

a spatiotemporal theory of turbulence computational challenges

Predrag Cvitanović and Matt Gudorf

working notes Georgia Tech

December 6, 2021

overview

- what this talk is about
- 2 turbulence in large domains
- space is time
- 4 bye bye, dynamics

how do clouds solve PDEs?

do clouds integrate Navier-Stokes equations?



are clouds Navier-Stokes supercomputers in the sky?

part 1

- turbulence in large domains
- space is time
- spacetime
- 4 bye bye, dynamics

goal: enumerate the building blocks of turbulence

Navier-Stokes equations

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = \frac{1}{B} \nabla^2 \mathbf{v} - \nabla \rho + \mathbf{f}, \qquad \nabla \cdot \mathbf{v} = 0,$$

velocity field $\mathbf{v} \in \mathbb{R}^3$; pressure field p ; driving force \mathbf{f}

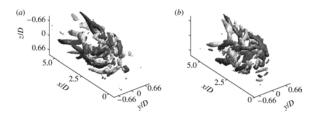
describe turbulence

starting from the equations (no statistical assumptions)

challenge: experiments are amazing

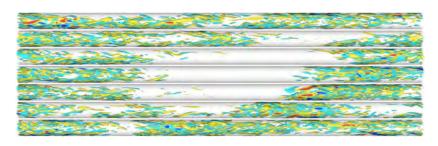


T. Mullin lab



B. Hof lab

can simulate arge computational domains



pipe flow close to onset of turbulence 1

but we have hit a wall:

exact coherent structures are too unstable to compute

¹M. Avila and B. Hof, Phys. Rev. **E 87** (2013)

goal: we can do 3D turbulence, but for this presentation

Navier-Stokes equations

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = \frac{1}{R} \nabla^2 \mathbf{v} + (\cdots)$$

velocity field $\mathbf{v}(\mathbf{x};t) \in \mathbb{R}^3$

not helpful for developing intuition

we cannot visualize 3D velocity field at every 3D spatial point

look instead at 1D 'flame fronts'

(1+1) spacetime dimensional "Navier-Stokes"

Navier-Stokes equations

(1822)

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = \frac{1}{R} \nabla^2 \mathbf{v} + (\cdots)$$



Kuramoto-Sivashinsky (1+1)-dimensional PDE

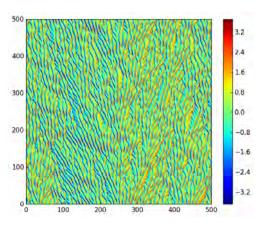
1975)

$$u_t + u \nabla u = -\nabla^2 u - \nabla^4 u, \qquad x \in \mathbb{R},$$

describes spatially extended systems such as

- flame fronts in combustion
- reaction-diffusion systems
- ...

an example: Kuramoto-Sivashinsky on a large domain

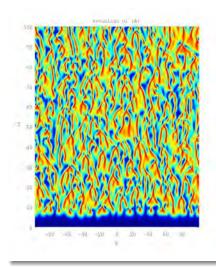


[horizontal] space $x \in [0, L]$ [up] time evolution

- turbulent behavior
- simpler physical, mathematical and computational setting than Navier-Stokes

another example of large spacetime domain simulation

complex Ginzburg-Landau

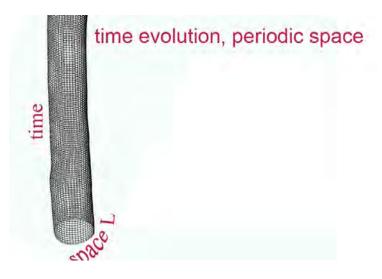


(will return to this)

[horizontal] space $x \in [-L/2, L/2]$

[up] time evolution

compact space, infinite time cylinder



so far : Navier-Stokes on compact spatial domains, all times

compact space, infinite time

Kuramoto-Sivashinsky equation

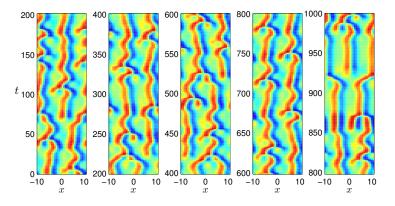
$$u_t = -(+\nabla^2 + \nabla^4)u - u\nabla u, \qquad x \in [-L/2, L/2],$$

in terms of discrete spatial Fourier modes

N ordinary differential equations (ODEs) in time

$$\dot{\tilde{u}}_k(t) = (q_k^2 - q_k^4) \, \tilde{u}_k(t) - i \frac{q_k}{2} \sum_{k'=0}^{N-1} \tilde{u}_{k'}(t) \, \tilde{u}_{k-k'}(t) \, .$$

evolution of Kuramoto-Sivashinsky on small L=22 cell



horizontal: $x \in [-11, 11]$

vertical: time

color: magnitude of u(x, t)

part 2

- turbulence in large domains
- space is time
- spacetime
- bye bye, dynamics

yes, but

is space time?

