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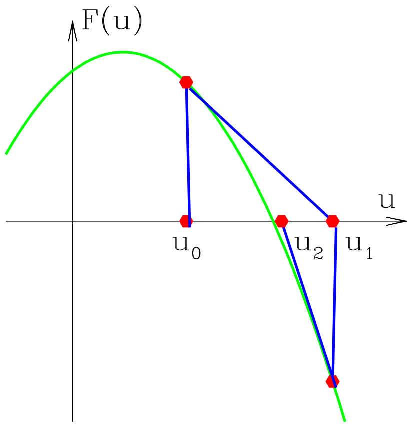
Numerical Methods for Differential Equations in Physics

Time stepping: $\partial_t U = F(U)$

Steady state solving: $0 = F(U)$

Newton's method



$$0 = F(U - u) \approx F(U) - F'(U)u$$

$$\begin{cases} u = F(U)/F'(U) \\ U \leftarrow U - u \end{cases}$$

Newton's Method converges quadratically

$$U_{n+1} = U_n - \frac{F(U_n)}{F'(U_n)}$$

$$F(\overline{U}) = 0 = F(U_n) + F'(U_n)(\overline{U} - U_n) + \tfrac{1}{2}F''(U_n)(\overline{U} - U_n)^2 + \dots$$

$$0 = \frac{F(U_n)}{F'(U_n)} + \frac{F'(U_n)}{F'(U_n)}(\overline{U} - U_n) + \tfrac{1}{2}\frac{F''(U_n)}{F'(U_n)}(\overline{U} - U_n)^2 + \dots$$

$$0 = \frac{F(U_n)}{F'(U_n)} + (\overline{U} - U_n) + \tfrac{1}{2}\frac{F''(U_n)}{F'(U_n)}(\overline{U} - U_n)^2 + \dots$$

$$0 = -U_{n+1} + \overline{U} + \tfrac{1}{2}\frac{F''(U_n)}{F'(U_n)}(\overline{U} - U_n)^2 + \dots$$

$$U_{n+1} - \overline{U} = \tfrac{1}{2}\frac{F''(U_n)}{F'(U_n)}(\overline{U} - U_n)^2 + \dots$$

$$\epsilon_{n+1} = \tfrac{1}{2}\frac{F''(U_n)}{F'(U_n)}\epsilon^2 + \dots$$

Typical sequence: $\epsilon = 10^{-1}, 10^{-2}, 10^{-4}, 10^{-8}, 10^{-16}$

Much faster than timestepping:

$$\begin{aligned} U(t) &= \overline{U} + ce^{-\lambda t} \\ U(t_n) - \overline{U} &= ce^{-\lambda t_n} \\ U(t_{n+1}) - \overline{U} &= ce^{-\lambda(t_n+\Delta t)} = e^{-\lambda \Delta t}(U(t_n) - \overline{U}) \end{aligned}$$

Linear convergence: $\epsilon_{n+1} \sim c\epsilon_n$ **with** $|c| \lesssim 1$ **since** $\Delta t \ll 1$

Typical sequence: $\epsilon = 0.95, 0.95^2, 0.95^3, 0.95^4, 0.95^5 = 0.77$

In addition to converging faster than timestepping,
Newton's method can converge to unstable states.

Secant Method

$$F'(U_n) \approx \frac{F(U_n) - F(U_{n-1})}{U_n - U_{n-1}}$$

Superlinear convergence: $\epsilon_{n+1} \sim \epsilon_n^{1.618}$ **(golden mean)**

Multidimensional Newton's Method

$$0 = F(U - u) \approx F(U) - DF_U u$$

$$\begin{cases} DF_U\ u = F(U) \\ U \leftarrow U - u \end{cases}$$

where

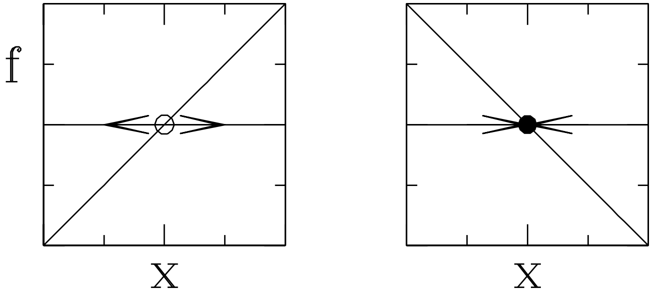
$$[DF]_{ij} \equiv \partial F_i / \partial U_j$$

