Unstable periodic orbits for the Navier-Stokes equations

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Contents

1 – Unstable Periodic Orbits

- Role of UPO's has been acknowledged since the work of Poincaré ("founder" of modern dynamical systems theory);

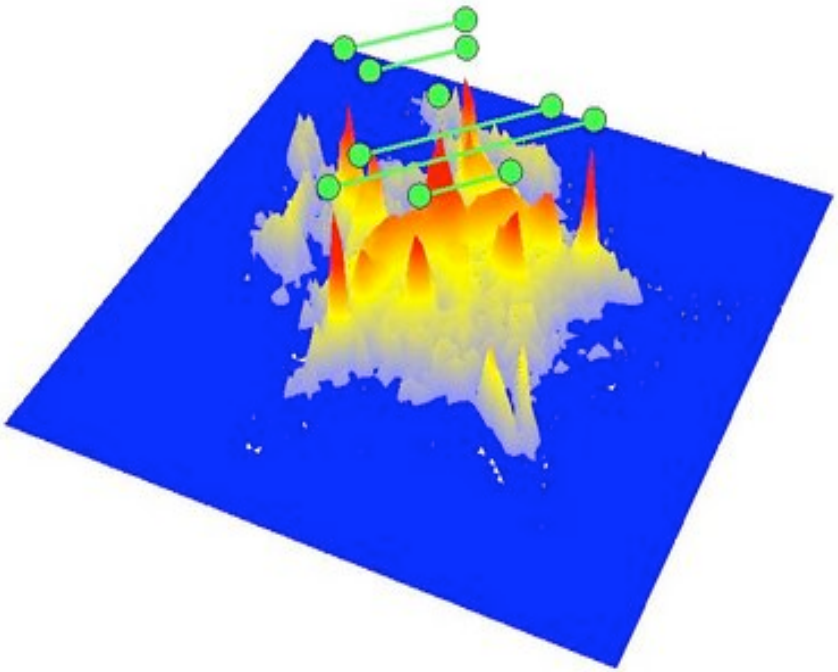
- Typical trajectory will wander incessantly in a sequence of close approaches to the UPOs;

- Analogy from statistical mechanics in physics: set of UPO's can be viewed as the microstates from which a macroscopic description of the system can be calculated;

- Accuracy of predictions is limited by the (non-composite) UPO of smaller period which we fail to include;

http://www.chaosbook.org/ by Cvitanovic *et al.*

1 – Unstable Periodic Orbits



• Abstract "dynamical landscape" with peaks representing the UPOs;

• Chaotic trajectory can be visualized as being the motion of a ball rolling on this abstract dynamical landscape;

• Motion will be strongly affected by the sharpness of the peak (stability of the UPOs);

• Strange attractor is closure of the set of all the UPOs (in the neighborhood of which the system will spend most of the time)

from: http://www.scholarpedia.org/article/Unstable_periodic_orbits

Curator: Dr. Paul So, George Mason University, Fairfax, VA

1 – Unstable Periodic Orbits

• Kawahara & Kida[1] found 2 periodic solutions in plane Couette flow, simulated using spectral methods;

• Novel efficient algorithm to locate UPOs (Boghosian *et al*, preprint), based on previous work by Lan and Cvitanovic[2];

• Tested on Lorenz model and several low-dimensional systems;

good convergence to the UPOs, including 2D fluid;

• Plot Δ(t,T): find initial guess (minimum) for whole trajectory, and value of T;

$$\Delta(t,T) = \| \; r(t+T) - r(t) \; \| \geq 0$$

• Numerically relax minima (in 4D) towards finding UPO;

1. *J. Fluid Mech.*, **449**, 291-300, 2001 **2.** *Phys. Rev. E*, **69** (1): 016217, 2004

2– Dynamical Zeta function

- In "traditional" fluid turbulence, observables are computed as averages over many time frames:

$$\langle A\rangle = \lim_{t\to\infty}\frac{1}{t}\int_0^t A(\rho(\tau))d\tau.$$

- Alternative approach would be to using a generating function:

$$s(\beta) = \lim_{t\to\infty}\frac{1}{t}\ln\left\langle e^{\beta\cdot A^t}\right\rangle,$$

$$\left\langle e^{\beta\cdot A^t}\right\rangle = \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} dx\, e^{\beta\cdot A(f^t(x))}.$$

- Then the moments of the PDF of an observable A are:

$$\left.\frac{\partial s}{\partial\beta}\right|_{\beta=0} = \langle A\rangle\,,$$

$$\left.\frac{\partial^2 s}{\partial\beta^2}\right|_{\beta=0} = \left\langle A^2\right\rangle - \langle A\rangle^2$$

2 – Dynamical Zeta function

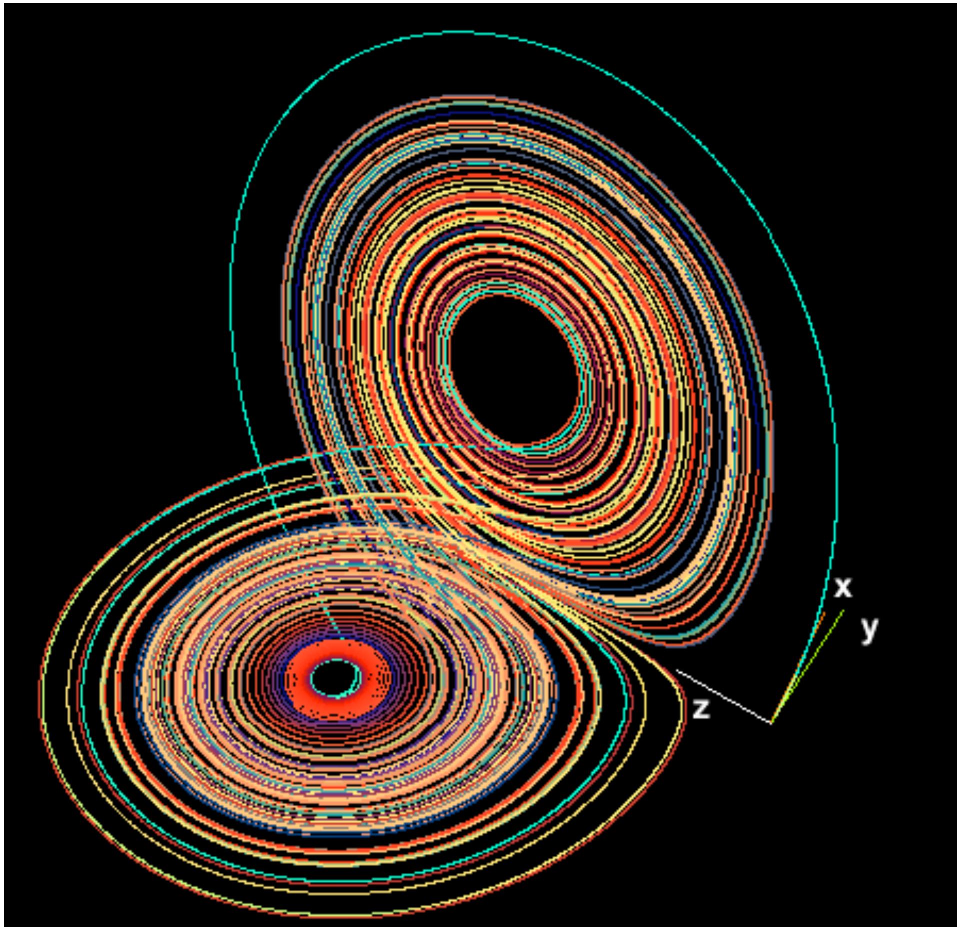
- DZF expression $\zeta^{-1}(s,\beta) = \lim_{T_{\max}\to\infty} \prod_{\{P(T<T_{\max})\}} 1 - e^{-sT_p+\beta A_p - \log(\Lambda_p)}$

  - product runs over all UPO's with period $T < T_{\max}$
  - T_p : period of the UPO.
  - A_p : average value of the observable on the UPO.
  - Λ_p : stability eigenvalue of the UPO.