compact time, infinite space

rewrite Kuramoto-Sivashinsky

$$u_t = -uu_x - u_{xx} - u_{xxxx}$$

as 4-fields vector

$$\mathbf{u}^{\top} = (u, u', u'', u''')$$

where $u' \equiv u_x$, $u'' \equiv u_{xx}$, $u''' \equiv u_{xxx}$

equation $\frac{d}{dx}\mathbf{u}(x) = \mathbf{v}(x)$ now 1st order in spatial derivative

Kuramoto-Sivashinsky = four coupled 1st order PDEs

$$\begin{array}{rcl} \frac{d\,u}{dx} & = & u'\,, & \frac{d\,u'}{dx} = u'' \\ \frac{d\,u''}{dx} & = & u'''\,, & \frac{d\,u'''}{dx} = -u_t - u'' - u\,u' \end{array}$$

compact time, infinite space

1st order in spatial derivative

evolve four 1st order PDEs for u(x) in x,

$$\frac{d}{dx}\mathbf{u}(x)=\mathbf{v}(x)$$

compact in time, periodic boundary condition

$$u(x,t) = u(x,t+T)$$

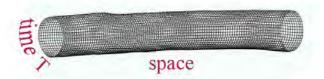
initial data

$$\mathbf{u}_{0}^{\top}=(u(x_{0},t),u^{'}(x_{0},t),u^{''}(x_{0},t),u^{''}(x_{0},t))$$

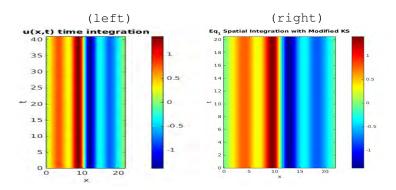
specified for all $t \in [0, T)$, at a fixed space point x_0

can do : compact time, infinite space cylinder

space evolution, periodic time

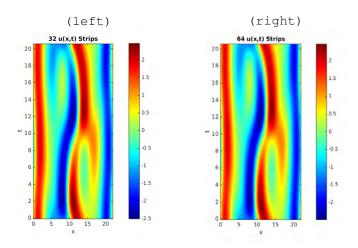


a time-invariant equilibrium, spatial periodic orbit



evolution of EQ_1 : (left) in time, (right) in space initial condition for the spatial integration is the time strip $u(x_0, t)$, t = [0, T), where time period T = 0, spatial x period is L = 22.

a spacetime invariant 2-torus integrated in either time or space



(left) old : time evolution. (right) new : space evolution x = [0, L] initial condition : time periodic line t = [0, T]

Gudorf 2016

but integrations are uncontrollably unstable

neither time nor space integration works for large domains

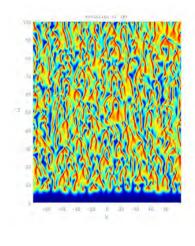
rethink the calculation

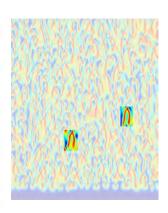
part 3

- turbulence in large domains
- 2 space is time
- spacetime
- bye bye, dynamics

complex Ginzburg-Landau on a large spacetime domain

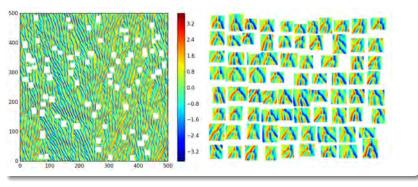
goal: enumerate nearly recurrent chronotopes





Kuramoto-Sivashinsky on a large spacetime domain

the same small tile recurs often in a turbulent pattern



goal: define, enumerate nearly recurrent tiles

chronotope²

In literary theory and philosophy of language, the chronotope is how configurations of time and space are represented in language and discourse.