$DF(U)$ **is the Jacobian matrix evaluated at state** U**.**

$$DF_U u \approx F(U + u) - F(U)$$

Fixed points and linear stability. $\dot{x} = f(x)$

unstable



stable

$0 = f(\bar{x})$ **Fixed point $\bar{x}$**

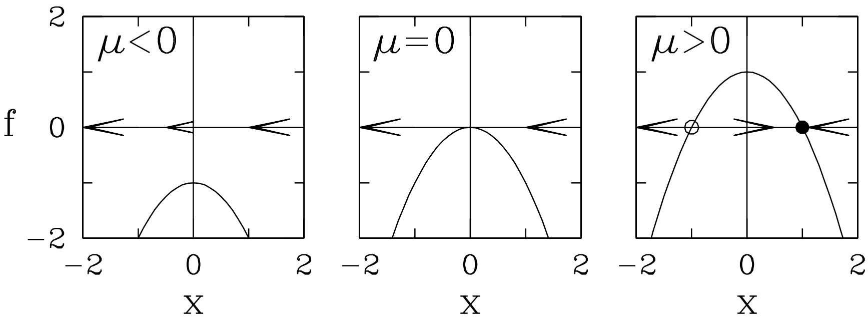
$$\frac{d}{dt}(\bar{x} + \epsilon(t)) = f(\bar{x} + \epsilon)$$

Linear stability of $\bar{x}$

$$\dot{\epsilon} = f(\bar{x}) + f'(\bar{x})\epsilon + \frac{1}{2}f''(\bar{x})\epsilon^2 + \cdots \approx f'(\bar{x})\epsilon$$

$$\epsilon(t) = e^{tf'(\bar{x})}\epsilon(0) \begin{cases} \text{increases if } f'(\bar{x}) > 0 \\ \text{decreases if } f'(\bar{x}) < 0 \end{cases}$$

Saddle-node Bifurcations



$$\dot{x} = f(x) = \mu - x^2$$

Fixed points:

$$\bar{x}_{\pm} = \pm\sqrt{\mu} \qquad \text{for } \mu > 0$$

Stability:

$$f'(\bar{x}_{\pm}) = -2\bar{x}_{\pm} = -2(\pm\sqrt{\mu}) = \mp 2\sqrt{\mu}$$

$$f'(\bar{x}_{+}) = f'(\sqrt{\mu}) = -2\sqrt{\mu} < 0 \implies \bar{x}_{+} \text{ stable}$$

$$f'(\bar{x}_{-}) = f'(-\sqrt{\mu}) = 2\sqrt{\mu} > 0 \implies \bar{x}_{-} \text{ unstable}$$

Newton's method finds steady states independently of their stability

Where might saddle-node bifurcations occur?

Swift-Hohenberg equation

$$\partial_t u = \mu u - \left(q_c^2 + \Delta\right)^2 u - u^3$$

Derived by J. Swift and P.C. Hohenberg (Phys. Rev. A 15, 319 (1977)) to describe pattern formation in convection