- Generating function: $s = s(\beta)$: $\zeta^{-1}(s(\beta),\beta) = 0.$

- Computation of expectation value: $\left.\frac{\partial s}{\partial \beta}\right|_{\beta=0} = \langle A \rangle$

Example of a strange attractor: Lorenz system



$$\frac{dx}{dt} = \sigma(y - x)$$

$$\frac{dy}{dt} = x(\rho - z) - y$$

$$\frac{dz}{dt} = xy - bz$$

ρ = Prandtl number

σ = Rayleigh number

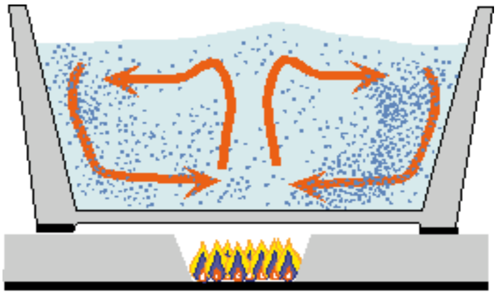
ρ = 28

σ = 10

β = 8/3

x: proportional to intensity of convection

y: proportional to temperature difference

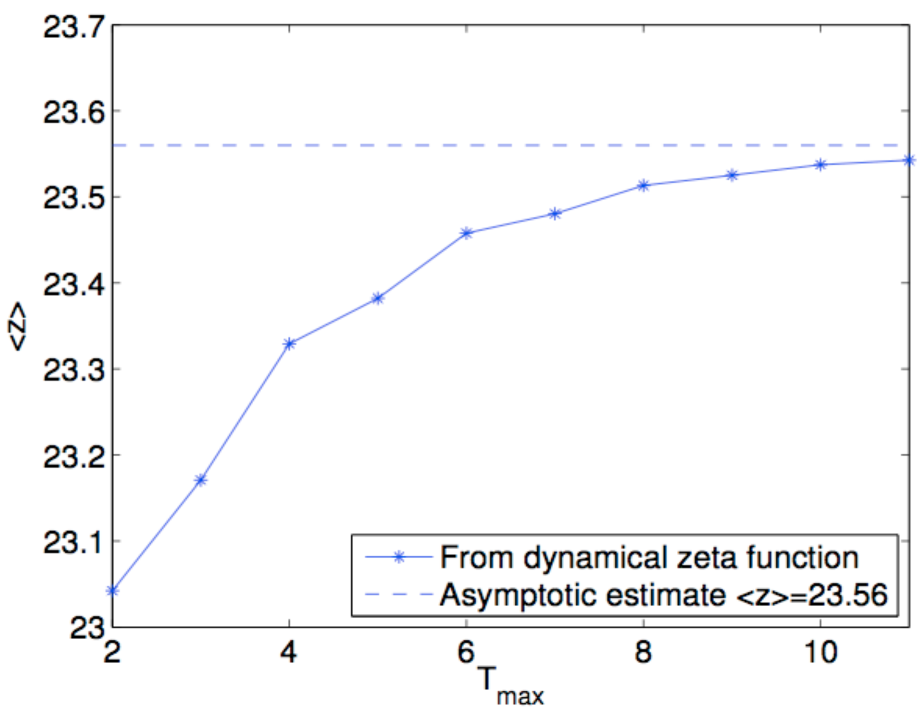


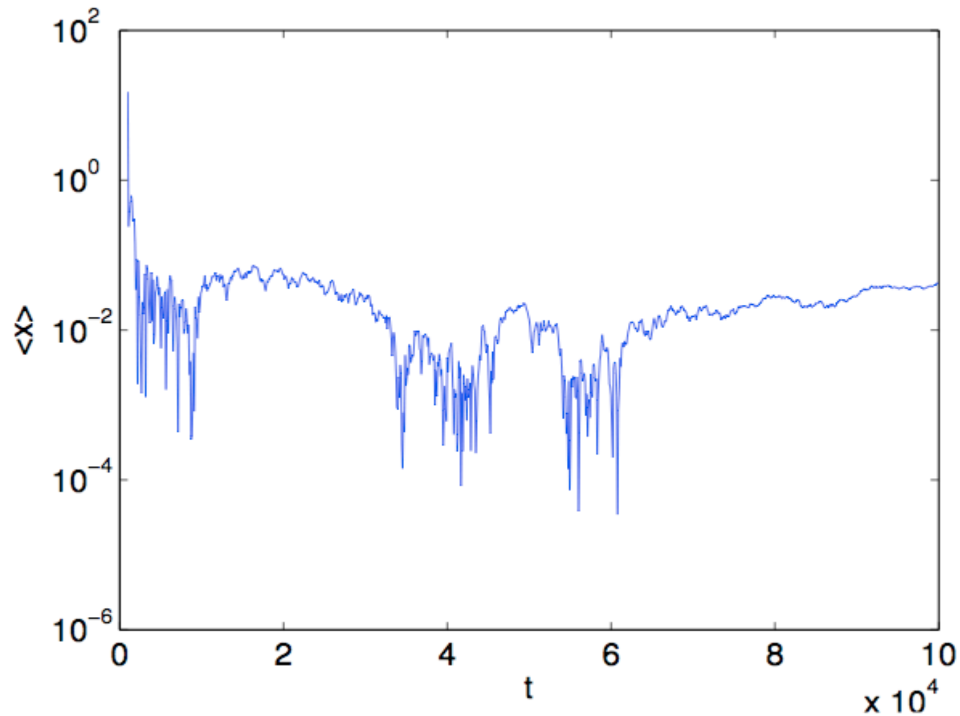
SINGLE CONVECTION CELL

- each of the lobes corresponds to a steady state
- but there are transitions, including reversal of direction: hot air descends, cold air ascends!

"Deterministic nonperiodic flow"
E. N. Lorenz, J. Atmos. Sci. 20 130 (1963)
Picture: **http://en.wikipedia.org/wiki/Lorenz_attractor**

2 – Dynamical Zeta function





- Comparison between the 2 approaches for the Lorenz equations: exact polynomial expansion (left) versus “noisy” time-integration (right).

2 – Dynamical Zeta function

(Main)Advantages in this approach:

- Degree of accuracy is high and converges quickly, with the number of known lower period UPOs
- No need to redo initial value problem every time we wish to compute the average of some quantity
- Averages are no longer stochastic in nature, we have an exact expansion to compute them

3 – Lower-dimensional systems

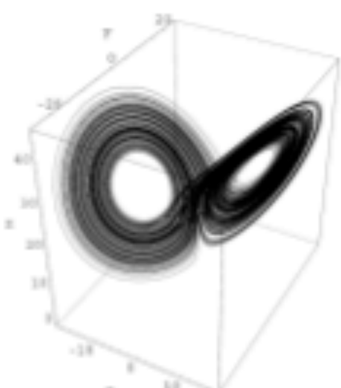
Dynamical system :

$$\dot{\rho}(t) = f(\rho(t))$$

Lorenz equation

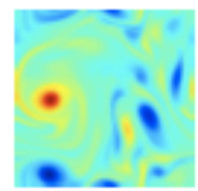
State ρ : point in 3D space

Orbit : Time-evolution of 3D point.

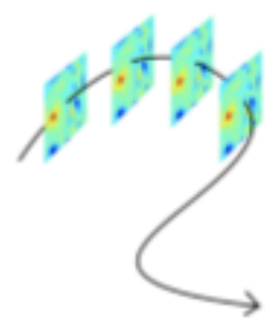


2D force-driven turbulent flow

State ρ : velocity distribution $u(x,y)$ at a given time (infinite-dimensional space).



Orbit : Time-evolution of Fluid.