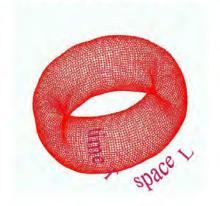
- Wikipedia: Chronotope

Mikhail Mikhailovich Bakhtin (1937)

²S. Lepri et al., J. Stat. Phys. **82**, 1429–1452 (1996).

use spatiotemporally compact solutions as chronotopes

periodic spacetime : 2-torus



this 'exact coherent structure' shadows a small patch of spacetime solution u(x, t)

periodic orbits generalize to d-tori

1 time, 0 space dimensions

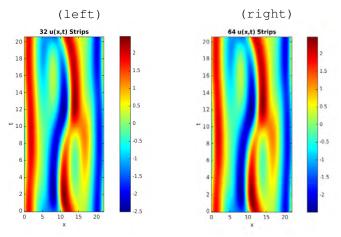
a state space point is periodic if its orbit returns to it after a finite time T;

such orbit tiles the time axis by infinitely many repeats

1 time, d-1 space dimensions

a state space point is *spatiotemporally periodic* if it belongs to an invariant d-torus \mathcal{R} ; such torus tiles the spacetime by infinitely many repeats

a spacetime invariant 2-torus integrated in either time or space



(left) old: time evolution t = [0, T]

initial condition : space periodic line x = [0, L]

(right) new: space evolution x = [0, L]

initial condition : time periodic line t = [0, T]

Gudorf 2016

every compact solution is a fixed point on a discrete lattice

discretize $u_{nm} = u(x_n, t_m)$ over NM points of spatiotemporal periodic lattice $x_n = nL/N$, $t_m = mT/M$, Fourier transform :

$$ilde{u}_{k\ell} = rac{1}{NM} \sum_{n=0}^{N-1} \sum_{m=0}^{M-1} u_{nm} \, \mathrm{e}^{-i(q_k x_{n} + \omega_\ell t_m)} \,, \quad q_k = rac{2\pi k}{L} \,, \; \omega_\ell = rac{2\pi \ell}{T} \,.$$

Kuramoto-Sivashinsky is no more a PDE, but an algebraic $[N \times M]$ -dimensional problem of determining global solution \mathbf{u} to

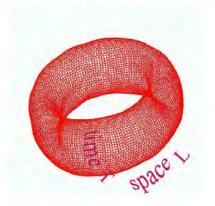
fixed point condition

$$\left(-i\omega_{\ell}-(q_{k}^{2}-q_{k}^{4})\right)\tilde{u}_{k\ell}+i\frac{q_{k}}{2}\sum_{k'=0}^{N-1}\sum_{m'=0}^{M-1}\tilde{u}_{k'm'}\tilde{u}_{k-k',m-m'}=0$$

every calculation is a spatiotemporal lattice calculation

field is discretized as $\tilde{u}_{k\ell}$ values over NM points of a periodic lattice

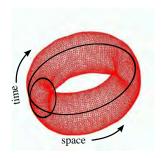
periodic spacetime : 2-torus



professor Zweistein forgets to take his meds

statement : HA!

You are imposing by hand the space & time periods L, T!



answer: NO! nature chooses *L* & *T*, they are free parameters.

there is no more time evolution

solution to Kuramoto-Sivashinsky is now given as

condition that

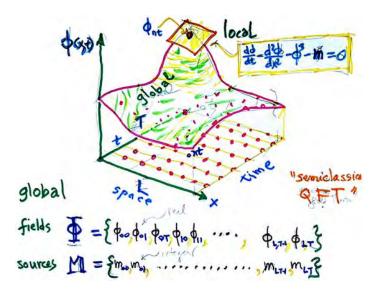
at each lattice point $k\ell$ the tangent field at $\tilde{u}_{k\ell}$

satisfies the equations of motion

$$\left[-i\omega_{\ell}-(q_{k}^{2}-q_{k}^{4})\right]\tilde{u}_{k\ell}+i\frac{q_{k}}{2}\sum_{k'=0}^{N-1}\sum_{m'=0}^{M-1}\tilde{u}_{k'm'}\tilde{u}_{k-k',m-m'}=0$$

this is a local tangent field constraint on a global solution

think globally, act locally



for each symbol array M, a periodic lattice state X_{M}

unexpected gift from nature

robust : no exponential instabilities as there are no finite time / space integrations

no need for $\sim 10^{-11}$ accuracies,

SO

accuracy to a few % suffices,
you only need to get the shape of a solution right

part 4

- turbulence in large domains
- space is time
- spacetime
- spacetime computations
- bye bye, dynamics

