Microscopic and Macroscopic Rayleigh – Bénard Flows : Continuum and Particle Simulation -- Fluctuations, Time Reversibility, Uniqueness and Lyapunov Instability

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Talk Outline

1. **What is Turbulence ; Why is it important ?**
2. **The Rayleigh-Bénard problem :**
   Dimensionless Control Parameters and Scale Models
3. **Numerical Methods and Results**
   - **Molecular Dynamics**
   - **SPAM**
   - **Fixed-Grid Continuum Mechanics**
4. **Summary, Conclusions, Research Directions**

1.1 Turbulence is Violent --- it is the unsteady and Lyapunov unstable motion of a fluid .

Windmills near LLNL

British Airways Photo

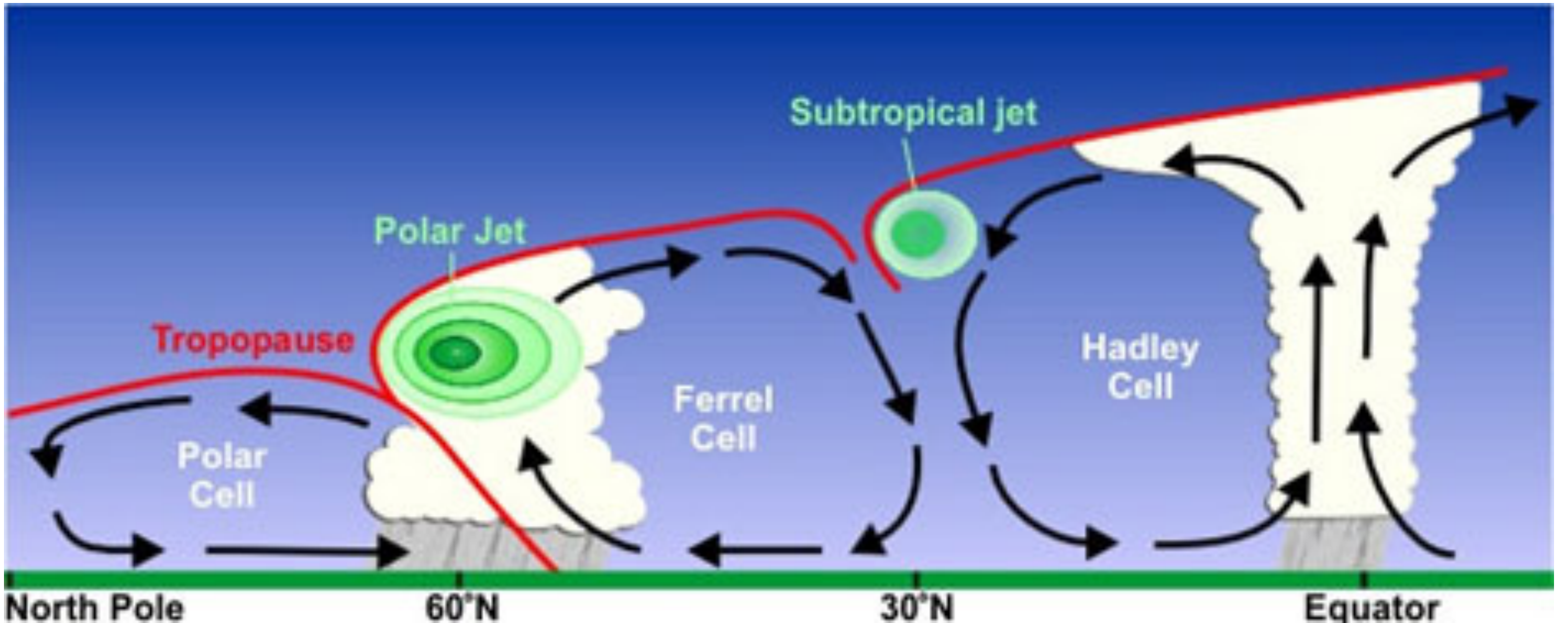
1.2 Cloud Streets off the Coast of Hokkaido

Cumulus clouds 300 meters high and 100 kilometers long ; Japanese Coast Guard photograph .

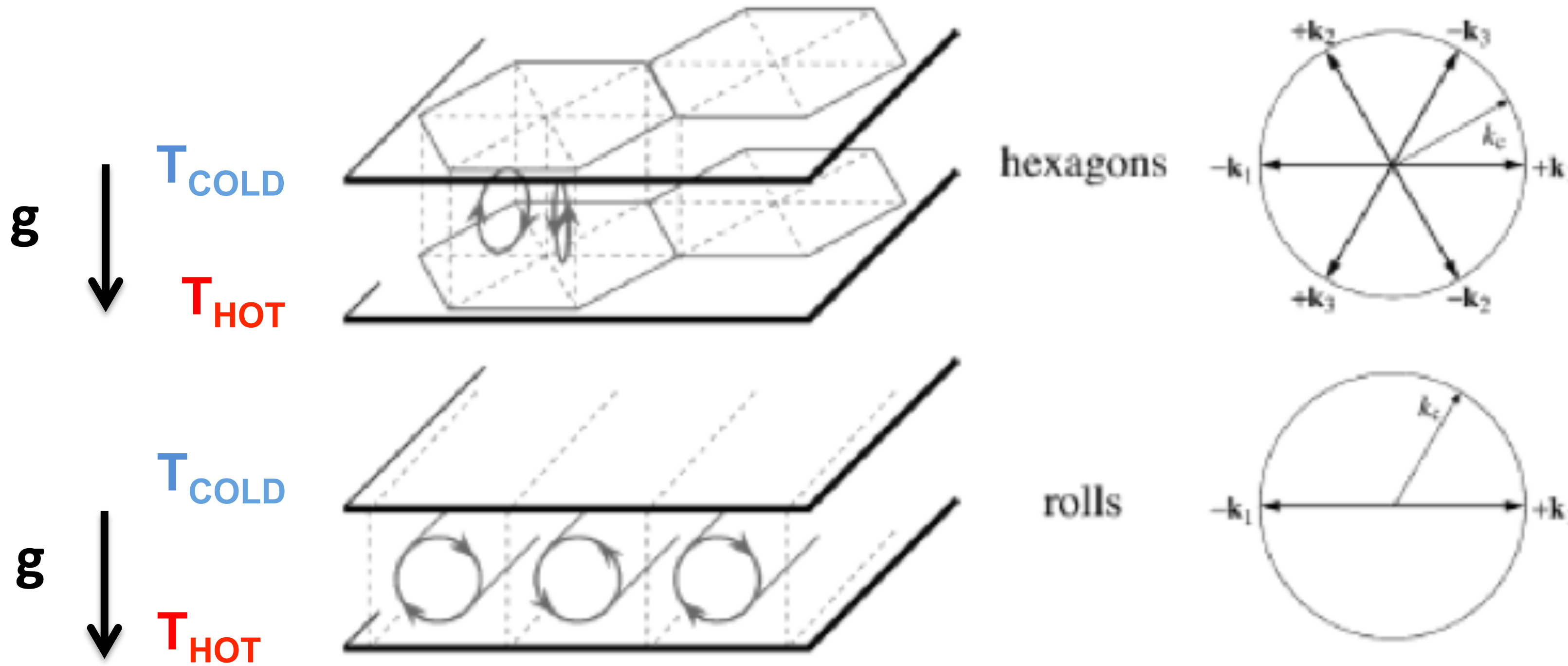
1.3 Turbulence is important in Real-Life situations .

1. Thunderstorms
2. Flow around mountains
3. Jet stream boundary layers
4. Flow in the Earth and Sun

Pictures from NASA Langley Research Center
Printed in Popular Mechanics, August 7, 2009



2.1 Rayleigh-Bénard Flow is a Simpler model problem with which to study Turbulence .



P. Manneville, Rayleigh-Bénard convection, thirty years of experimental, theoretical, and modeling work in Dynamics of Spatio-Temporal Cellular Structures – Henri Benard Centenary Review, 2005.

2.2 Fluid Flow is usefully characterized by several Dimensionless Control parameters

The *Rayleigh Number* $\mathcal{R}$ includes four mechanisms for energy density change with ΔT and g .

1. Gravitational Energy : $\rho g v$, v is flow velocity .
2. Viscous Work : $\eta(v/h)^2$.

   Ratio (1/2) : $gh^2/(v\,\nu)$, where $\nu = \eta/\rho$.

3. Convective Heat Transport: $\rho C \Delta T v/h$.
4. Differential Heat Flux: $\kappa T/h^2$.

   Ratio (3/4) : $vh\Delta T/DT$, where $D = \kappa/(\rho C)$.

Ratio Product : (1/2)(3/4) : $\mathcal{R} = g(\Delta T/T)h^3/(D\nu)$.

2.3 Kolmogorov's famous idea :

Spectrum e(k) [with units of L^3/t^2]
depends upon only two things (for an inviscid fluid) :

energy rate [L^2/t^3] and
wavenumber k [1/L] .

Dimensional Analysis gives the form of the Spectrum :

$$[\ L^3/t^2\ ] = [\ L^2/t^3\ ]^{2/3}[1/L]^{-5/3}$$

There is a 3D ultraviolet catastrophe :
the energy in the range dk is $k^2/k^{5/3} = k^{1/3}$

There is a 2D infrared catastrophe :
the energy in the range dk is $k/k^{5/3} = k^{-2/3}$