3 – Lower-dimensional systems: 2D fluid

- Magnetohydrodynamic forcing in a thin layer of conducting fluid

- Fluid flow simulated using OpenLB, with a sinusoidal force, to reproduce experimental work (quasi-2D)[1]. Colours represent the vorticity field: red is large negative value (counterclockwise), blue is large positive value (clockwise).

1. N. T. Ouellette and J. P. Gollub, Phys. Rev. Lett. 99 (19), 2007, 194502

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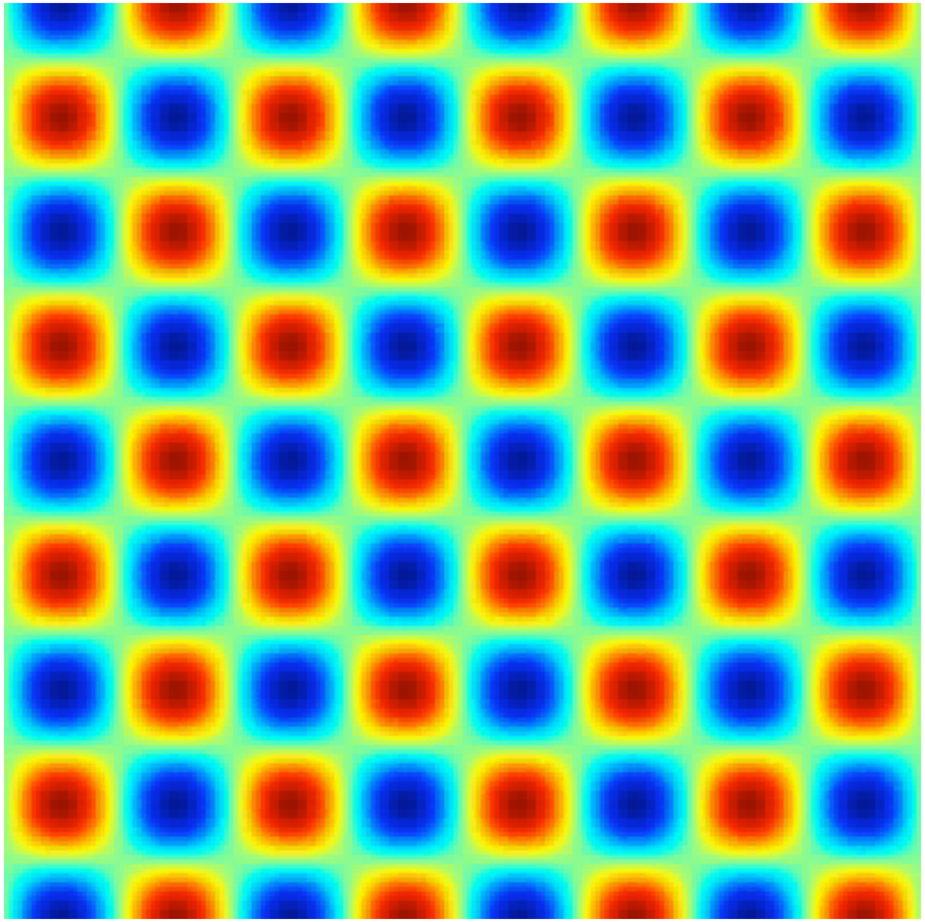

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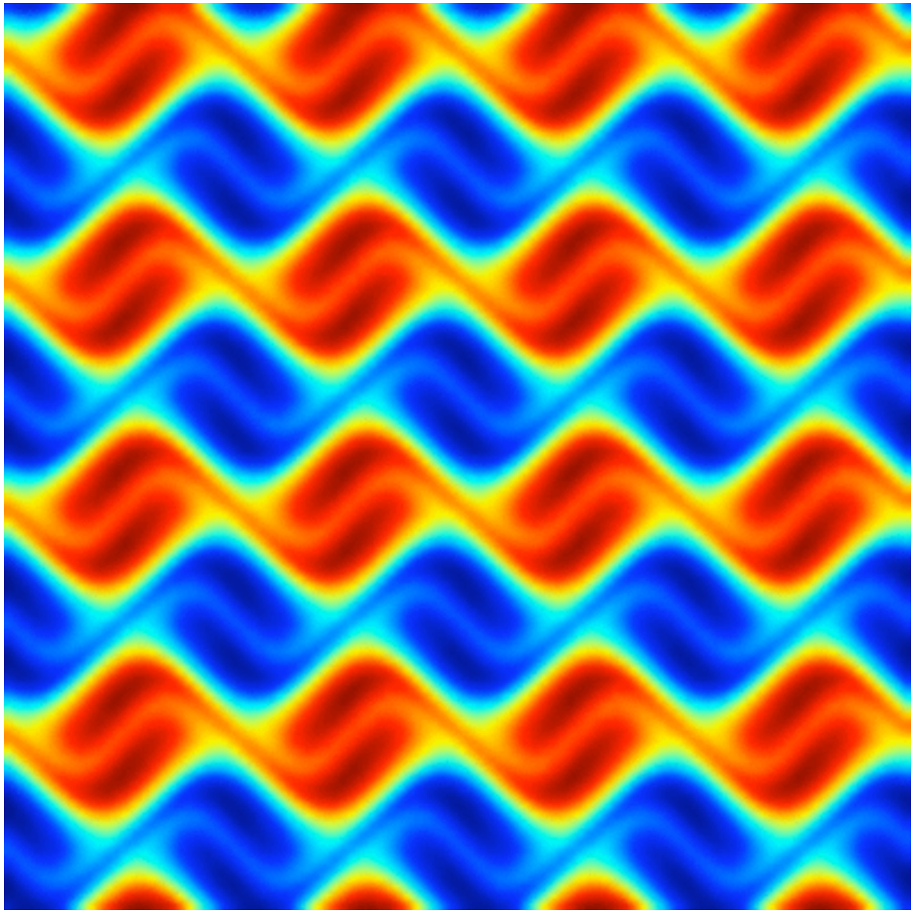
3 – Lower-dimensional systems: 2D fluid revisited

- Same system as previous slide. Red denotes large negative vorticity (counterclockwise rotation), blue is large positive vorticity (clockwise rotation). Periodic solution shown here (found analytically) is highly unstable.

3 – Lower-dimensional systems: 2D fluid revisited



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4 – Lattice Boltzmann Method

(or why stream and collide is all it takes)

- Fluid flow (nearly incompressible NSE) is simulated using the Lattice Boltzmann Method[1,2]

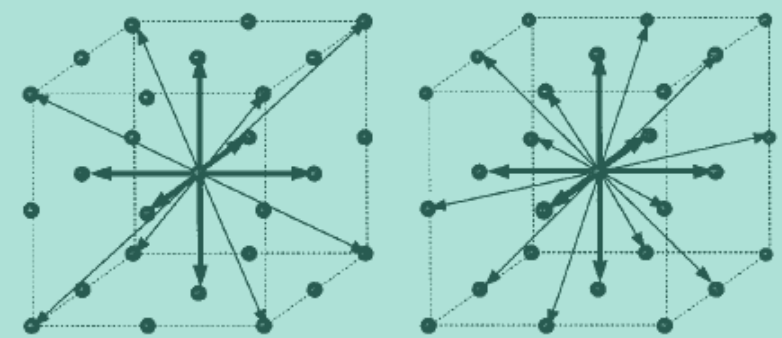


FIG. 1. Lattice structure of d3q15 (left) and d3q18 (right).