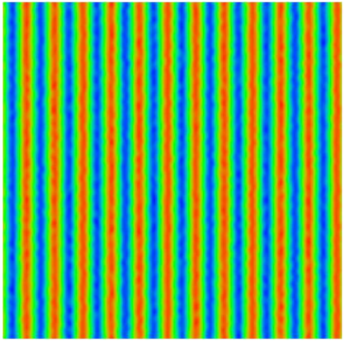
Add quadratic term to obtain hexagons

$$\partial_t u = \mu u - \left(q_c^2 + \Delta\right)^2 u + g_1 u^2 - u^3$$

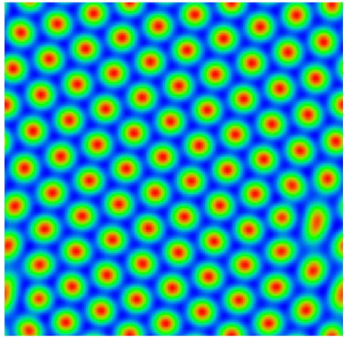
Include q_c and $q_c' = 1$ to obtain quasipatterns

$$\partial_t u = \mu u - \left(q_c^2 + \Delta\right)^2 (1 + \Delta)^2 u + g_1 u^2 - u^3$$

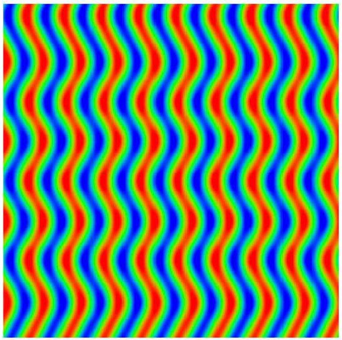
2D Patterns produced by Swift-Hohenberg equation