2.4 Rayleigh-Bénard Length Scaling

Making Scaled Flow Models, all with the Same Rayleigh Number :

$$\mathcal{R} = gL^3(d\ln V/d\ln T)_P/(\nu D)\ ;$$

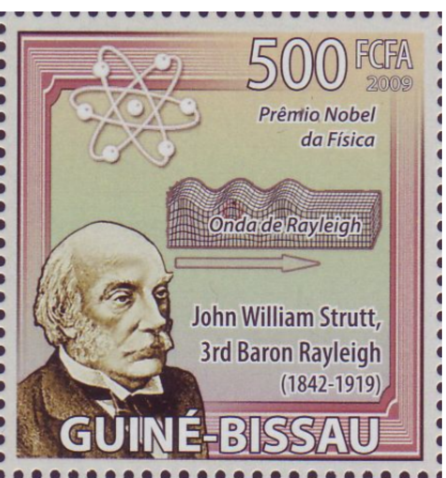
$$P = \rho kT \text{ and constant } \rho \rightarrow g = kT/mL\ ;$$

$$\text{Choose } \Delta T = \langle T \rangle\ ;$$

ν, D proportional to L

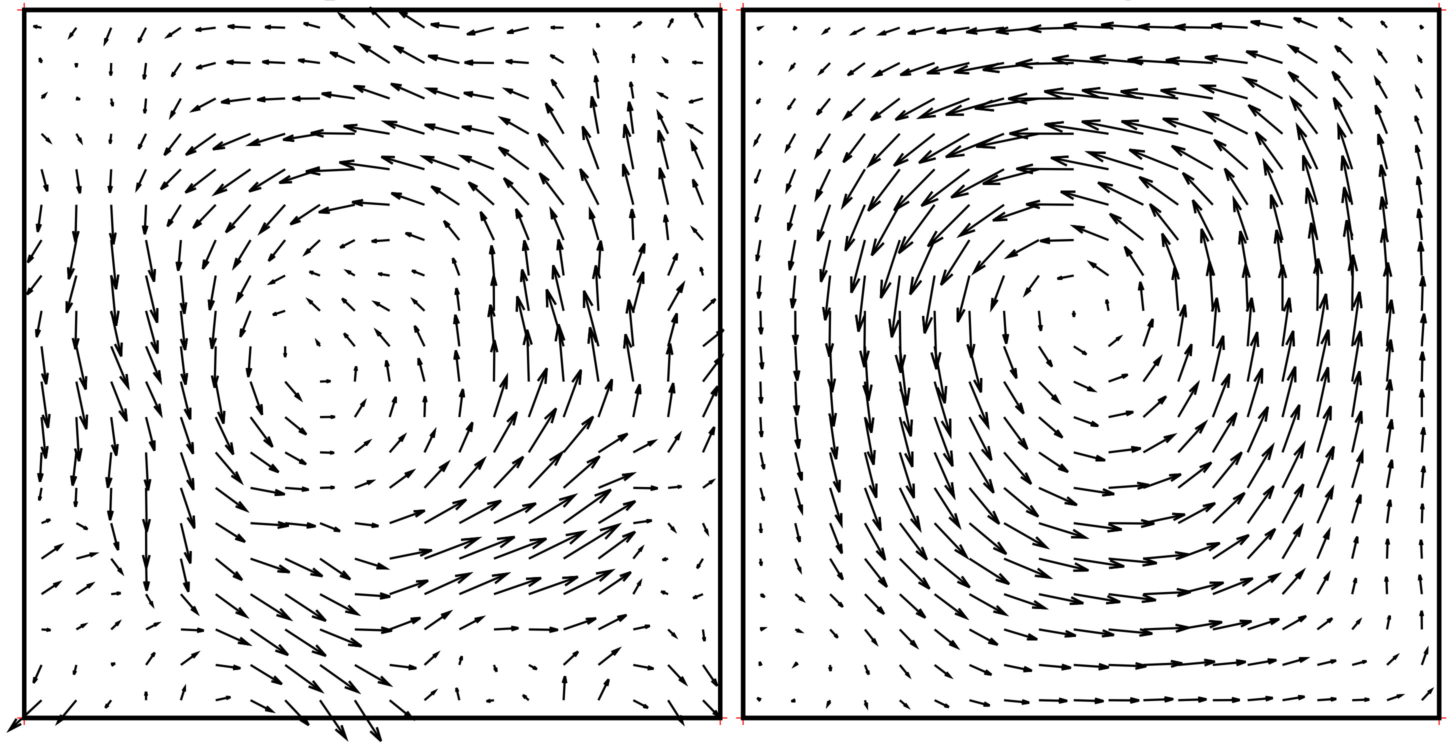
gives

$v(y/L)$, $Q(y/L)$, $\rho(y/L)$



3.1 Numerical Methods and Results: Two-Dimensional Moleculer Dynamics using SPAM for Spatial Averages .

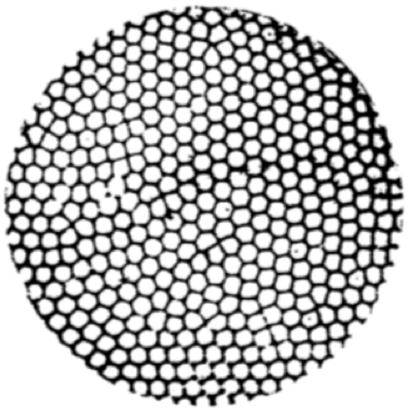
Last Snapshot (N=23,700) Averaged Flow



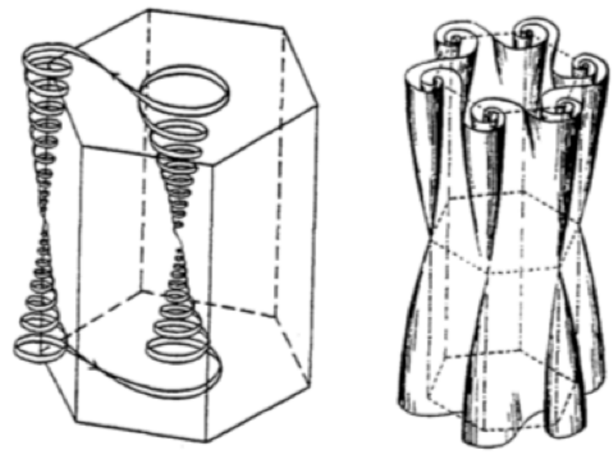
-150 < (x,y) < +150   -150 < (x,y) < +150

Fluctuations dominate Molecular Dynamics , Making Comparisons Complicated .

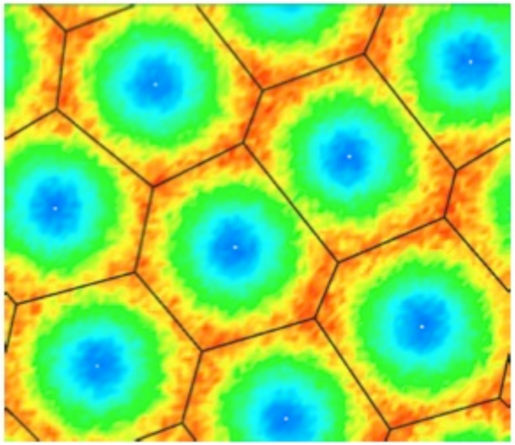
3.2 Rayleigh-Bénard flows in three dimensions can form Hexagonal cells or Longitudinal rolls .



Bénard's experiment

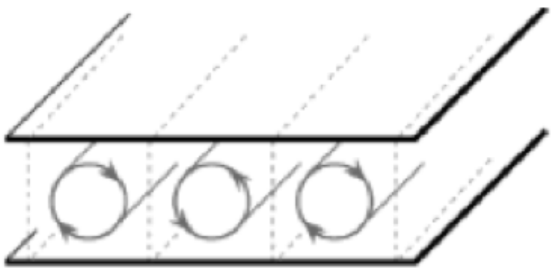


Chandrasekhar

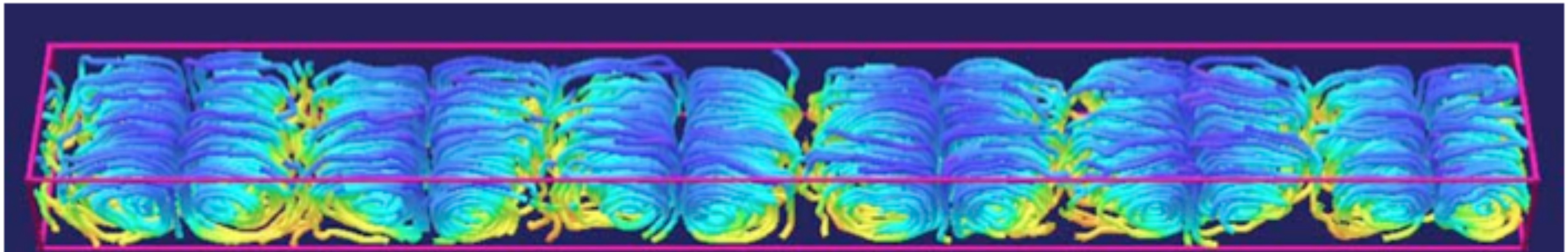


Rappaport

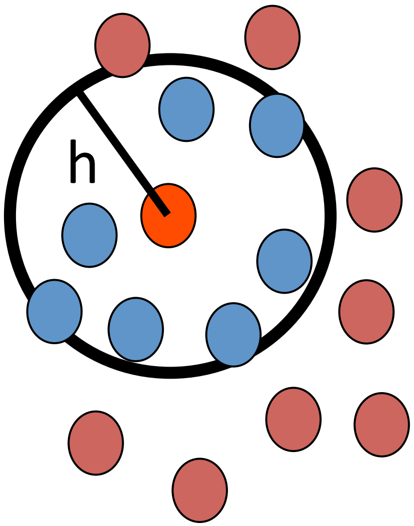
3 507 170 atoms ↑



Rappaport 506 696 particles ↓



3.3 SPAM is a Particle Method .



Particle density from neighbors within a smoothing length

$$\rho_J = \sum_K m_K w(|r_J - r_K|) \;,\; |r_J - r_K| \le h$$

Properties of the weight function:

Normalized; Continuous first and second derivatives

Lucy's weight function

$$w_{2D}(r < h) = (5/\pi h^2)(1 + 3x)(1 - x)^3 \;,\; x = r / h \;; \quad h = 3$$

Function approximation

$$f_R = \sum f_J m_J w_{RJ} / \rho_R \;,\; |r_J - r_K| \le h$$

3.4 Smooth-Particle Equations

Continuity Equation is automatically satisfied.

Equation of Motion:

$$m_J(du_J /dt) = -\sum m_J m_K[(P/\rho^2)_J + (P/\rho^2)_K] \cdot \nabla w_{JK}$$

Energy Equation:

