructed from parts of naturally occurring forms

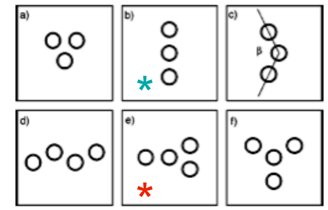
Note: Many of these are not yet thoroughly tested

Relation to Other Work:

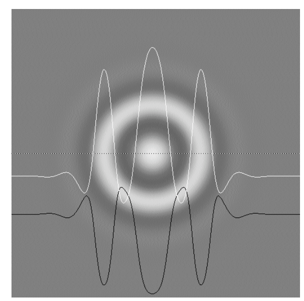
"Negaton" Clusters and Targets

- Spots and "target" patterns very similar to the Gray-Scott "negatons" are seen in papers by Schenk, Purwins, et al.
- In a 1998 work, a 2-component R-D system is studied; the spots are stationary and are reported to "bind" into stable groupings with specific geometrical configurations (as shown). There are differences between this system and Gray-Scott, evident in which "molecules" are reported as stable.
- In a 1999 work (by Schenk alone) a 3-component R-D system includes a "target" pattern with a very similar cross-section.

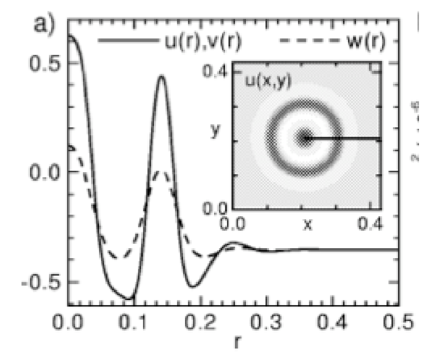




From Schenk et al. "Interaction of self-organized quasiparticles..." (*Physical Review E* **57(6)** 1998), fig. 1 and 5
The pattern marked * is stable in Gray-Scott at {*k*=0.0609, *F*=0.06}, the pattern marked is * not.



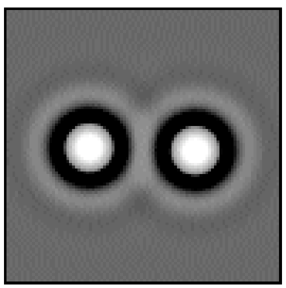
Target pattern in Gray-Scott, *k*=0.0609, *F*=0.06, with *U* and *V* levels at cross-section through center



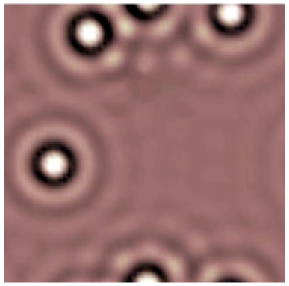
Target pattern from C. P. Schenk (PhD dissertation, WWU Münster, 1999) p. 116 fig. 4.37

Relation to Other Work: Halos

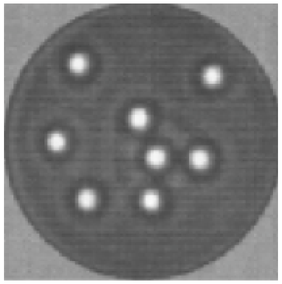
- The light and dark “rings” or “halos” are seen in physical experiments and numerical simulations intended to model both physical and biological systems
- When spots appear in these systems, as in Gray-Scott, the spots tend to be seen at certain “quantized” distances
- Halo amplitudes, spot spacings and relative sizes differ; this also reflects changes seen in Gray-Scott as the *k* and/or *F* parameters are changed



Negatons with halos (Gray-Scott system, *k*=0.0609, *F*=0.06, lighter = higher *U*; exaggerated contrast)