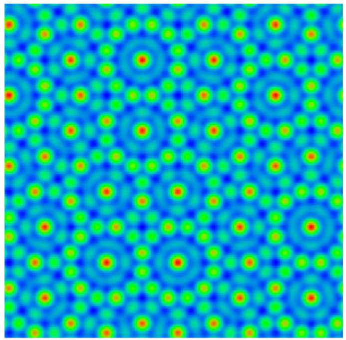
Stripes



Hexagons

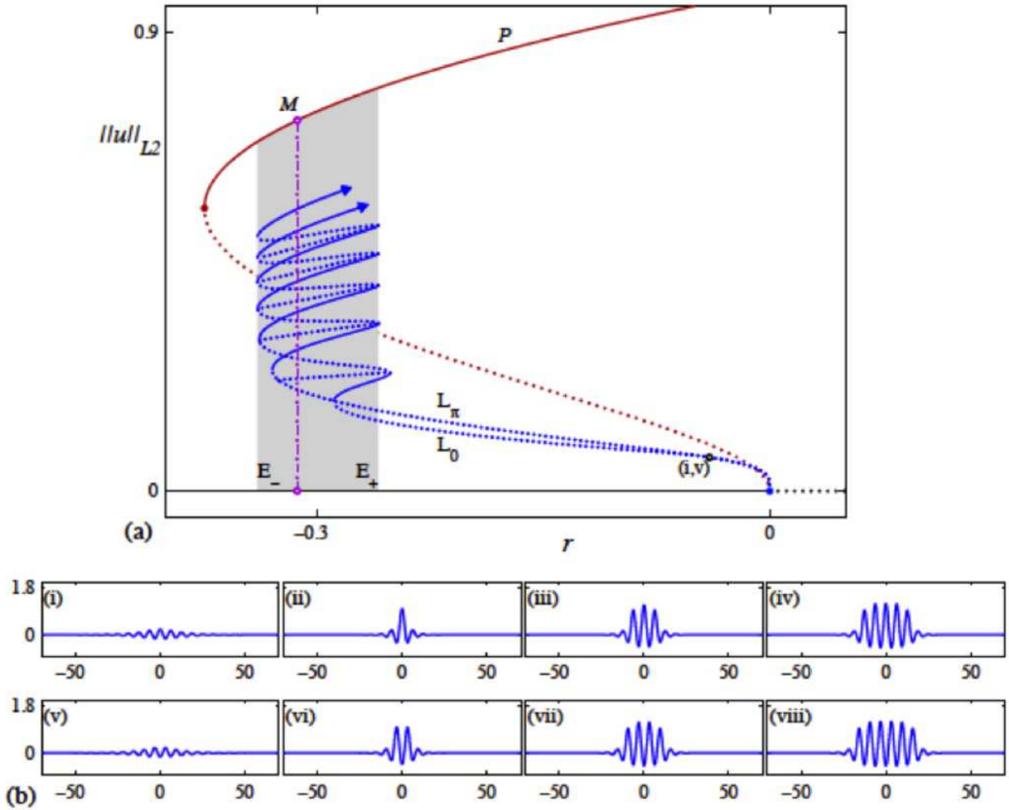


Zigzag instability

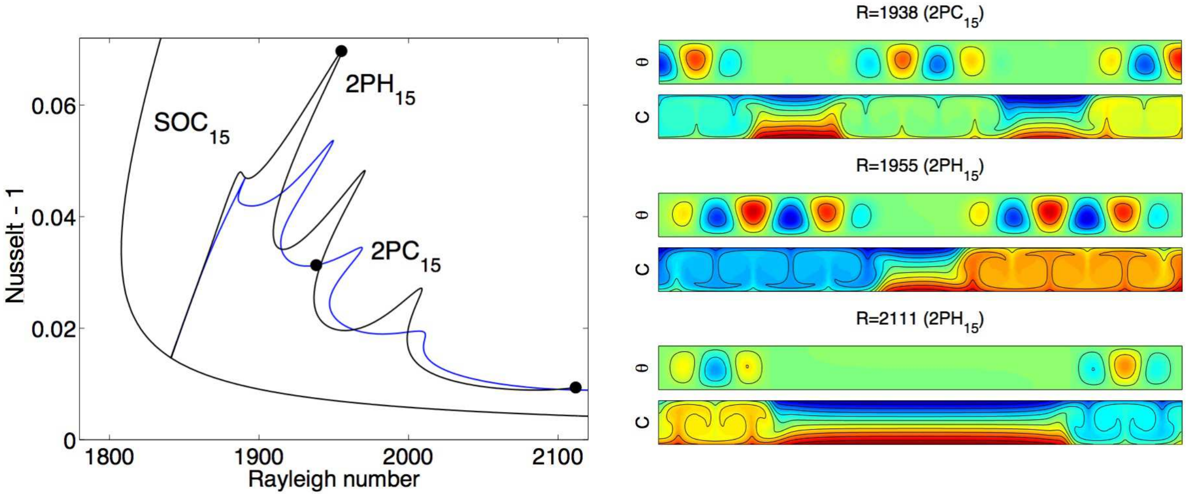


Quasicrystals

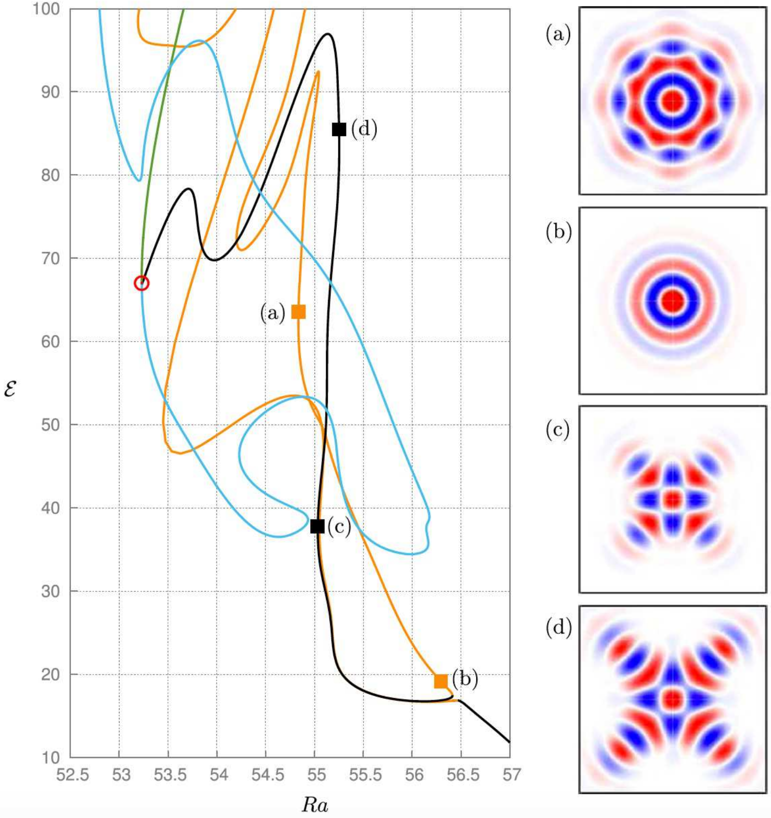
Snaking in 1D Swift-Hohenberg Equation



Thermosolutal Convection: Patterns with 1D snaking



Thermosolutal Convection: Patterns with 2D snaking



Newton's method: example

Swift-Hohenberg equation:

$$\partial_t U = F(U) = \mu U - \left(q_c^2 + \Delta\right)^2 U - U^3$$

Equation for steady state:

$$0 = F(U) = \mu U - \left(q_c^2 + \Delta\right)^2 U - U^3$$

Loop: calculate and compare with ϵ:

$$||F(U)|| \equiv ||\mu U - \left(q_c^2 + \Delta\right)^2 U - U^3|| < \epsilon \ ?$$

If $||F(U)|| \not< \epsilon$, then U not solution, so try $U - u$:

$$0 = \mu(U - u) - \left(q_c^2 + \Delta\right)^2 (U - u) - (U - u)^3$$
$$= \mu U - \left(q_c^2 + \Delta\right)^2 U - U^3 - \left(\mu u - \left(q_c^2 + \Delta\right)^2 u - 3U^2 u - 3U u^2 - u^3\right)$$

Newton step: truncate at first order in u and solve for $u(x)$:

$$\underbrace{\left[\mu - \left(q_c^2 + \Delta\right)^2 - 3U^2\right]}_{DF(U)} u = \underbrace{\mu U - \left(q_c^2 + \Delta\right)^2 U - U^3}_{F(U)}$$

Replace $U \leftarrow U - u$

Solving Linear Systems Ax=b

DIRECT METHOD::