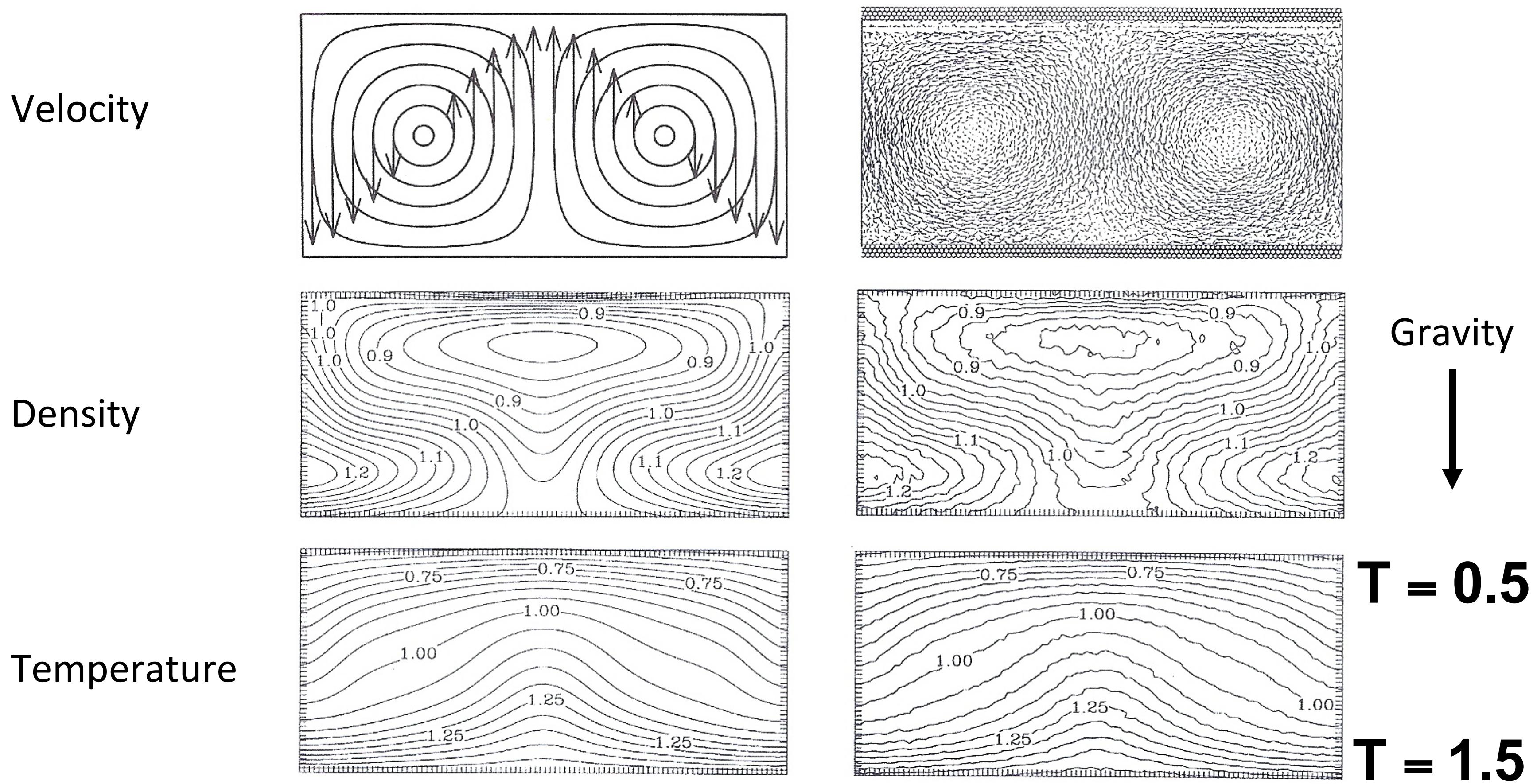
$$m_J(de_J/dt) = \text{heat in} - \text{work done}$$

Work and heat are computed from pressure and gradients of the velocity, temperature, and heat flux .

Time integration with 4^{th} order Runge-Kutta

Wm. G. Hoover, *et ux, SPAM-Based Recipes for Continuum Simulations,* Computing in Science & Engineering, p. 78 (2001) .

3.5 Rayleigh-Bénard Flow (Gravity & T gradient) Finite-Difference (left) & Smooth Particles (right)



Rolls form for $R_c = \frac{gL^4(d\ln T/dy)}{\upsilon D_T}$ **& 5000 smooth particles**

Kum, Hoover, & Posch, PRE 52, 4899-4908 (1995) .

Conclusions:
Molecular Dynamics and SPAM

Molecular Dynamics is *not* Appropriate .

MD requires *both* Time *and* Space Averages .

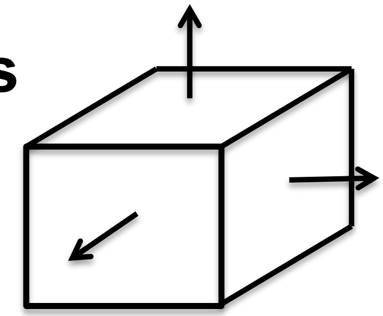
SPAM is Much Better , but still Tedious .

Both Methods are Correct in Principle (only) .

Continuum Mechanics is a Better Way .

3.6 Back to Basics ! Continuum Mechanics from the three Conservation laws .

Mass, momentum, energy flow through surfaces in a fixed volume



Eulerian (fixed frame)

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho u)$$

Lagrangian (comoving frame)

$$\frac{\mathbf{d}}{\mathbf{dt}} = \frac{\partial}{\partial \mathbf{t}} + \mathbf{u} \cdot \nabla$$

Continuity equation

$$d\rho/dt = -\rho\nabla \cdot \mathbf{u}$$

Equation of motion

$$\rho du/dt = -\nabla \cdot \mathbf{P} + \rho \mathbf{g}$$

Energy equation

$$\rho de/dt = -\nabla \mathbf{u} : \mathbf{P} - \nabla \cdot \mathbf{Q}$$

Constitutive equations

$$\mathbf{P} = \mathbf{P}(\rho, e, \nabla u) \; ; \; \mathbf{Q} = \mathbf{Q}(\rho, e, \nabla T)$$

3.7 Newton-Fourier Constitutive Model

Ideal-Gas Equation of State with Newtonian Shear viscosity η and with zero Bulk Viscosity .

$$P_{eq} = \rho e = NkT/V \text{ with } \eta + \lambda = 0 \,.$$

$$P_{xx} = P_{eq} - \eta\,[\,(du_x/dx) - (du_y/dy)\,]$$

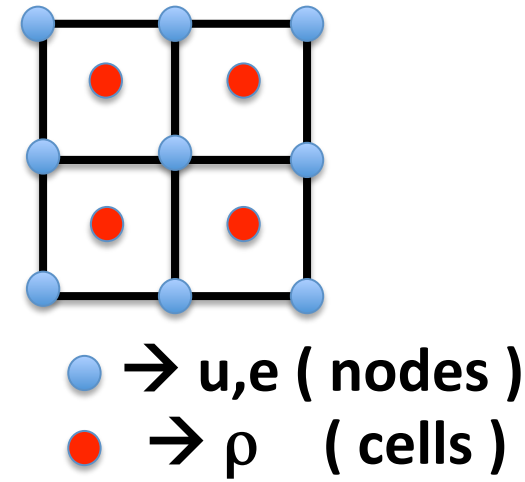
$$P_{yy} = P_{eq} - \eta\,[\,(du_y/dy) - (du_x/dx)\,]$$

$$P_{xy} = -\eta\,[\,(du_x/dy) + (du_y/dx)\,]$$

$$Q_x = -\kappa\,(dT/dx)$$

$$Q_y = -\kappa\,(dT/dy)$$

3.8 Finite-Difference Method



0. [Single-Grid Solutions are not Stable .]
1. Use Linear Interpolation throughout .
2. Use Centered Differences for (u,e) Gradients .
3. Get P and Q from the (u,e) Gradients .
4. Get Gradients for the (ρ,u,e) Evolutions .
5. Integrate (ρ,u,e) with Runge-Kutta Integration .

3.9 Simplest Possible Numerical Approach

Ideal gas: $P = \rho kT = \rho e$ L x L box

$$\rho g = -dP/dy = -\rho k dT/dy \longrightarrow g = [T_{hot} - T_{cold}]/L$$

Boundary Values

$$u_x = u_y = 0 \;;\; e = [T_{hot} + T_{cold}]/2 + (y/L)[T_{cold} - T_{hot}]$$

$$\mathcal{R} = gL^4 (d\ln T/dy)/\nu D_T$$

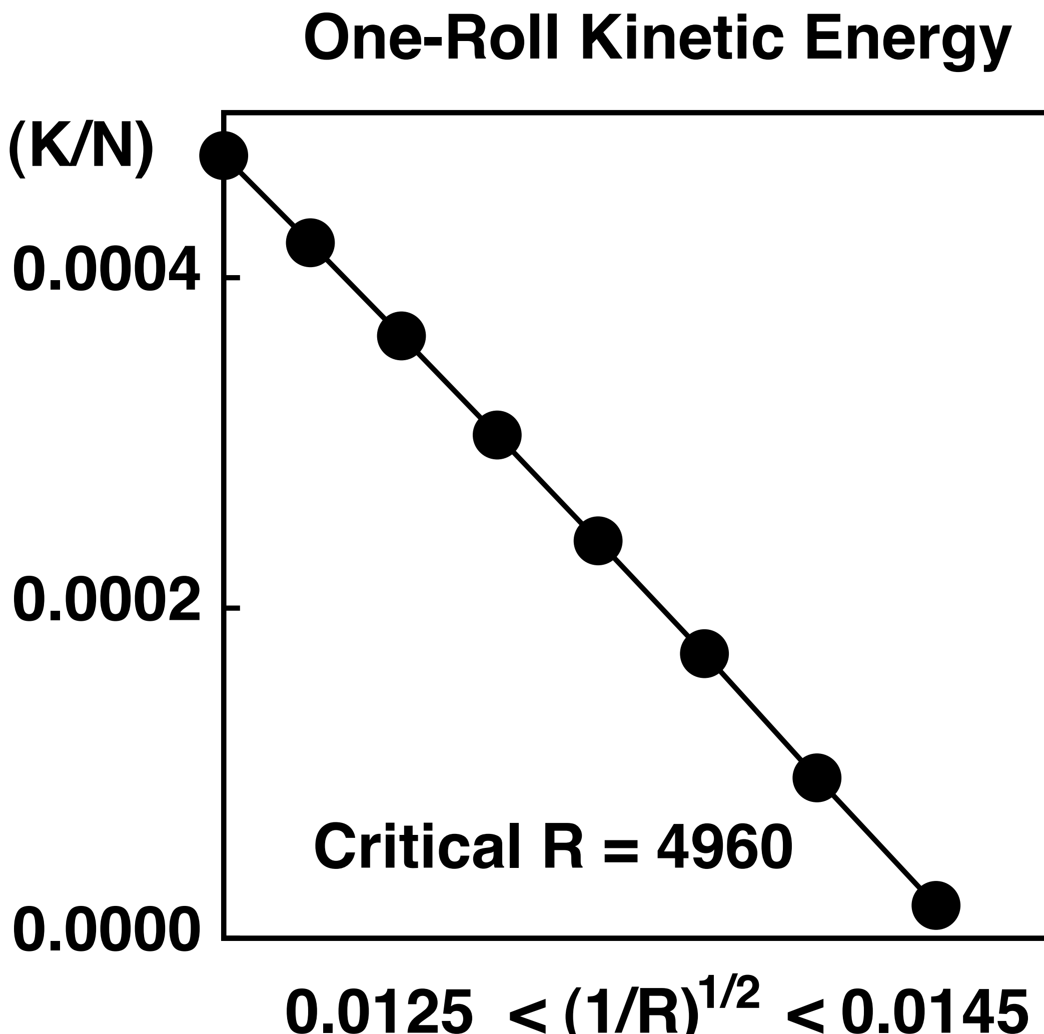
Choose $T_{hot} = 1.5$ $T_{cold} = 0.5$; $T = 1.0$

$$\mathcal{R} = gL^3/\nu D_T$$

Note: We can scale up the problem size (L) by keeping the Rayleigh number the same , changing either temperature or transport properties .