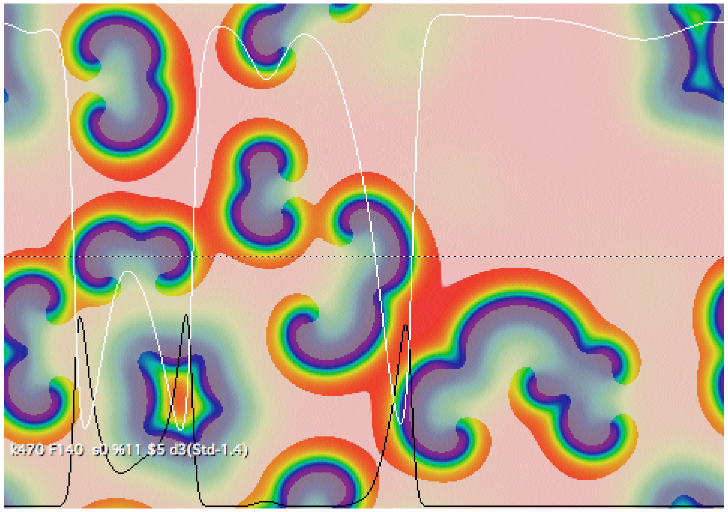
Spots with halos in numerical simulation by Barrio et al. “Modeling the skin patterns of fishes” (*Physical Review E* **79** 031908 2009) fig. 11



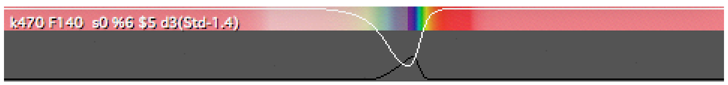
Spots with halos in gas-discharge experiment by Lars Stollenwerk (“Pattern formation in AC gas discharge systems”, website of the Institute of Applied Physics, WWU Münster, 2008) fig. 3d

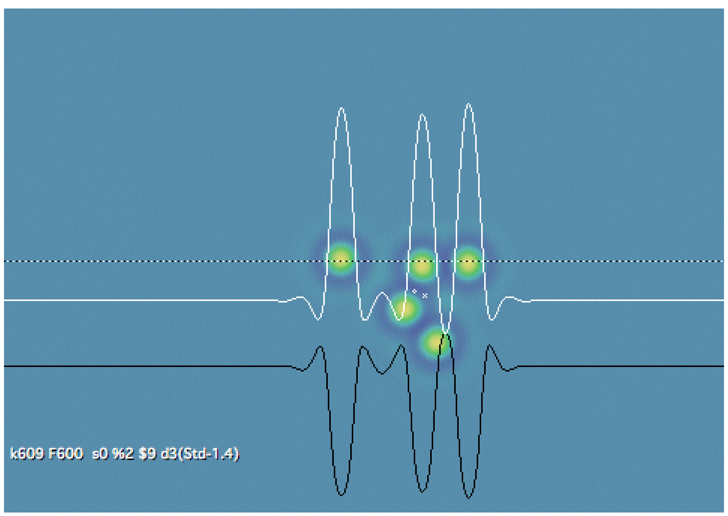
Halos also appear in models by Schenk, Purwins, et al (ibid., 1998 and 1999, shown elsewhere) in work related to gas discharge experiments

One-Dimensional Gray-Scott Model

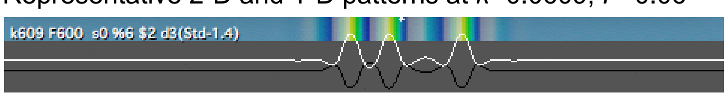


2-D spirals and 1-D pulse at k=0.047, F=0.014



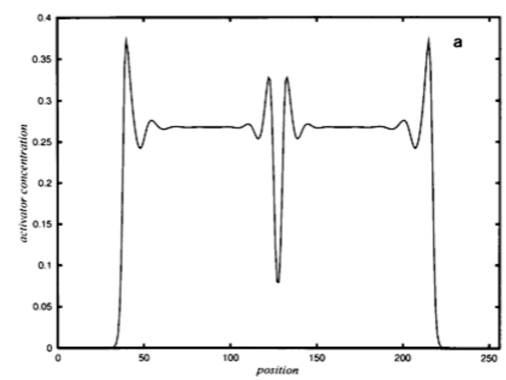


Representative 2-D and 1-D patterns at k=0.0609, F=0.06



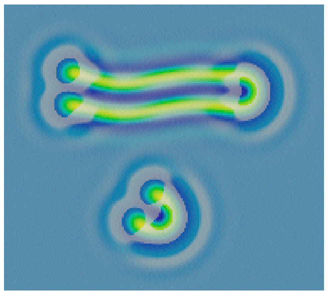
- There are extensive results on the 1-D system based on rigorous mathematical analysis (most are for higher ratios D_U/D_V than in the systems presented here)
- The "spiral wavefront" observed at many parameter values in the 2-D system is also a viable self-sustaining stable moving pattern in the 1-D system at the same parameter values
- For many parameter values that support "negative stripes" in the 2-D system, certain asymmetrical clumps of "negatons" form stable moving patterns in the 1-D system
- Negatons in 1-D were reported (shown) as early as 1996