LU decomposition = Gaussian elimination

$$A = LU \qquad O(M^3)$$

$$Ly = b \qquad O(M^2)$$

$$Ux = y \qquad O(M^2)$$

But we are talking about REALLY BIG M, e.g.

$$M = N_x \times N_y \times N_z = 100 \times 100 \times 100 = 10^6$$

There exist fast techniques for Laplacian matrices

But what about Jacobian matrices, which are more general than Laplacians?

ITERATIVE METHODS: MATRIX SPLITTING

$$A = D + L + U$$

Jacobi:

$$Dx^{(k+1)} = b - (U + L)x^{(k)} \qquad O(M)$$

Gauss-Seidel:

$$(D + L)x^{(k+1)} = b - Ux^{(k)} \qquad O(M^2)$$

converges if diagonally dominant or symmetric positive definite

SOR (Successive over-relaxation):

$$(D + \omega L)x^{(k+1)} = \omega b - [\omega(D + U) + D]\, x^{(k)} \qquad O(M^2)$$

Faster convergence than Gauss-Seidel, strategies for choosing ω

ITERATIVE METHODS: KRYLOV SPACE METHODS

Act repeatedly on right-hand-side b

$$\mathcal{K} \equiv \text{span}\{b,\, Ab,\, A^2b,\, A^3,\, \ldots A^{K-1}b\}$$

Represent solution in Krylov space:

$$x \approx \sum_{k=0}^{K-1} c_k A^k b$$

Matrix-vector multiplication: $O(M^2)$
Generating M independent directions $\longrightarrow O(M^3)$

BUT for matrices resulting from PDE discretization
Matrix-vector multiplication takes between $O(M^\alpha)$ with $1 < \alpha < 2$