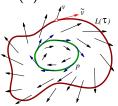
how to find solutions? an ODE example

the law of motion:

$$\dot{x} = v(x)$$

guess loop tangent $\tilde{v}(\tilde{x}) \neq v(\tilde{x})$

periodic orbit
$$\tilde{v}(\tilde{x})$$
, $v(\tilde{x})$ aligned



cost function

$$F^2[\tilde{x}] = \oint_I ds (\tilde{v} - v)^2; \quad \tilde{v} = \tilde{v}(\tilde{x}(s, \tau)), \ v = v(\tilde{x}(s, \tau)),$$

penalize³misorientation of the loop tangent $\tilde{v}(\tilde{x})$ relative to the true dynamical flow tangent field $v(\tilde{x})$

³Y. Lan and P. Cvitanović, Phys. Rev. E **69**, 016217 (2004).

how do clouds solve PDEs?

clouds do not NOT integrate Navier-Stokes equations



do clouds satisfy Navier-Stokes equations?

yes!

they satisfy them locally, everywhere and at all times

the equations imposed as local constraints

Kuramoto-Sivashinsky equation

$$F(u) = u_t + u_{xx} + u_{xxxx} + uu_x = 0$$

for example, minimize over the entire 2-torus

cost function

$$G \equiv \frac{1}{2} |F(u)|_{L \times T}^2$$

need your help!

adjoint descent

cost function

$$G = \frac{1}{2}\mathbf{F}^{\mathsf{T}}\mathbf{F}$$
.

introduce fictitious time (τ) flow by differentiation of cost function.

$$\partial_{ au} G = (J^{ op} \mathbf{F})^{ op} (\partial_{ au} \mathbf{x})$$

"adjoint descent" method defined by chosing4

$$\partial_{ au}\mathbf{x} = -(J^{ op}\mathbf{F})$$

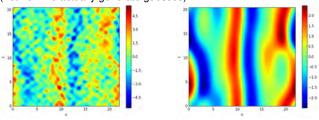
⁴M. Farazmand, J. Fluid M. **795**, 278–312 (2016).

does it work at all?

add strong noise to a *known* solution, twice the typical amplitude

only the first test

(not how we actually generate guesses)



(left) initial guess: a known invariant 2-torus

$$(L_0, T_0) = (22.0, 20.5057459345) + \text{strong random noise}$$

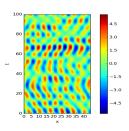
(right) the resulting adjoint descent converged invariant 2-torus

$$(L_f, T_f) = (21.95034935834641, 20.47026321555662)$$

initial guess generation?

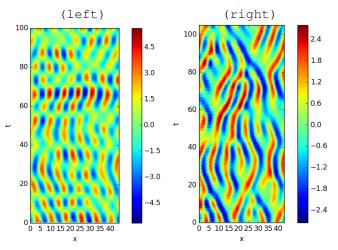
the time scale: the shortest 'turnover' scale characterized by the period of the shortest periodic orbit? Or perhaps the Lyapunov time?

the spatial scale : $\bar{L}=2\pi\sqrt{2}$, the most unstable spatial wavelength of the Kuramoto-Sivashinsky



initial: spatial \bar{L} -modulated random guess

KS invariant 2-torus found variationally



(left) initial : $\bar{L}=2\pi\sqrt{2}$ spatially modulated "noisy" guess (right) adjoint descent : converged invariant 2-torus

Gudorf 2018

initial guesses, embedded in ergodic sea?

Historically,

guesses extracted from close recurrences observed in long turbulent simulations

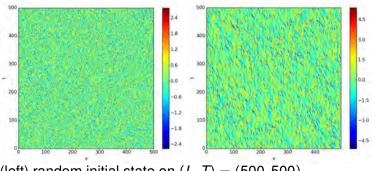
- inefficient, finds only the shortest, least unstable orbits^{5,6}
- can integrate only not far in time

need spatiotemporal guesses

⁵D. Auerbach et al., Phys. Rev. Lett. **58**, 2387–2389 (1987).