3.10 Results: Critical Rayleigh Number

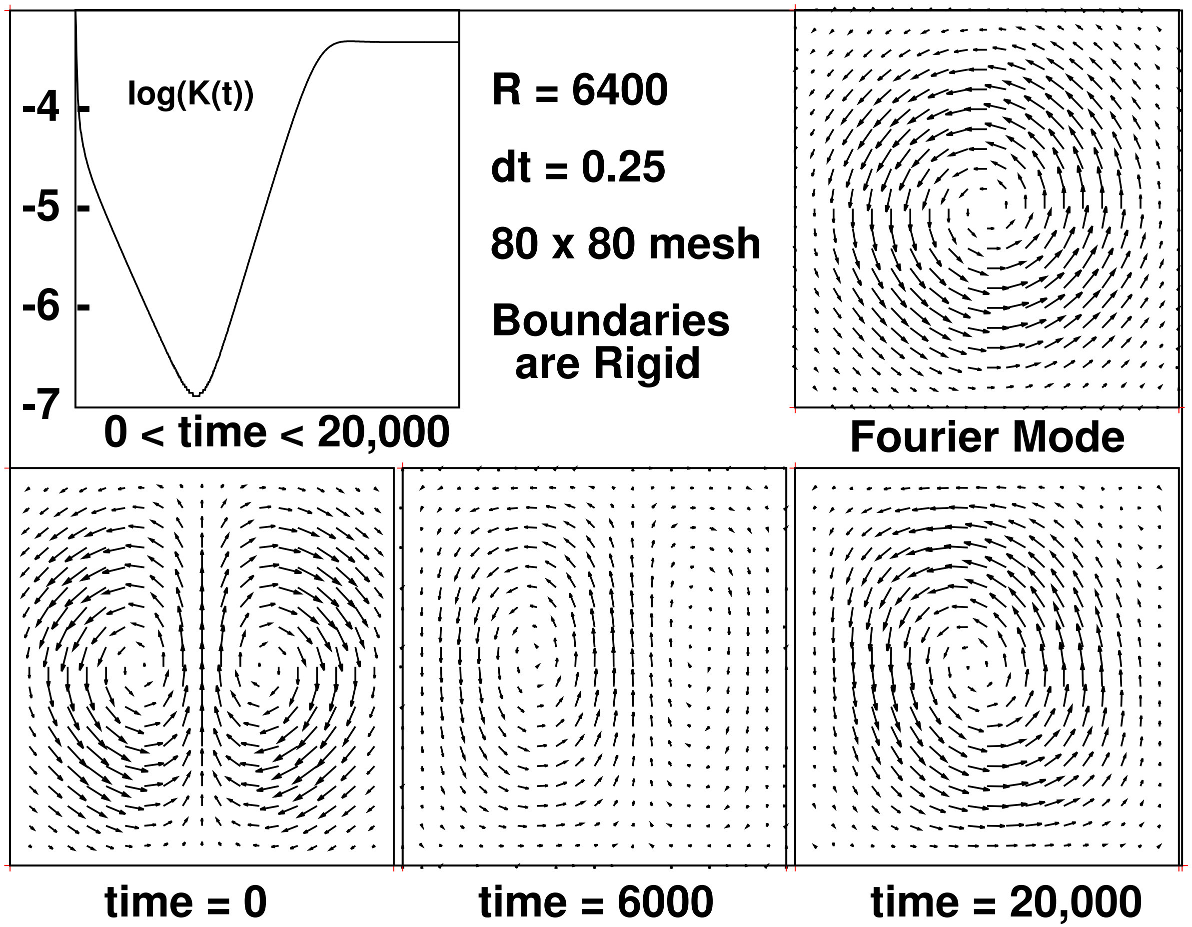
The "Critical" Rayleigh number for Convection gives A Linear variation of Kinetic energy with $(1/\mathcal{R})^{1/2}$.



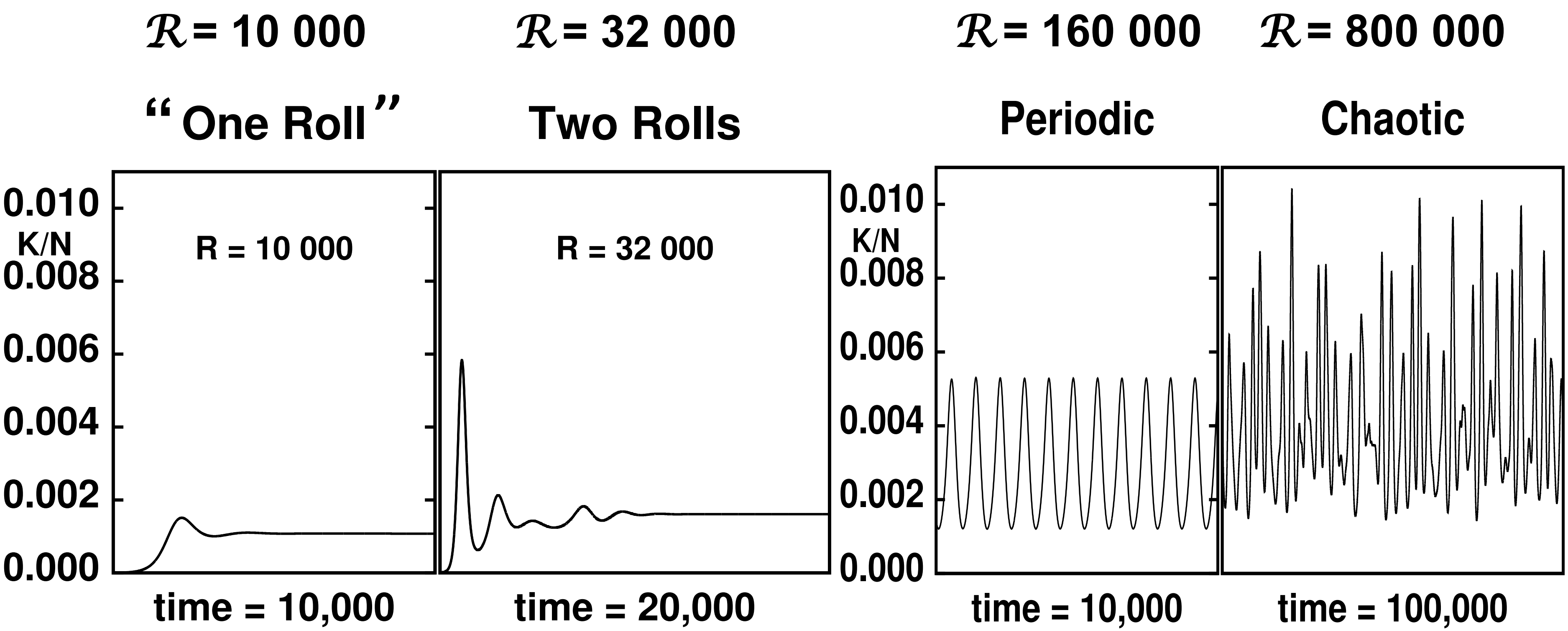
3.11 Comparison: Analytic Mode with Simulation

Lowest k Fourier mode :

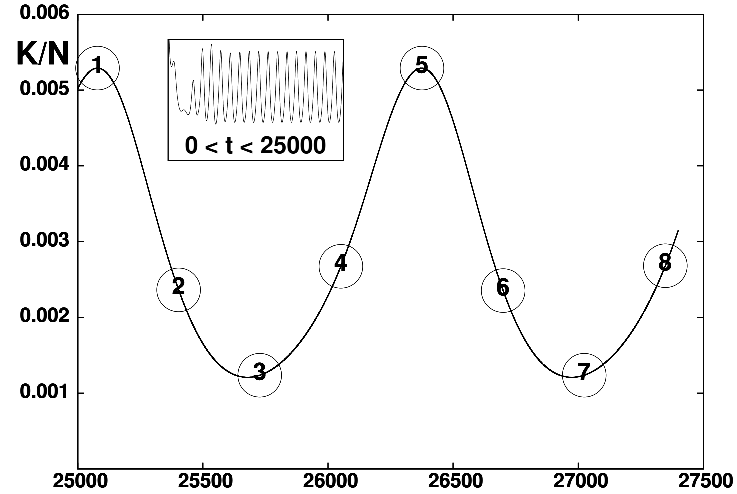
$$\{ u_x \propto \cos(kx)\sin(2ky) \; ; \; u_y \propto -\sin(2kx)\cos(ky) \} \; ; \; k \equiv (\pi/L)$$