Find way to require many fewer than M directions

CG (Conjugate Gradient) for SPD (Symmetric Positive Definite) matrix A

$$\text{Minimize } f(x) \equiv \frac{1}{2} x^T A x - x^T b$$

$$f(x) \equiv \frac{1}{2} \sum_{jk} x_j A_{jk} x_k - \sum_j x_j b_j$$

$$\partial_{x_1} f(x) = \frac{1}{2} \sum_{j \neq 1} x_j A_{j1} + \frac{1}{2} \sum_{k \neq 1} A_{1k} x_k + A_{11} x_1 - b_1$$

$$= \sum_j A_{1j} x_j - b_1 = (Ax - b)_1$$

$$\nabla f(x) = Ax - b$$

$$\text{Hessian of } f(x) = A$$

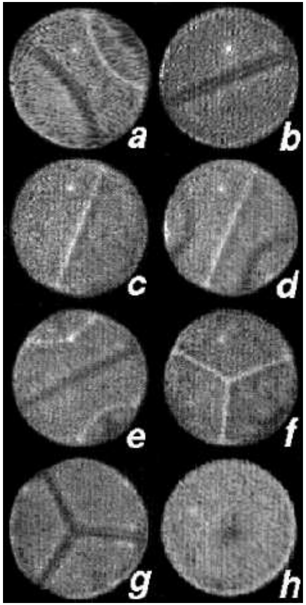
Critical point $\bar{x}$ of f (i.e. such that $\nabla f(\bar{x}) = 0$) is minimum of f if its Hessian matrix A (i.e. such that $A_{ij} = \partial_{x_i x_j} f$) is positive definite.

Generalizations for non-SPD matrices:

GMRES (Generalized Minimal Residual), BCGSTAB (Biconjugate Gradient Stabilized), IDR (Induced Dimension Reduction)

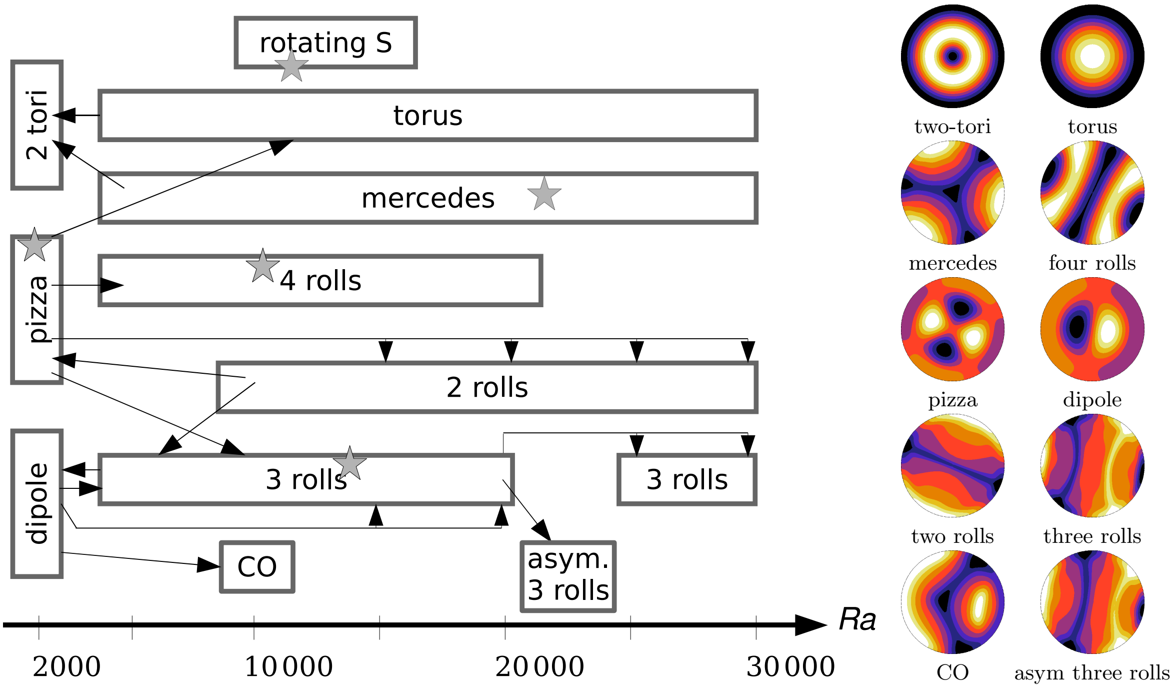
Extreme Multiplicity in Cylindrical Rayleigh-Bénard Convection