⁶J. F. Gibson et al., J. Fluid Mech. **611**, 107–130 (2008).

guesses extracted from large spacetime domains

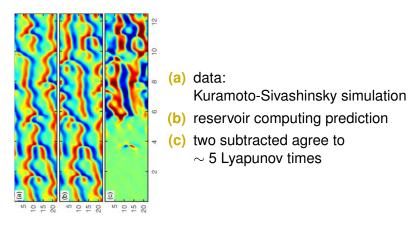


(left) random initial state on (L, T) = (500, 500)(right) adjoint descent \rightarrow typical Kuramoto-Sivashinsky state

finite windows are our starting guesses for invariant 2-tori

another, much twittered: machine learning guesses

"reservoir computing" example⁷



Q: how would you learn this data?

⁷J. Pathak et al., Phys. Rev. Lett. **120**, 024102 (2018).

embarrassment of riches

what to do?

Matthew N. Gudorf

has 1 000's of such invariant 2-tori

part 5

- turbulence in large domains
- space is time
- spacetime
- fundamental tiles
- bye bye, dynamics

building blocks of turbulence

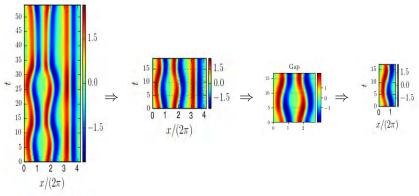
how do we recognize a cloud?



by recurrent shapes!

so, construct an alphabet of possible shapes

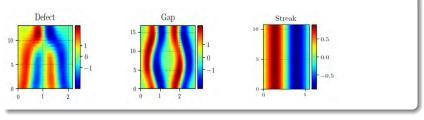
extracting a fundamental tile



- 1) invariant 2-torus
- 2) invariant 2-torus computed from initial guess cut out from 1)
- 3) "gap" invariant 2-torus, initally cut out from 2)
- 4) the "gap" prime invariant 2-torus fundamental domain

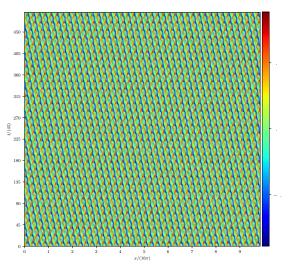
a trial set of prime (rubber) tiles

an alphabet of Kuramoto-Sivashinsky fundamental tiles



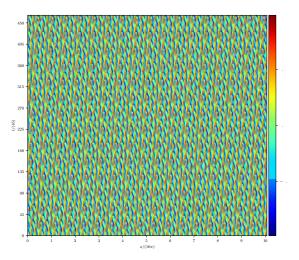
utilize also discrete symmetries : spatial reflection, spatiotemporal shift-reflect, · · ·

Kuramoto-Sivashinsky tiled by a small tile



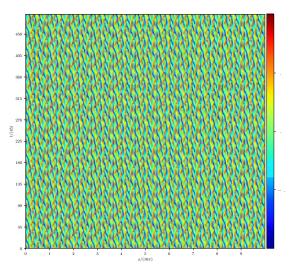
tiling by relative periodic invariant 2-torus (L, T) = (13.02, 15)

spacetime tiled by a larger tile



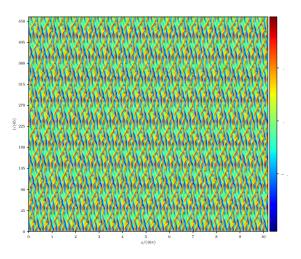
tiling by relative periodic invariant 2-torus (L,T)=(33.73,35)

spacetime tiled by a tall tile



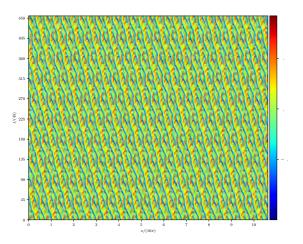
tiling by shift-reflect invariant 2-torus (L, T) = (55.83, 24)

spacetime tiled by a larger tile



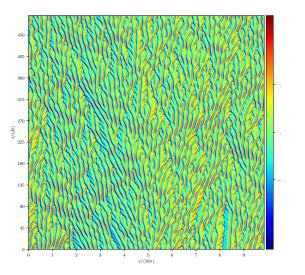
tiling by relative periodic invariant 2-torus (L, T) = (32.02, 51)

spacetime tiled by a larger tile



tiling by relative periodic invariant 2-torus (L, T) = (44.48, 50)

any particular tiling looks nothing like turbulent Kuramoto-Sivashinsky!