$$f_i(\vec{r}+\vec{c}_i, t+1) = f_i(\vec{r}, t) + \Omega_i(\vec{r}, t),$$

$$\rho = \sum_{i=1}^{b} f_i, \rho\vec{u} = \sum_{i=1}^{b} f_i \vec{c}_i.$$

$$\sum_{i=1}^{b} \Omega_i = 0, \sum_{i=1}^{b} \Omega_i \vec{c}_i = \vec{0}.$$

$$f_i^{eq}(\rho, \vec{u}) = \rho[a + b\vec{c}_i.\vec{u} + c(\vec{c}_i.\vec{u})^2 + du^2],$$

$$f_i(\vec{r}+\vec{c}_i, t+1) - f_i(\vec{r}, t) = S_{ij}(f_j(\vec{r}, t) - f_j^{eq}(\vec{r})),$$

$$\sum_{i=1}^{b} f_i^{eq} = \rho, \sum_{i=1}^{b} f_i^{eq} \vec{c}_i = \rho\vec{u},$$

$$f_i(\vec{r}+\vec{c}_i, t+1) - f_j(\vec{r}, t) = -\frac{1}{\tau}(f_i(\vec{r}, t) - f_i^{eq}(\vec{r})).$$

$$\nu = (\tau - \frac{1}{2})c_s^2 \Delta t,$$

1. S. Chen, G. D. Doolen, Annu. Rev. Fluid Mech., 30, 329-364, 1998
2. S. Succi, “The LBE for Fluid Dynamics and Beyond”, Oxford University Press, Oxford, 2001

4 – Lattice Boltzmann Method

- Basic premise: macroscopic dynamics is the result of collective behavior of many microscopic ones and the macroscopic dynamics not sensitive to underlying details is microscopic physics;

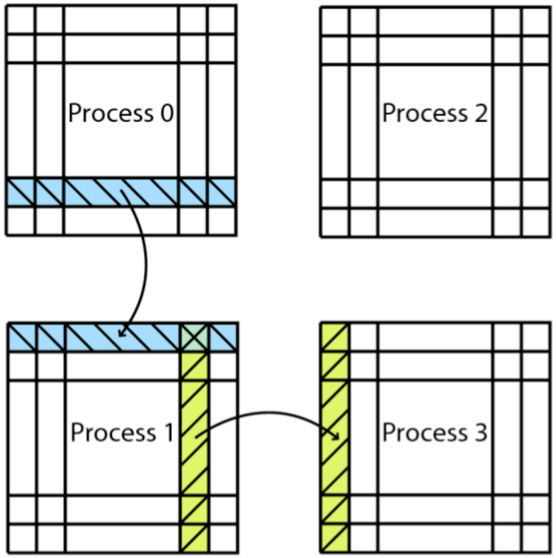
- How did we go from discrete velocities to hydrodynamics? Multi-scale (Chapman-Enskog) expansion, assuming diffusion time scale much slower than convection time scale;

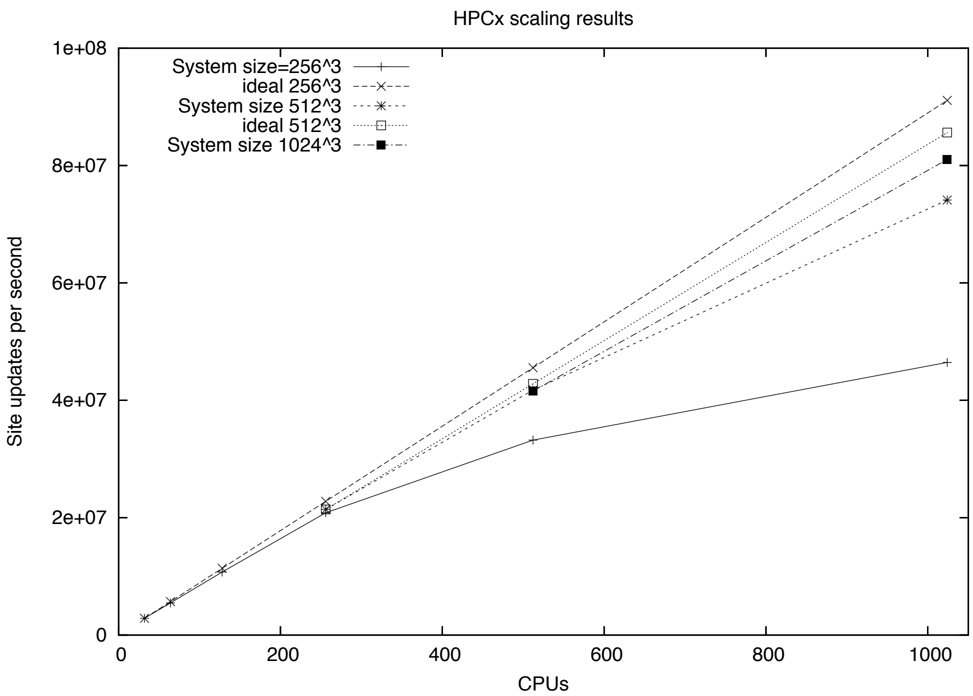
- Main areas of application: complex boundaries, interfacial dynamics, multiphase flows; Codes: OpenLB, LB3D (amphyphilic fluids), HemeLB (cerebral blood flow);

- Main advantages of LBM:
  - local collision operator + linear streaming operator (almost “embarrassingly” parallel);
  - minimal set of velocities, from which macroscopic quantities are computed;
  - no need for extra term for extra equation for pressure term, which so often requires extra numerical treatments (pressure is now eq. of state);

5 – HYPO4D[1]

- Communication pattern between processors: only the halo values need to be sent to nearest neighbors →





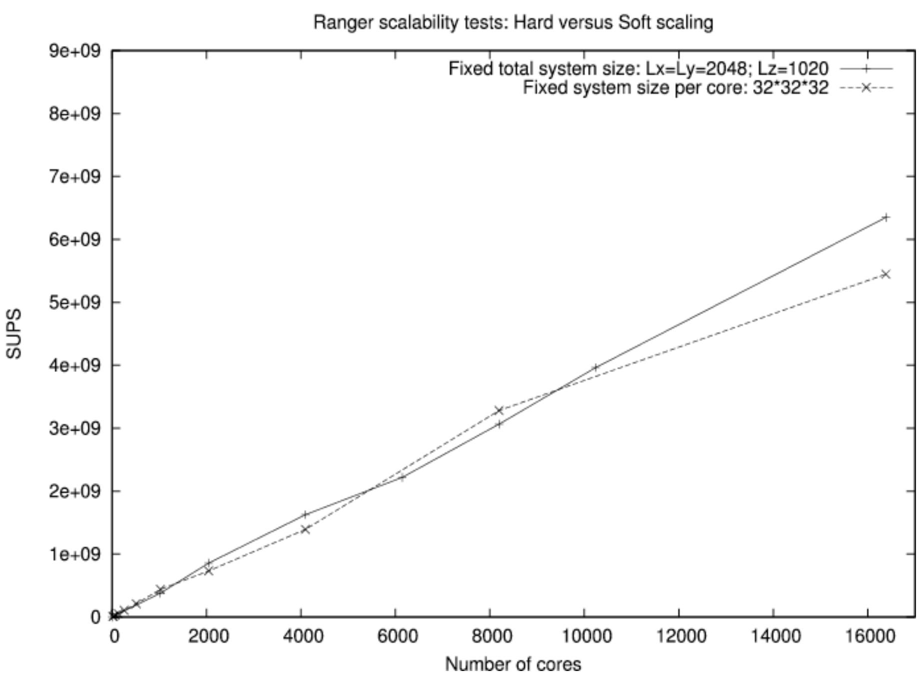
- Scalability tests at NGS and HPCx (Gold Star award)