with K. Borońska



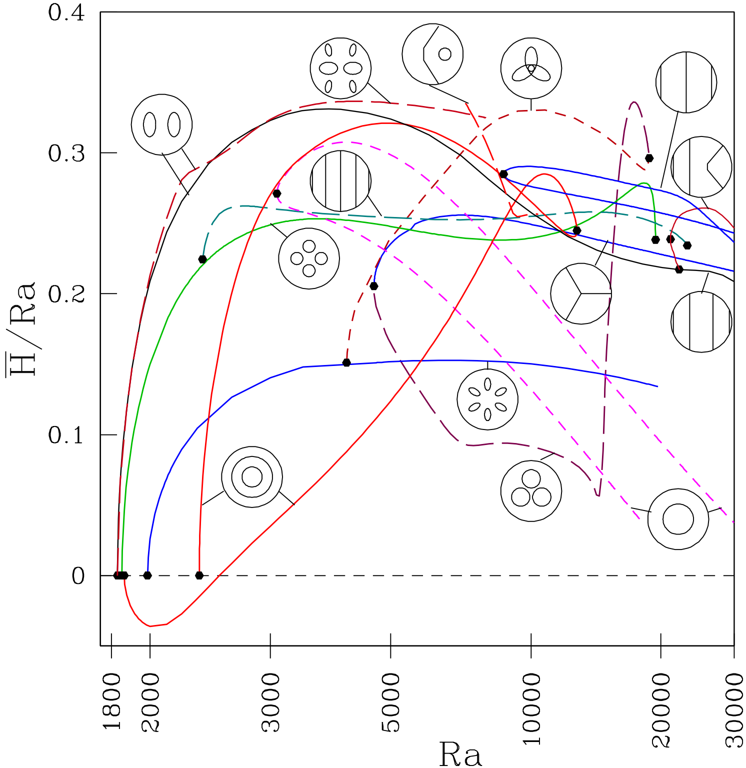
Hof, Lucas & Mullin, Phys. Fluids (1999)