3.12 Kinetic energy as a function of $\mathcal{R}$ reveals degeneracy [multiple solutions] .

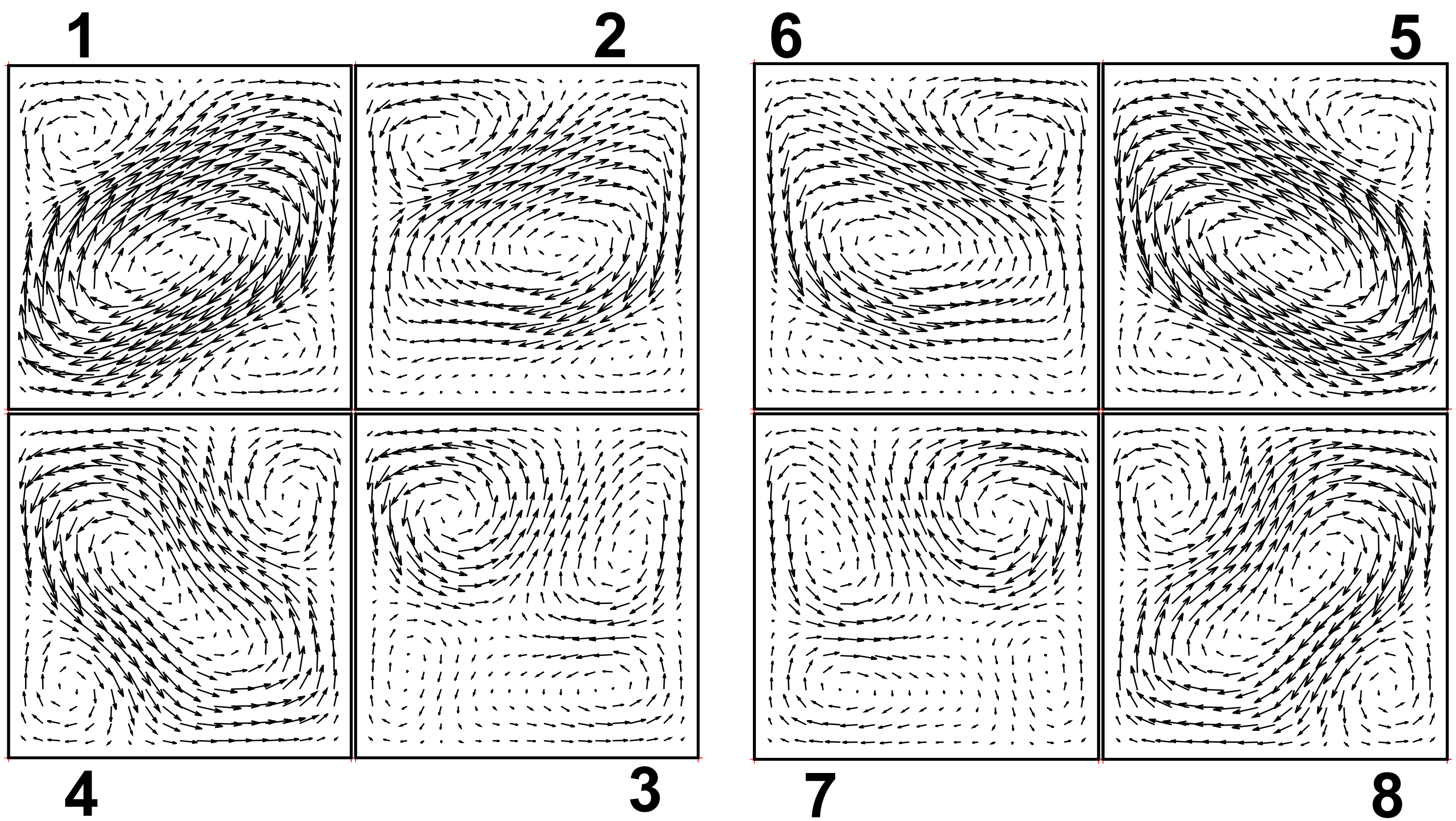


3.13 PERIODIC SOLUTIONS

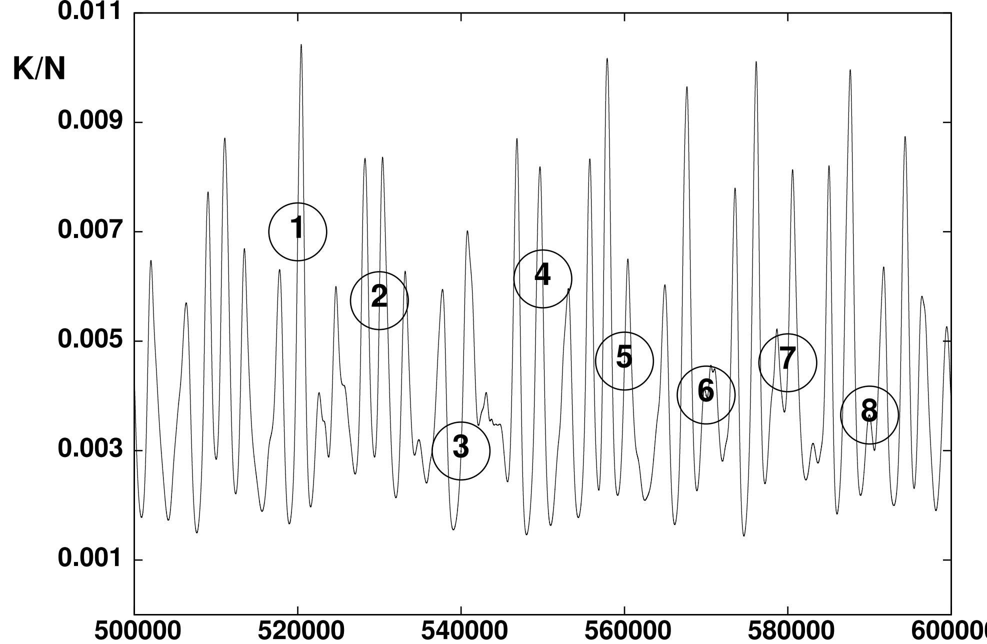


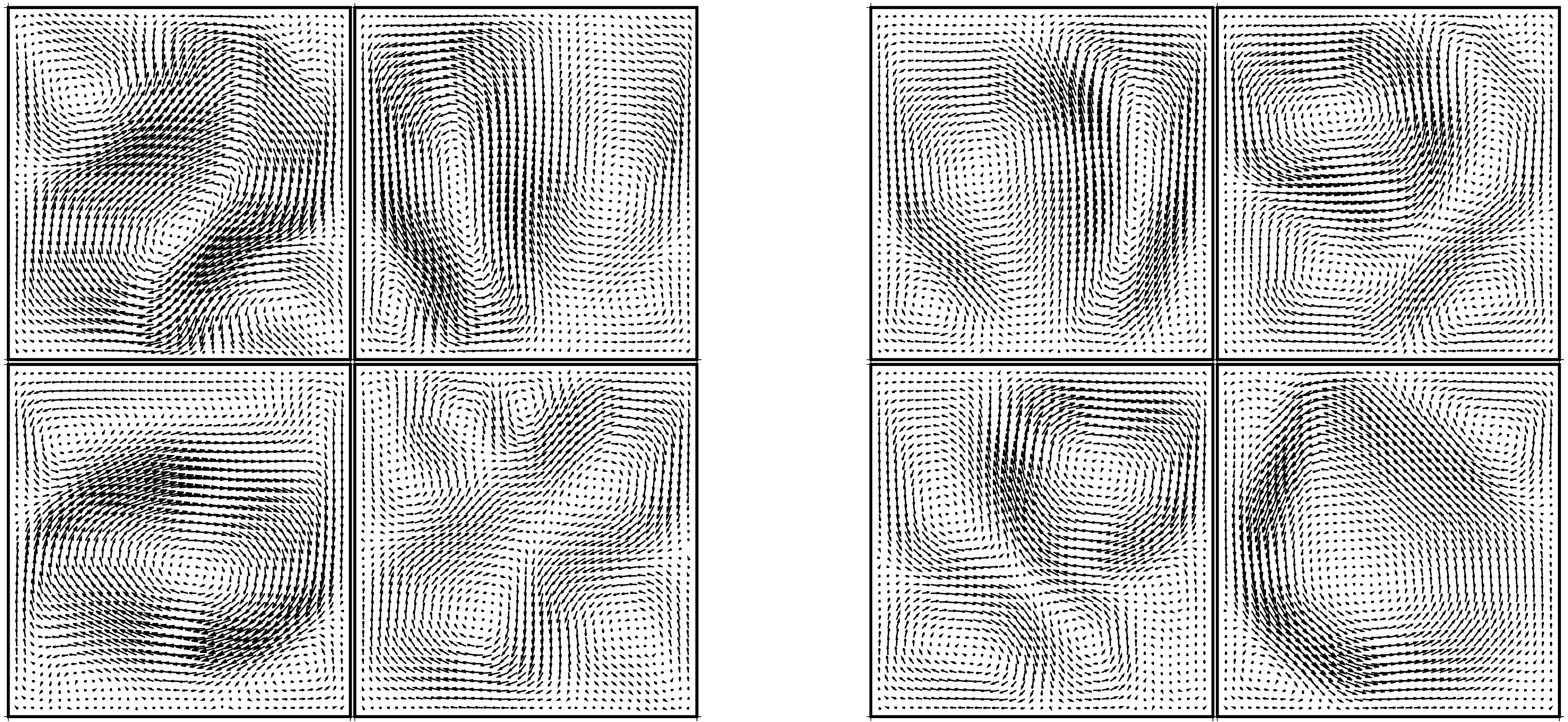
Periodic solutions display mirror symmetry.
At $\mathcal{R}$ = 160 000 the period is 2596.

Morphologies below correspond to points labeled on the kinetic energy curve.



$\mathcal{R}$ = 800 000 ; Is this chaotic?





3.14 How do the solutions depend on $\mathcal{R}$?

There are at least five different solution types :

1. **Static (below the critical $\mathcal{R}$) ,**
2. **“1-roll” stationary ,**
3. **2-roll stationary , perhaps “2-roll” ,**
4. **multiple roll periodic ,**
5. **multiple roll chaotic(?)**

[2 and 3 Coexist when $\mathcal{R}$ = 21,000 .]

How do Solutions depend on the mesh ? How can we locate Regions where the relative stabilities change ?

3.15 How do the solutions depend on $\mathcal{R}$?

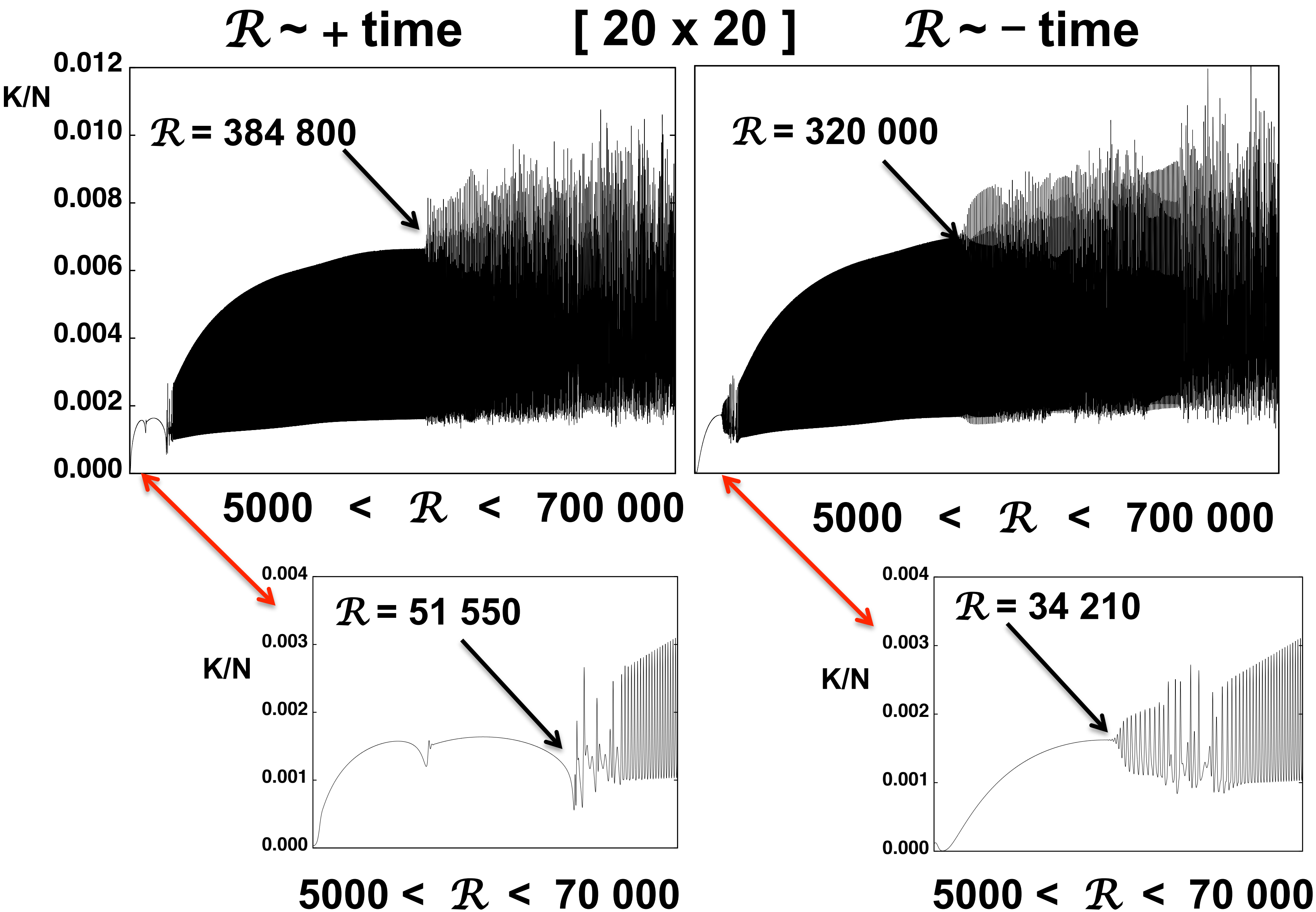
Maximum $\mathcal{R}$ for a given Mesh :