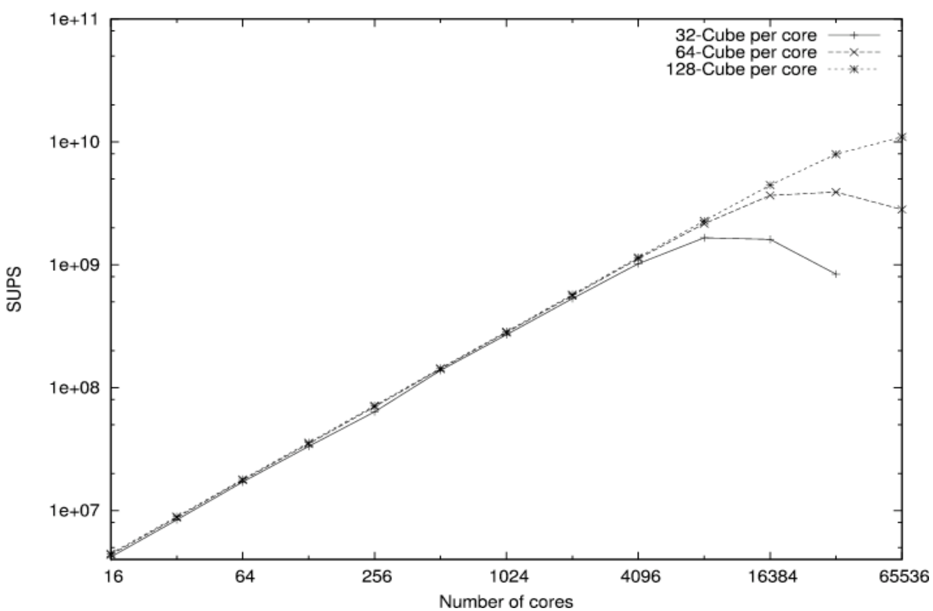
(i.e., ~1.9 speed-up for cubic lattice with L=1024, when going from 512 to 1024 processors)

1. R. S. Saksena, B. Boghosian, L. Fazendeiro et al., Phil. Trans. R. Soc. A 367:2557-2571, 2009

5 – HYPO4D: Ranger + Intrepid scaling

- In the halo-exchange step, all MPI communications are non- blocking, in order to prevent dead-lock;
- No aggressive optimization pursued, so that code can be deployed (almost) seamlessly on different platforms;
- Ranger @TACC: Sun Constellation Linux Cluster, 62976 AMD cores, 123 TB memory, 579.4 TFlops (theoretical) peak;
- Intrepid @Argonne: IBM BlueGene/P, 163 840 cores, 80 TB memory, 557 TFlops (theoretical) peak;





- Linear scaling up to 16K on Ranger (left) and 33K on Intrepid (right). Also close to linear up to 33K on Ranger and 65K on Intrepid;

6 – Turbulent flow

• Current approach: fluid starts from rest, periodic boundary conditions in all directions (isotropic, homogeneous turbulence), ABC type force applied:

$$\vec{\nabla} \cdot \vec{F} = 0$$

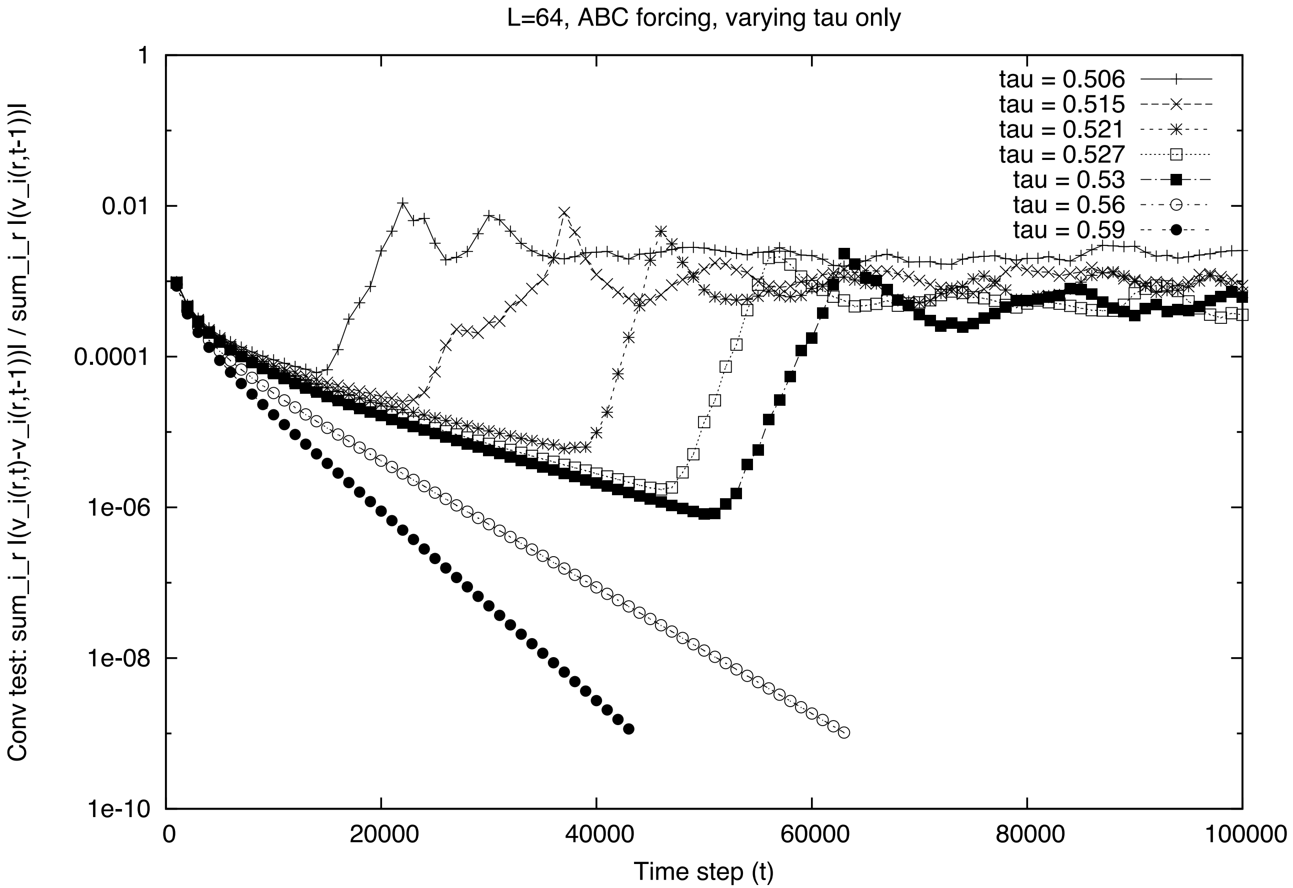
$$\vec{\nabla} \times \vec{F} = \vec{F}$$

• Numerical stability tests applied at all sites in the lattice at every time step, convergence tests and other quantities measured at regular intervals;

• After a certain threshold of LB viscosity, (weak) turbulent behavior sets in;

• HYPO4D = initial value problem (LB) + minimum search + 4D numerical relaxation (variational principle applied to LBE) + post-processing tools;

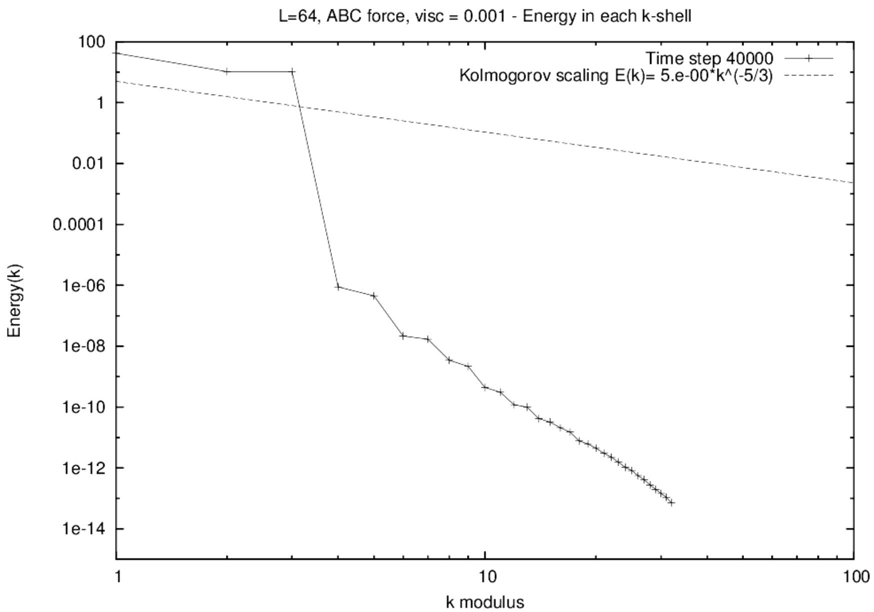
6 - Turbulent flow: Convergence test



- Cubic lattice, 64^3, varying kinematic (LB) viscosity;
- Maximum Re ~ 500, taking velocity averaged over many time, steps, but DNS, no modeling included;

- Convergence test for the velocity field, taken between consecutive time steps. Notice sharp increase after turbulent regime sets in (vertical axis scale is logarithmic).