Results from Time-Dependent Simulations

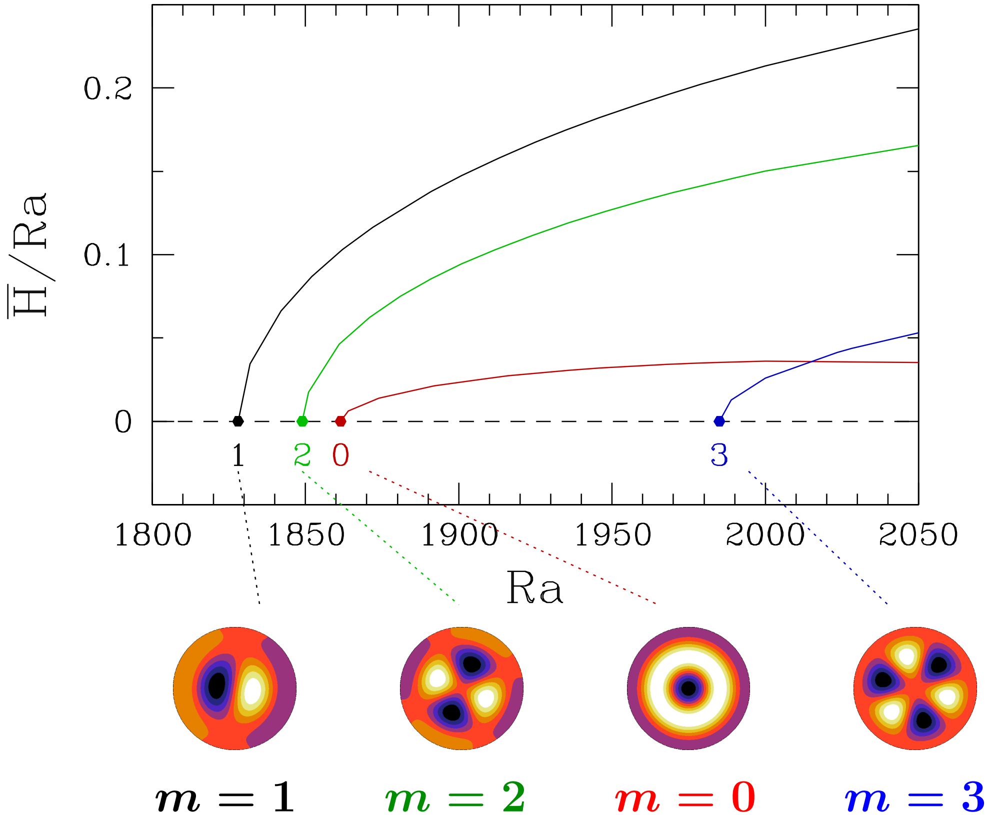


$$(U, V, W, T) = 4 \times N_r \times N_\theta \times N_z = 4 \times 40 \times 120 \times 20 = 384\,000$$

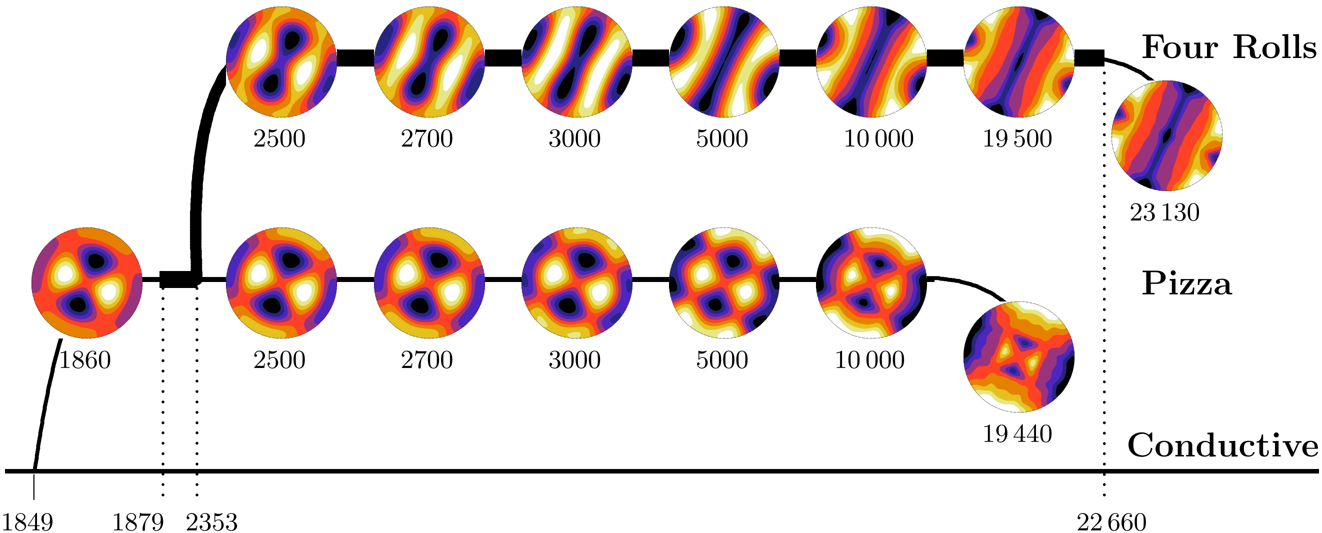
Complete Bifurcation Diagram



Thresholds from Conductive State



Pizza: Bifurcations from $m = 2$ mode



Trigonometric $\Longrightarrow$ *Rolls*

Flowers and Automobiles: Bifurcations from $m = 3$