715K	810K	840K	860K	905K	940K
16x16	24x24	32x32	48x48	64x64	96x96

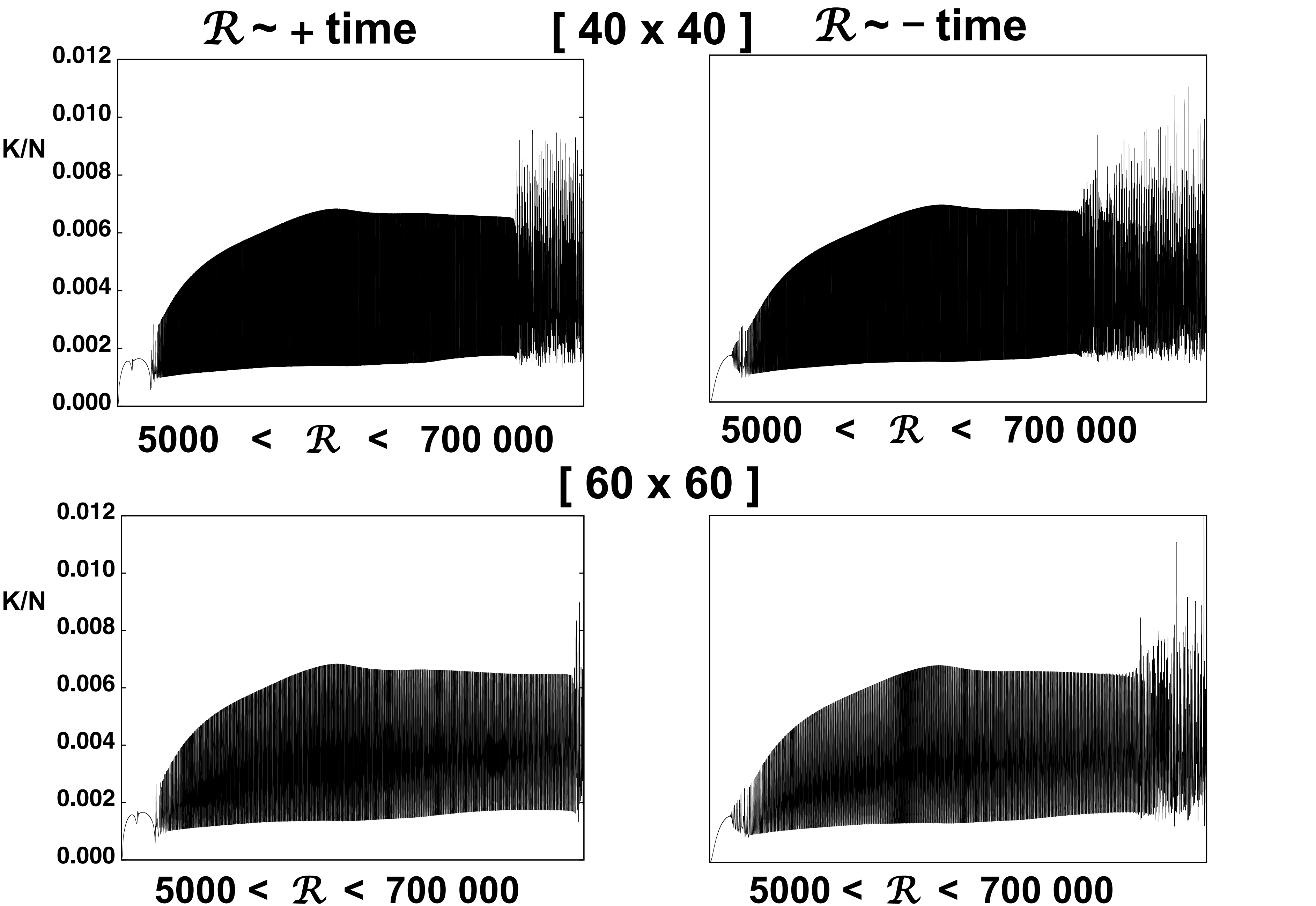
Searching for Morphological Changes :

- **Use (K/N) versus $\mathcal{R}$ to find $\mathcal{R}_c$**
- **Make $\mathcal{R}$ a function of *time* .**
- **Check the *reversibility* of the path .**
- **Check the *mesh size dependence* .**
- **Check the *rate dependence* .**

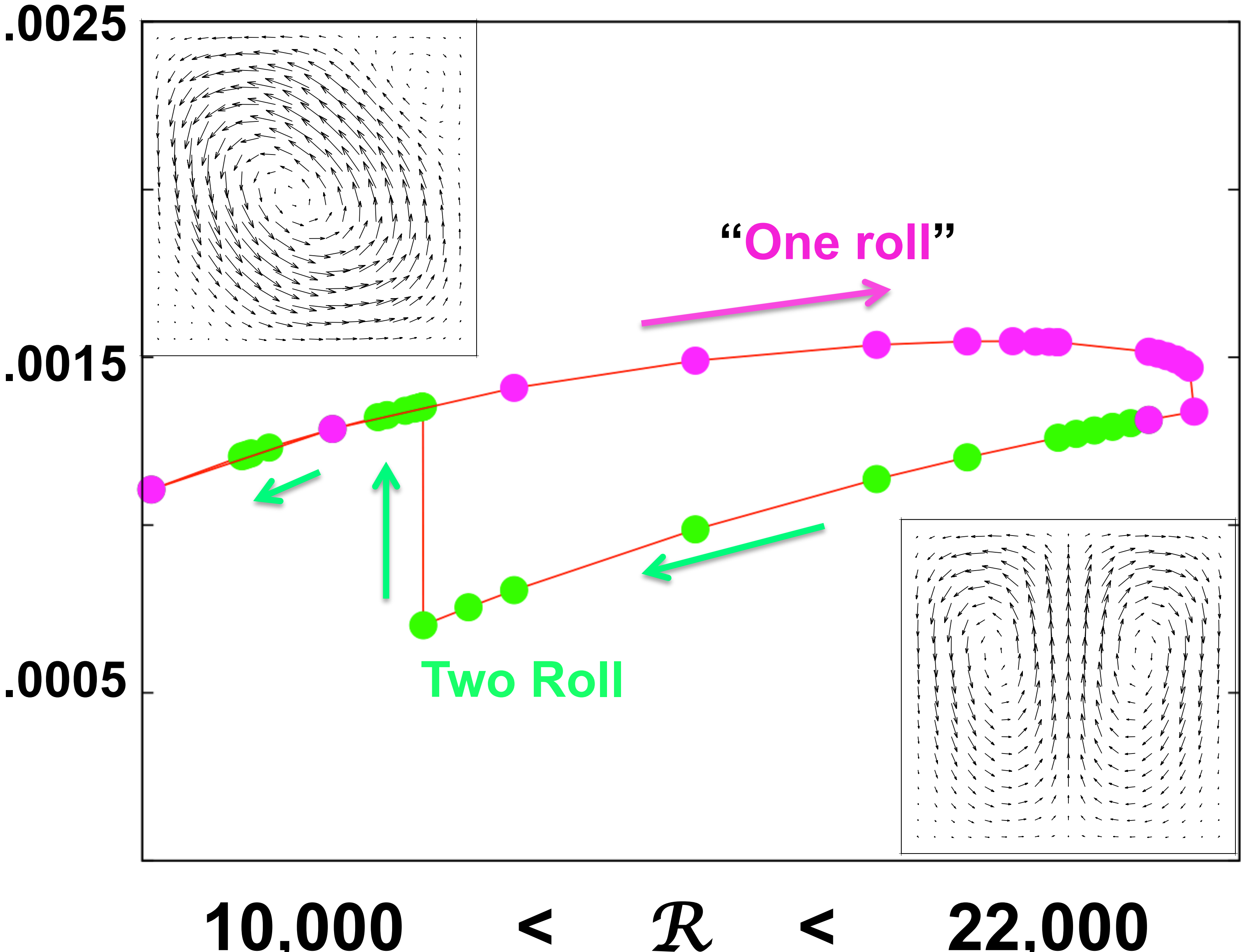
3.16 Vary $\mathcal{R}$ with time. Use the kinetic energy (K/N) profile to characterize the solution . Compare with finer mesh solutions .



3.16 Kinetic Energy Profile Dependence on Mesh .



3.17 K($\mathcal{R}$)/N Exhibits Hysteresis .

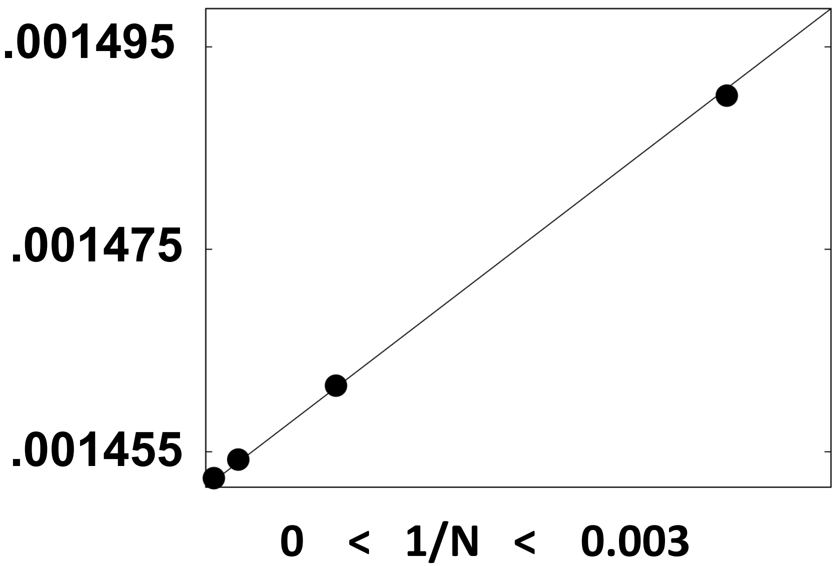


3.17 Mesh Convergence Tests, $\mathcal{R}$ = 16,000

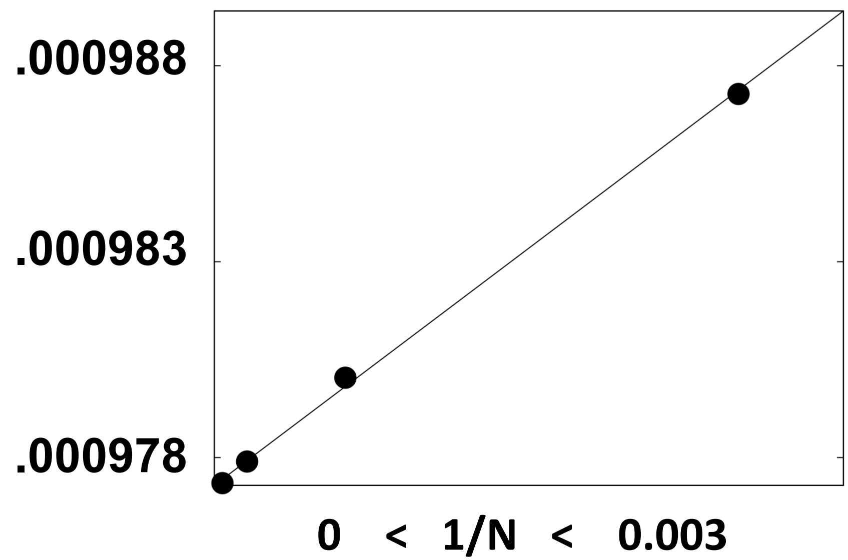
Solutions converging to machine accuracy show that the kinetic energy varies linearly with the inverse of the system size for system sizes .