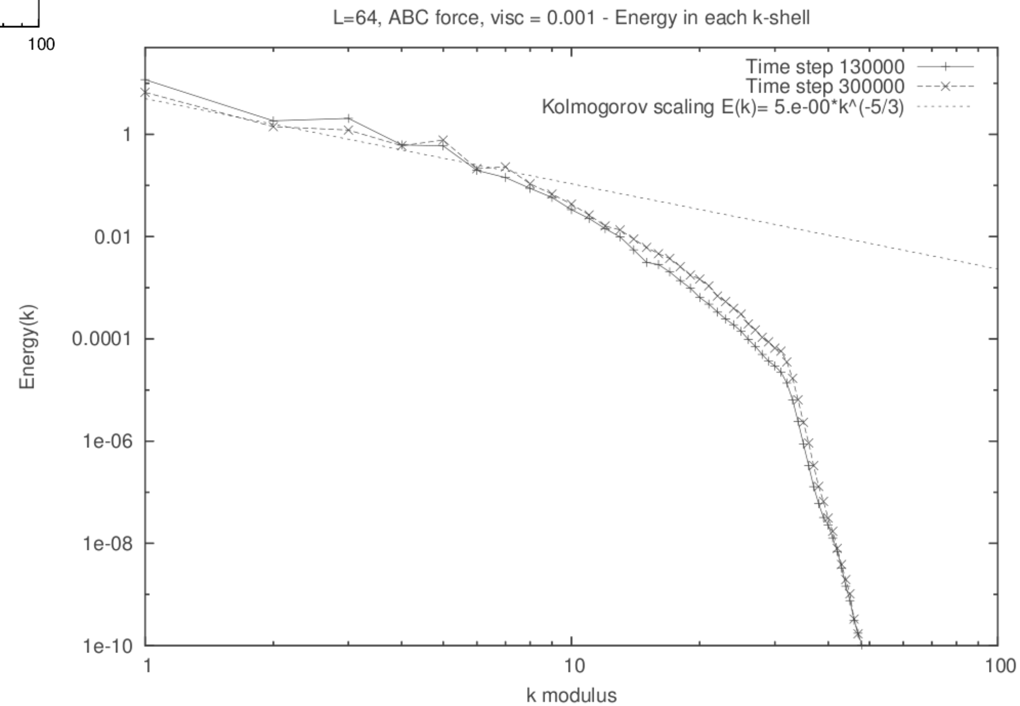
6 - Turbulent flow: Energy spectrum E(q)



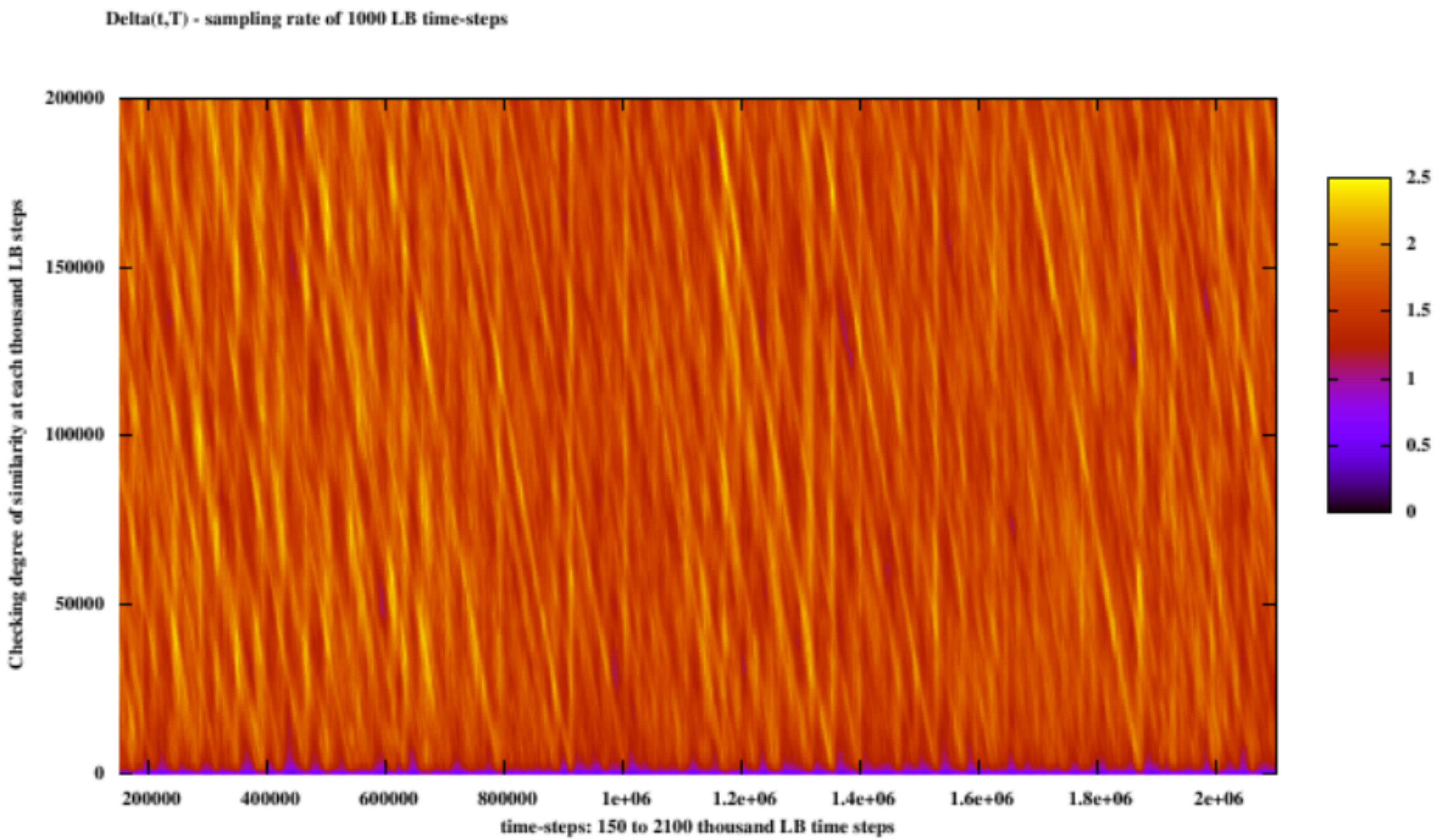
- Kolmogorov picture of turbulent flow divides it (roughly) into 3 different scales: kinetic, inertial, dissipative;

- Left plot shows energy spectrum E(q) before transition to time-dependent behavior;

- Right plot shows spectrum for two different time snapshots after the transition, with Kolmogorov fitting for visual aid;