Single 1-D negaton inside a growing region of solid "blue state" at k=0.06, F=0.05, from Mazin et al. "Pattern formation in the bistable Gray-Scott model" (*Math. and Comp. in Simulation* **40** 1996) fig. 9

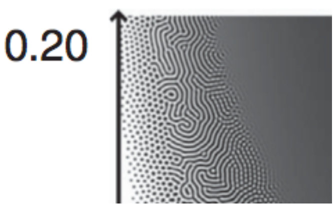


(Note: Non-existence results of Doelman, Kaper and Zegeling (1997) and of Muratov and Osipov (2000) are not applicable because they concern models with a much higher ratio D_U/D_V)

Open Questions

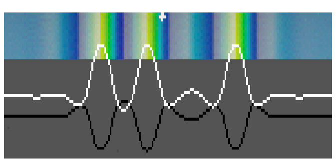

Double-stripe and U

- Why does the U-shaped pattern move and keep its shape?
  - As parameter *k* is increased, leading end of double-stripe (shown) moves faster, but trailing end moves slower and the object lengthens; in the other direction (decreasing *k*) the reverse is true
  - When these two speeds are closely matched, the U shape (shown) neither grows nor shrinks – why?



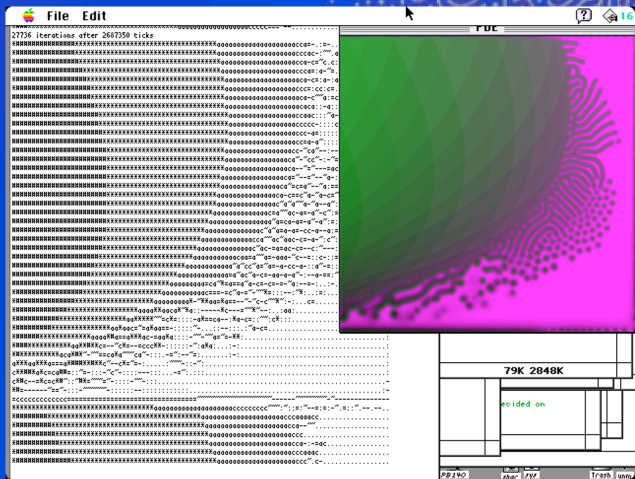
From Miyazawa (ibid. 2010)

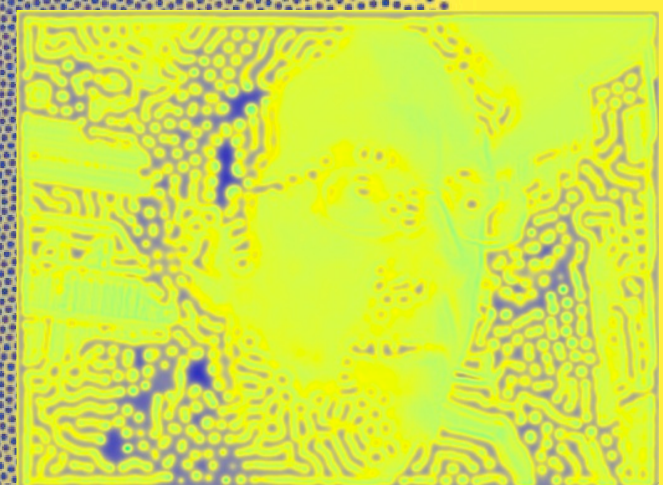
- Do these patterns appear in other reaction-diffusion models?
  - Universal presence of other pattern types suggests this; parameter space maps should make it easy to find; nearby Turing effect is possibly relevant


1-D moving pattern

- Can any of the special properties of these patterns be proven mathematically?
  - 1-D systems seem particularly well suited to this task
  - Shape of negaton "halos" is easy to solve
  - Most existing work applies conditions or limits that exclude the commonly studied D_U/D_V=2 systems

Discussion





Robert Munafo mrob.com/sci
mrob.com/pub/comp/xmorphia
mrob27(at)gmail.com 617-335-1321