{ 20 x 20 , 40 x 40 , 80 x 80 , 160 x 160 }

"One-Roll" Convergence



Two-Roll Convergence



Kinetic Energy in the continuum limit is (K/N) = 0.00145150 .

Kinetic Energy in the continuum limit is (K/N) = 0.000977293 .

3.18 Time averages reveal a 4-roll solution

$\mathcal{R}$ = 800 000

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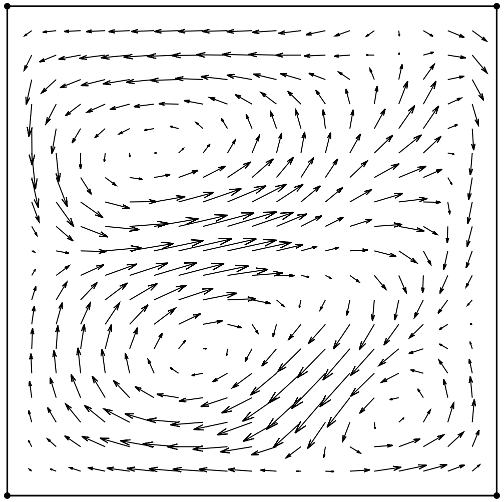

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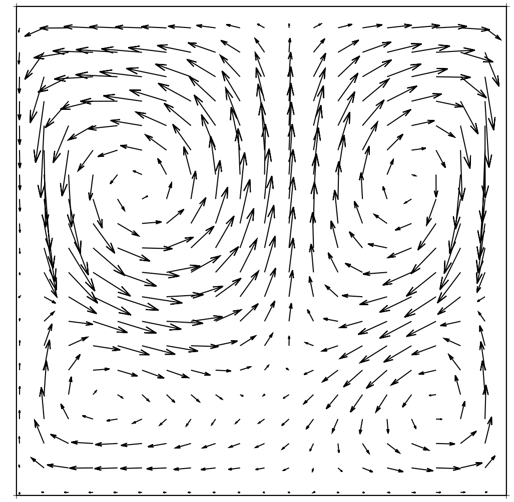

$\mathcal{R}$ = 160 000 ; Mirror Symmetry

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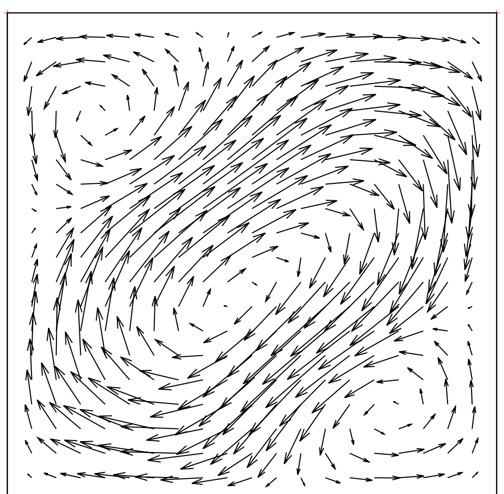

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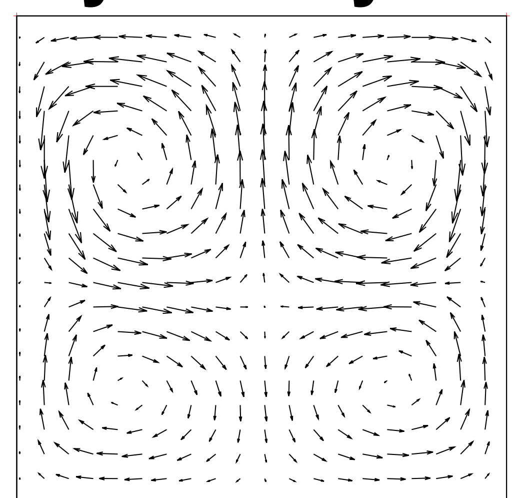


3.19 Summary of These Results

1. **Use $\mathcal{R}$(t) to generate a K($\mathcal{R}$) profile;**

   Check Rate and Mesh dependence .

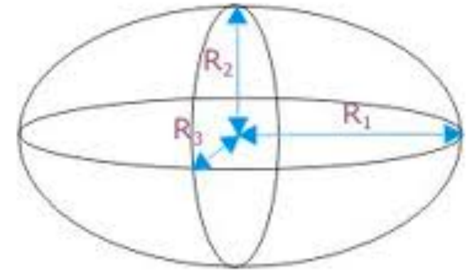
2. **Time averaged solutions reveal the underlying solutions as :**

   "1-roll" , 2 roll , and 4 roll .

3. **"One-" and two-roll stationary solutions coexist at the same $\mathcal{R}$ and form a hysteresis loop .**

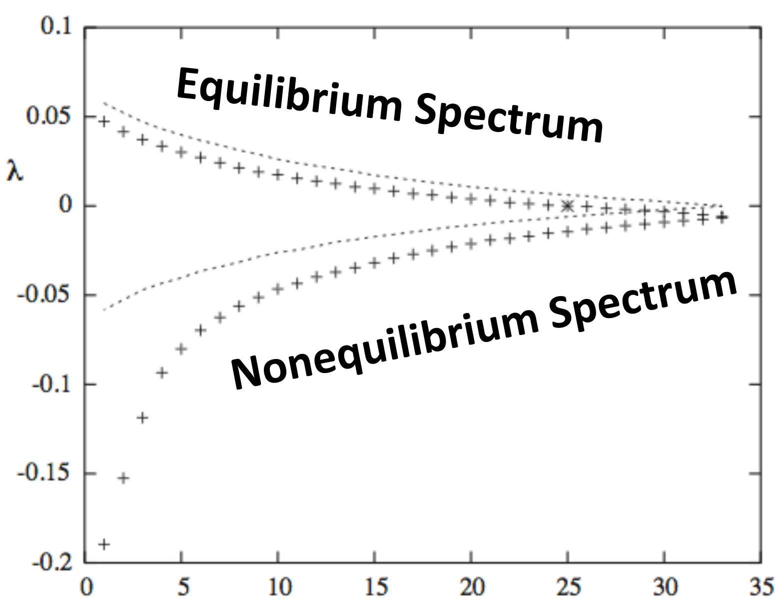
   Different approaches to the starting conditions make it possible to generate one- or two-roll stationary solutions for the same $\mathcal{R}$.

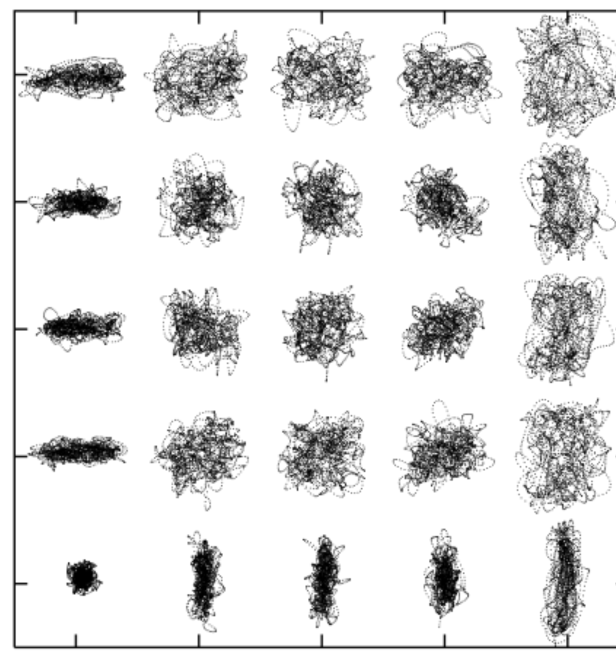
Lyapunov Instability



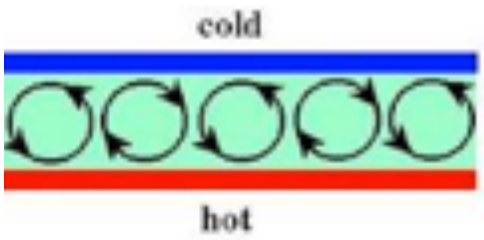
$$\delta = \delta_0 e^{+\lambda t}$$

In Molecular Dynamics with N Degrees of Freedom there are 2N Exponents Defining the Phase-Space Growth Rates. In Continuum Mechanics there is an Infinite Number!