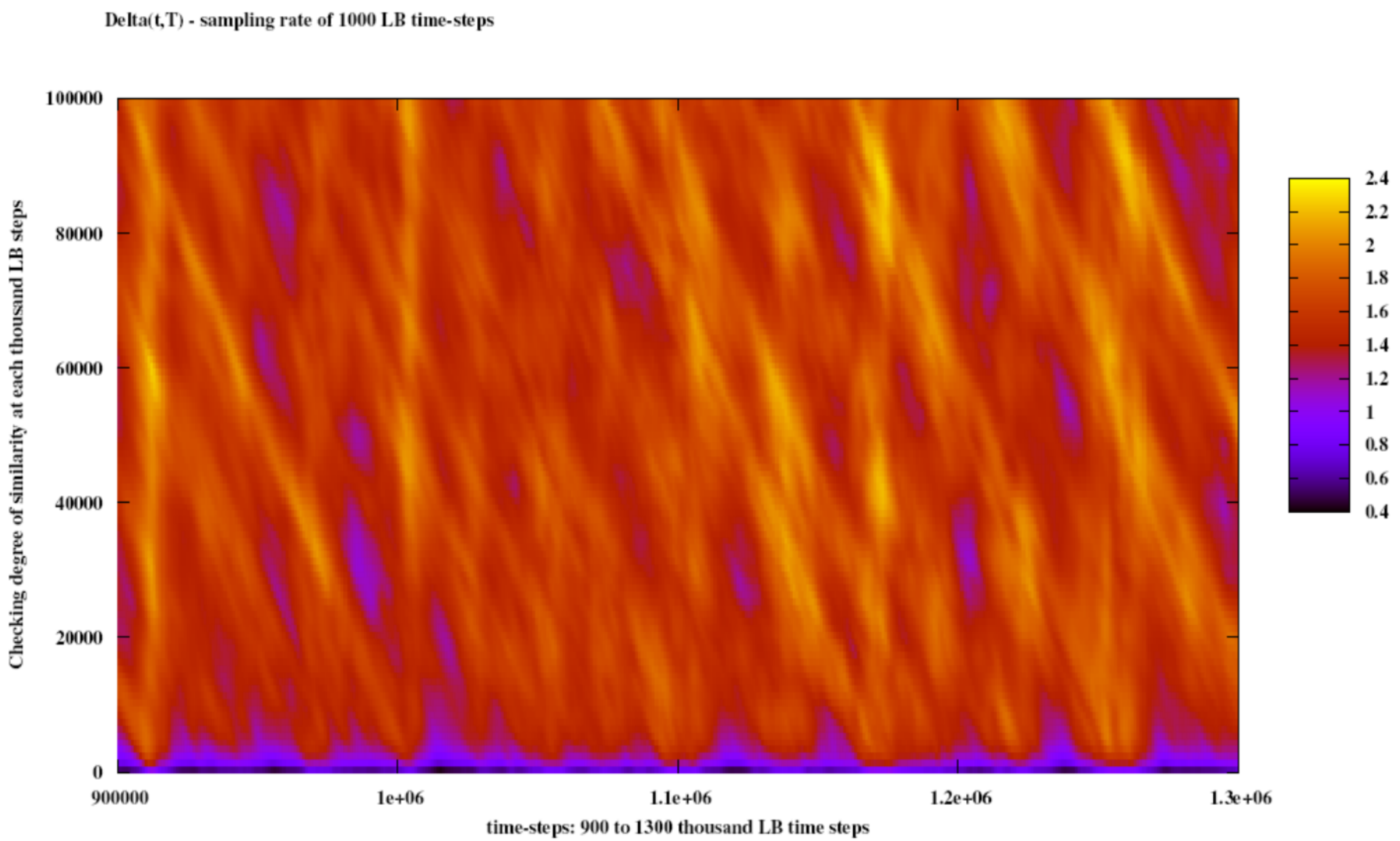
7 - 4D Numerical Relaxation: search for minima



- Vertical axis is T, horizontal axis is t, color code gives "delta" quantity:

$$\Delta(t,T) \equiv \sqrt{\sum_{\mathbf{r}} \sum_{i=1}^{l} (f_i(\mathbf{r}, t+T) - f_i(\mathbf{r}, t))^2},$$

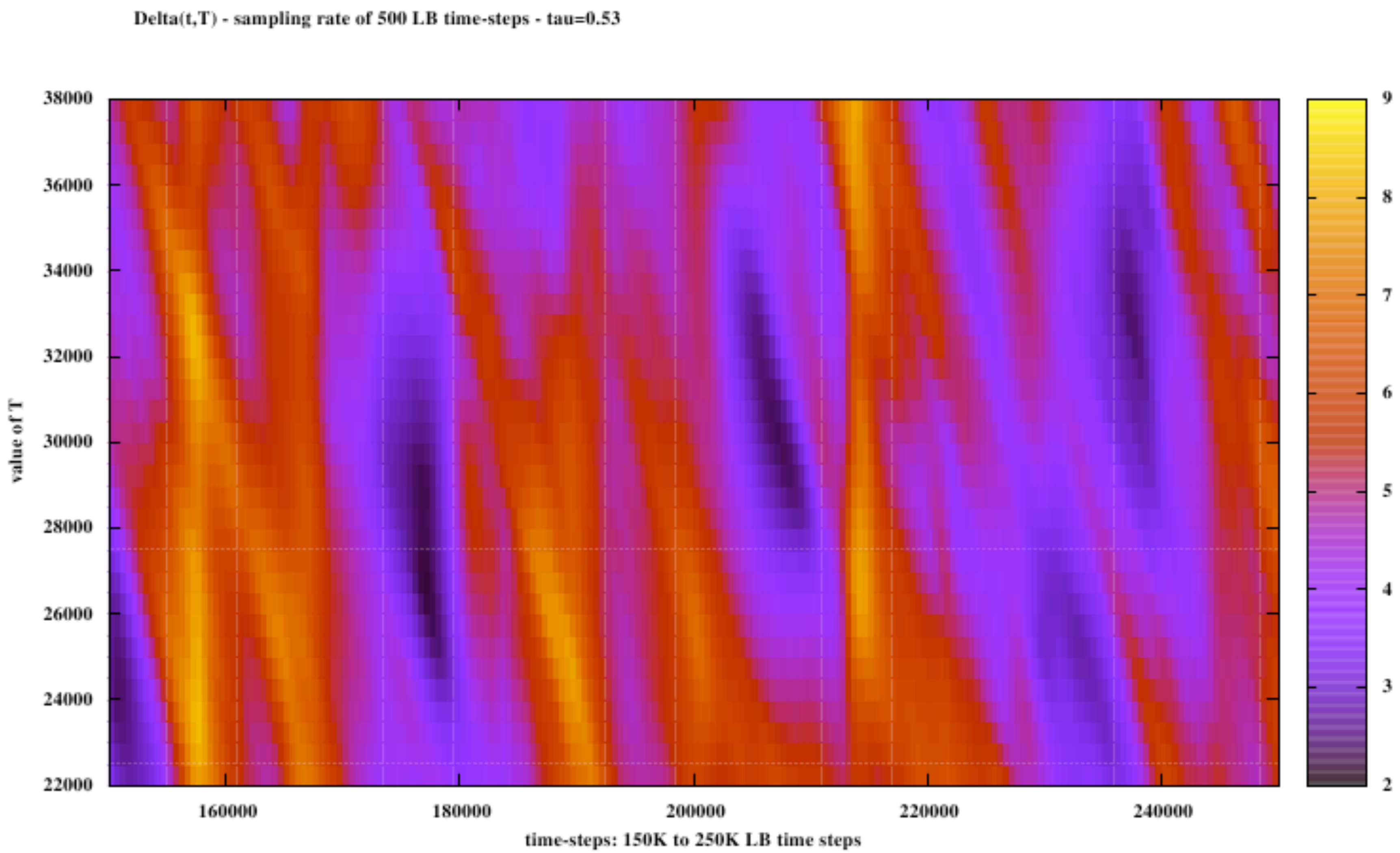
7 - 4D Numerical Relaxation: search for minima



- Detail of previous plot, showing several (purplish) minima/areas of interest, as well as hinting at some regularity in their distribution

7 - 4D Numerical Relaxation: search for minima

- New minima for v = 0.01



7 - 4D Numerical Relaxation

- Memory critical resource for the full 4D relaxation procedure;

- For the minimum shown T~26.5K, we have to keep in memory at least 64^3*19 (number of LB velocities)*8(double precision)*2.65* 10^4 variables ~ 1 TB; Then SD=5 copies and CG=8!!!!!!

- Minimization algorithm:

- define functional $\mathcal{F} \equiv \frac{1}{2} \sum_{t=0}^{T-1} \sum_{\vec{r}} \sum_{i=1}^{b} |\phi_i(\vec{r}, t)|^2$ with

$$\phi_i(\vec{r}, t) = f_i(\vec{r} + \vec{c}_i, t + 1) - f_i(\vec{r}, t) - \Omega_i(\vec{r}, t)$$

- compute gradient $\frac{\delta \mathcal{F}}{\delta f_k(\vec{s}, q)}$

7 - 4D Numerical Relaxation: algorithm

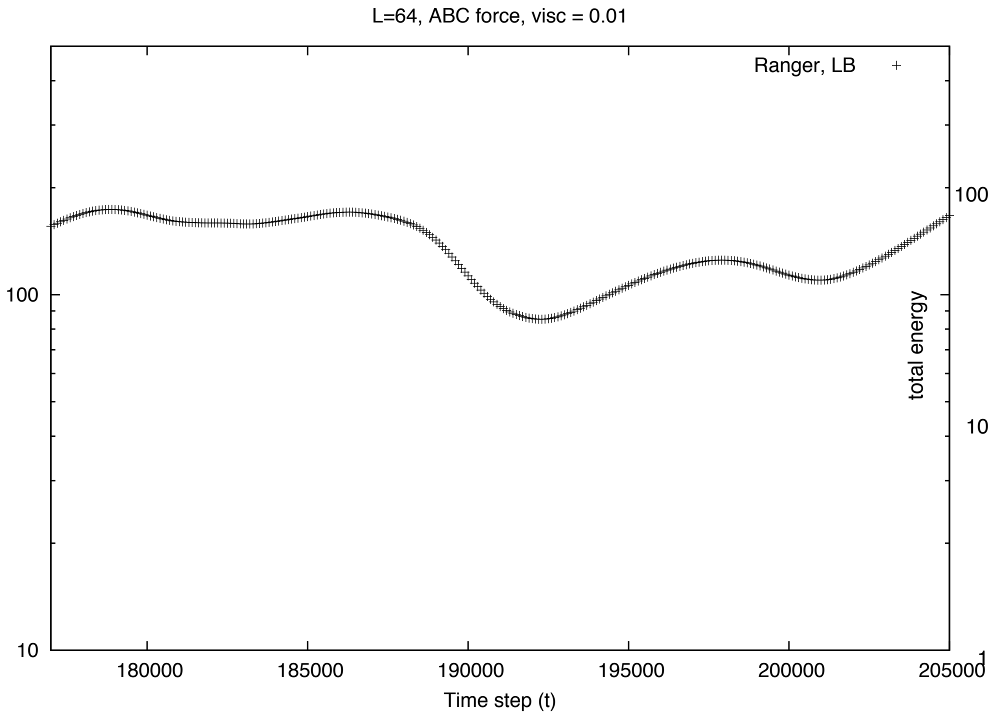
- Fill (4D) lattice with $f_i(\vec{r}, t)$ from $t = t_0, T - 1$
- 4D collide and stream (periodic time BC)
- Compute ϕ and initial $\mathcal{F}$
- Combination of SD and/or CG until $\mathcal{F}$ no longer varies
- SD algorithm :

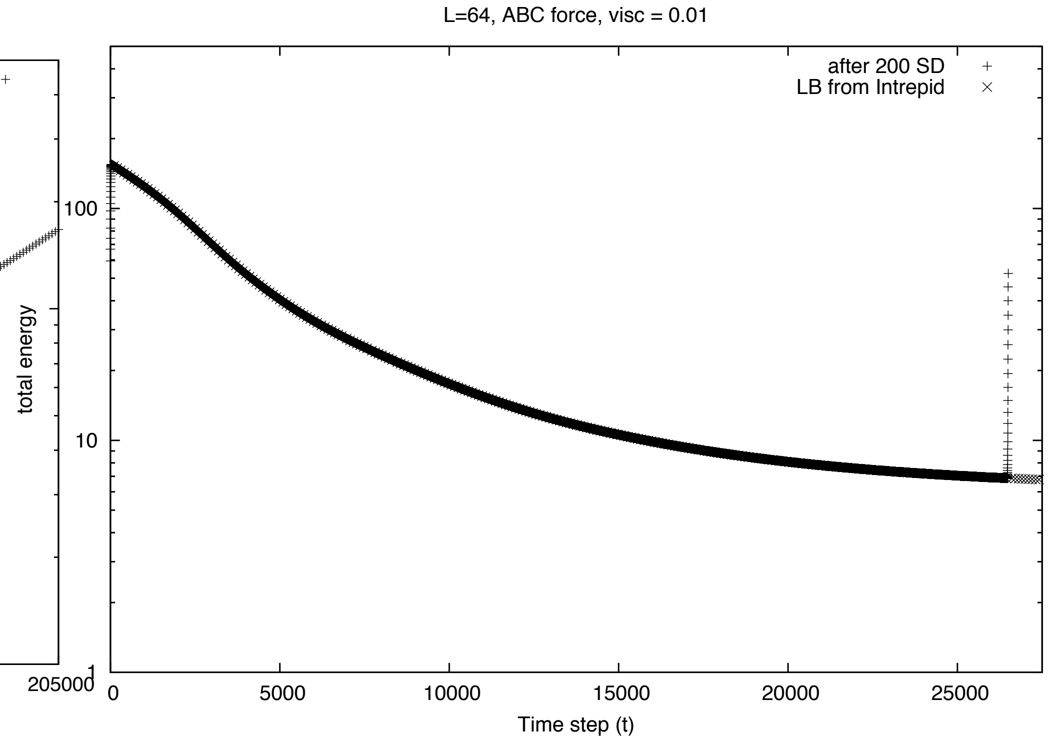
$$f_i(\vec{r}, t) - = \alpha * \frac{\partial \mathcal{F}}{\partial f_i(\vec{r}, t)}$$

- α found through golden mean search procedure, done at every step

7 - 4D Numerical Relaxation: failed experiment :(

- Left: initial 26.5K trajectory;
Right: after SD minimization, and also time-forwarding from checkpoint on same machine;
Y-axis: total energy in both cases;
- At every single SD step, $\mathcal{F}$ decreases!





8 - Prospects & Challenges

- Relaxation procedure in order to identify first (smaller period) UPOs in 3D NSE;
- Characterization of the UPOs (stability eigenvalues, but also energy dissipation rate, vorticity, enstrophy, etc);
- Compare averages from one or more UPOs with time forward averaging;
- Possible heteroclinic connections between periodic solutions, along which bursting (intermittency) may occur (K&K);
- Classification of the (prime) UPOs identified + creation and maintenance of a digital library of such orbits;
- Could a symbolic dynamics be devised from some of these UPOs, for 3D NSE turbulence?

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TACC

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NCSA

Pittsburgh Supercomputing Center

Manchester 1824 The University of Manchester

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LSU

LONI

Shreveport Ruston Monroe Lake Charles Lafayette Baton Rouge New Orleans

Science & Technology Facilities Council Daresbury Laboratory

NSF

SDSC San Diego Supercomputer Center