3.20 Scale Models with Fixed Temperatures



$0.5 < T < 1.5$; $< \rho > = 1$;

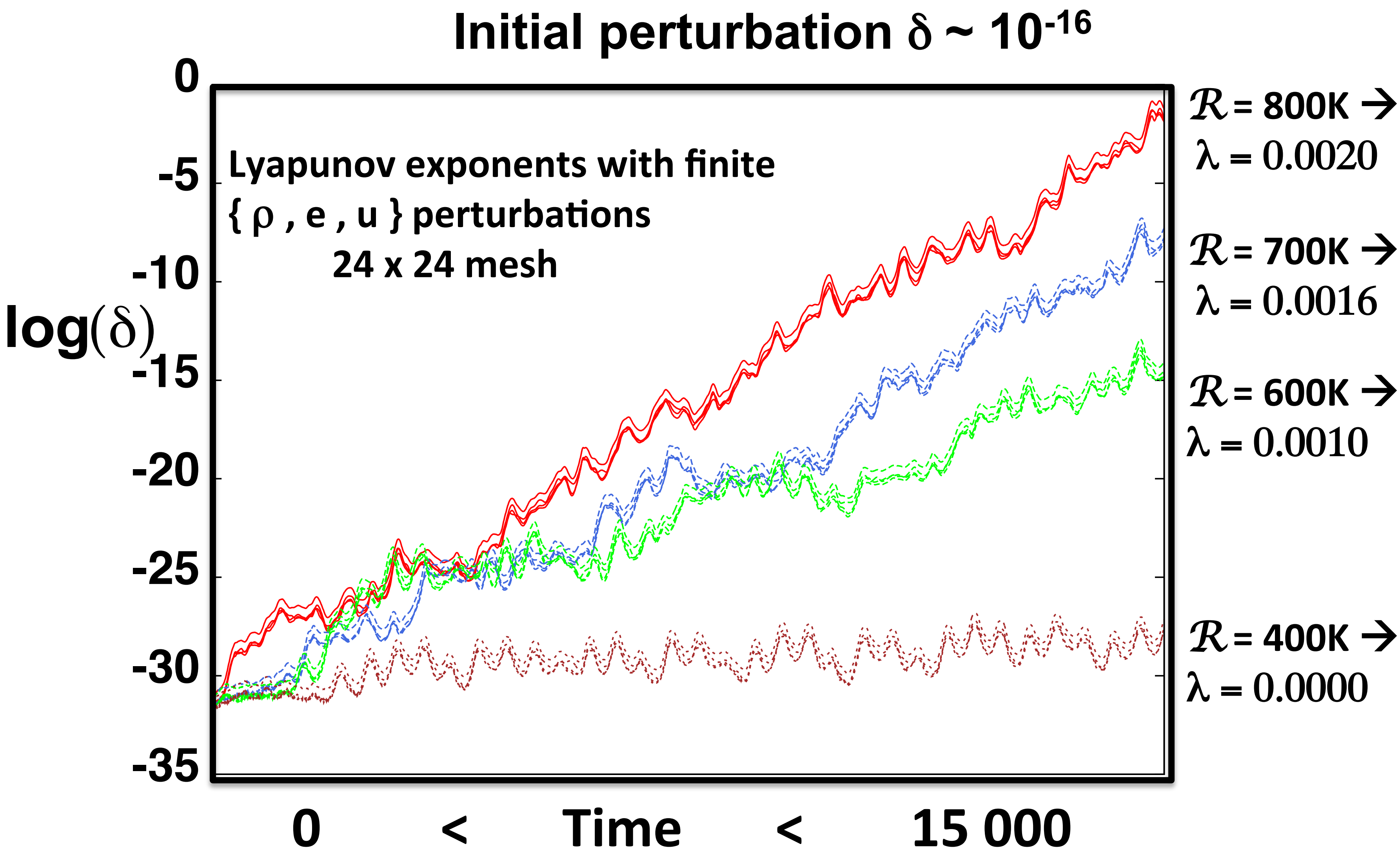
$g = 1/L$; $R = L^2/(\nu D)$

The flow variables depend upon space and time :

$\{ \rho(y/L), v(y/L), T(y/L) , P(y/L) , Q(y/L) \}$ with $L \approx \tau$

The transport coefficients are proportional to L so that the fluxes match and transit times are proportional to L . The time required for any feature to double in size is likewise proportional to L . Thus the Lyapunov spectrum of e-folding rates are frequencies ; $\{ \lambda \}$, varies as $(1/L)$.

3.21 Calculate separation from a reference trajectory .



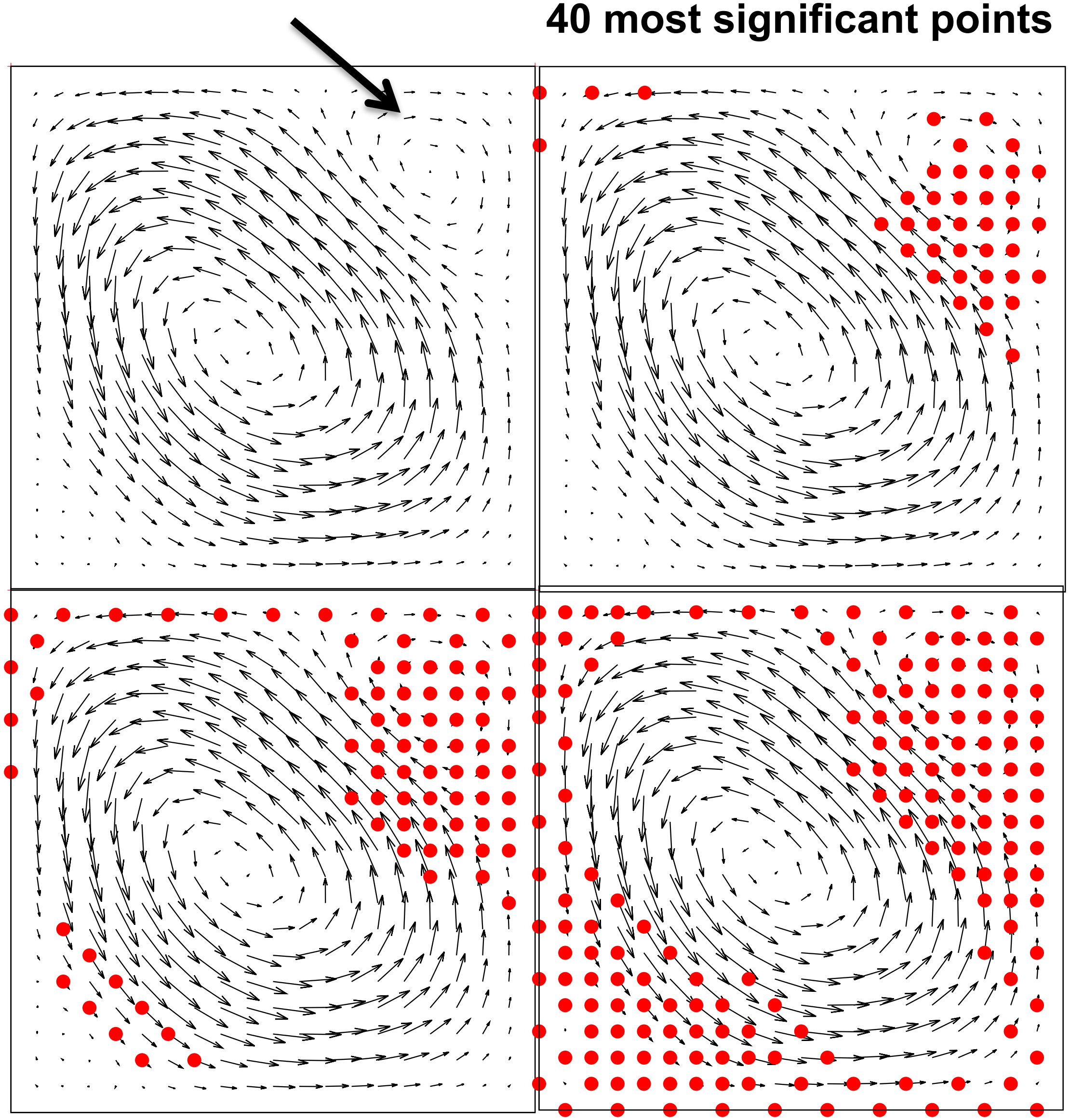
3.22 Measure the Lyapunov exponent for a “one-roll” solution with a weaker secondary roll

Strong single roll with a secondary weaker roll

441 mesh points

169 points with above average Lyapunov exponents

The largest growth is in the vicinity of the secondary roll



3.23 What Accounts for Rolls' Stability ?

Maximum Local (dS/dt) , Internal Energy ,
Kinetic Energy , Total Heat Flux , Growth Rate ?

Rolls	K_x/Nm	K_y/Nm	E/Nm	$Q_{boundary}$	W/τ
2	0.003730	0.00357	1.014	0.0120	1.42
4	0.001139	0.00410	1.018	0.0118	1.70 ✓
6	0.000274 ✓	0.00226 ✓	1.012 ✓	0.0106 ✓	1.25

Except for the 4-Roll Growth Rate , these Criteria Favor the (*Unstable*) 6-Roll Pattern ! Evidently Stability Isn't a Simple Question !

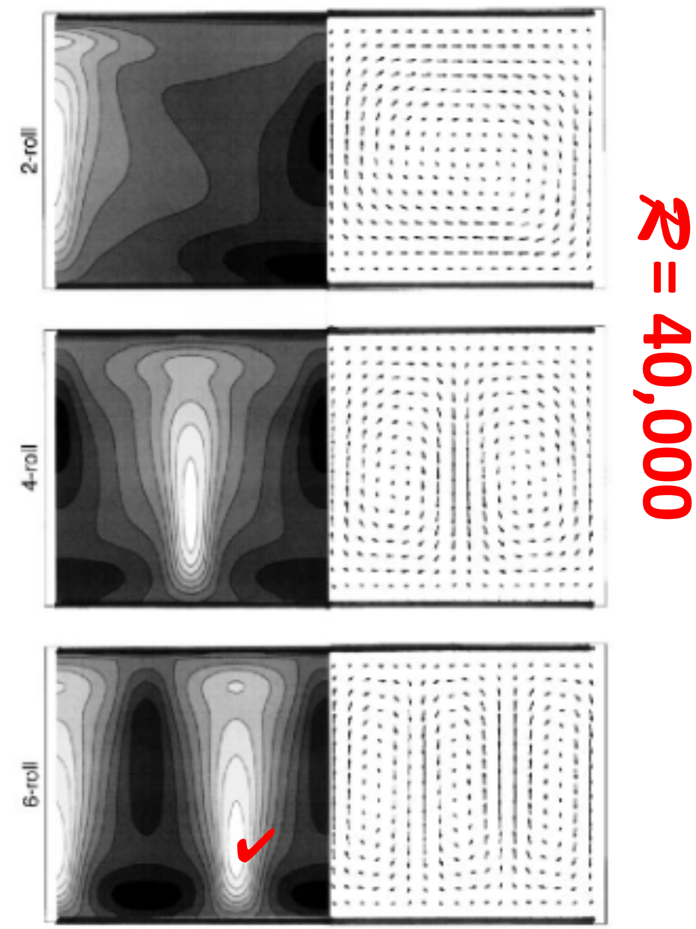


FIG. 1. For the (2, 4, 6)-roll flows, the local entropy production (left) and velocity field (right) is shown. The region of maximum local entropy production (white) corresponds to compression of the cooler fluid.

From Vic Castillo's PhD thesis, available online

4.0 Summary , Conclusions , and New Directions

Even 2D Rayleigh-Bénard is Challenging :

Scale Models Connect with Fractals .
Characterization of Solutions .
Flows are Fundamentally *Continuum* Problems .
Hydrodynamic and Lyapunov Instability .

Many Research Problems are Possible :

Relating Hydrodynamic & Lyapunov Instabilities .
Sources of Vorticity & Enstrophy .
Scaling of the Lyapunov Spectrum .
Spectrum of Turbulence 2D $\neq$ 3D .