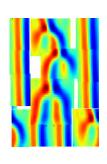
[horizontal] space $x \in [-L/2, L/2]$ [up] time evolution

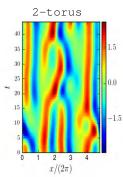
part 6

- turbulence in large domains
- 2 space is time
- spacetime
- fundamental tiles
- gluing tiles
- bye bye, dynamics

a qualitative tiling guess

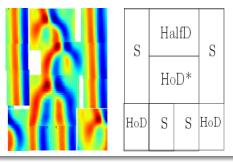
a tiling and the resulting solution





turbulence.zip: each solution has a unique symbolic name

symbolic dynamics is 2-dimensional!



0	2		0
0	1		0
0	1*		0
0			0
1	0	0	1
	0	0	

- each symbol indicates a corresponding spatiotemporal tile
- these are "rubber" tiles

part 7

- turbulence in large domains
- space is time
- bye bye, dynamics

in future there will be no future

goodbye

to long time and/or space integrators

they never worked and could never work

life outside of time

the trouble:

forward time-integration codes too unstable

multishooting inspiration: replace a guess that a point is on the periodic orbit by a guess of the entire orbit.

 \rightarrow

spatio-temporally periodic solutions of classical field theories can be found by variational methods

the equations solved as global optimization problems

impose the equations as local constraints

$$F(u) = u_t + u_{xx} + u_{xxxx} + uu_x = 0$$

minimize globally

perhaps using cost function

$$G \equiv \frac{1}{2} |F(u)|_{L \times T}^2$$

can computers

do this?

the answer is

scalability

compute locally, adjust globally

Navier-Stokes codes

- T. M. Schneider: developing a matrix-free variational Navier-Stokes code, machine learning initial guesses
- D. Lasagna and A. Sharma: developing variational adjoint solvers to find periodic orbits with long periods
- Q. Wang: parallelizing spatiotemporal computation is FLOPs intensive, but more robust than integration forward in time

it's rocket science^{8,9,10}

⁸T. M. Schneider, Variational adjoint methods coupled with machine learning, private communication, 2019.

⁹D. Lasagna et al., Periodic shadowing sensitivity analysis of chaotic systems, 2018.

¹⁰Q. Wang et al., Phys. Fluids **25**, 110818 (2013).

towards scalable parallel-in-time turbulent flow simulations

future:

processor speed \rightarrow limit $\mbox{number of cores} \rightarrow 10^6 \rightarrow \cdots$

Wang et al (2013)11:

next-generation: spacetime parallel simulations, on discretized 4D spacetime computational domains, with each computing core handling a spacetime lattice cell

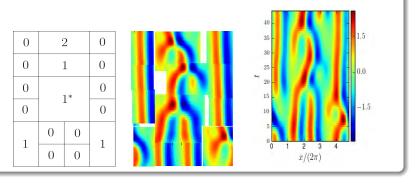
compared to time-evolution solvers: significantly higher level of concurrency, reduction the ratio of inter-core communication to floating point operations

⇒ a path towards exascale DNS of turbulent flows

¹¹Q. Wang et al., Phys. Fluids **25**, 110818 (2013).

enumerate hierarchically spatiotemporal patterns

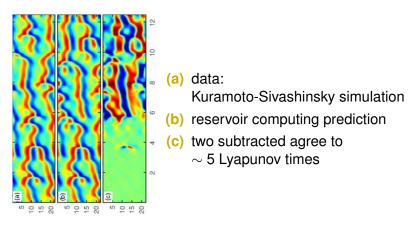
2D symbolic encoding \Rightarrow admissible solutions



- each symbol indicates a minimal spatiotemporal tile
- glue them in all admissible ways

machine learning will be needed

"reservoir computing" example 12



Q: how would you learn this data?

¹²J. Pathak et al., Phys. Rev. Lett. **120**, 024102 (2018).

take home: clouds do not integrate PDEs

do clouds integrate Navier-Stokes equations?



at any spacetime point Navier-Stokes equations describe the local tangent space

they satisfy them locally, everywhere and at all times

summary

- study turbulence in infinite spatiatemporal domains
- theory : classify all spatiotemporal tilings
- numerics : future is spatiotemporal

there is no more time there is only enumeration of spacetime solutions

spatiotemporally infinite spatiotemporal cat



part 8

- turbulence in large domains
- 2 space is time
- spacetime
- fundamental tiles
- gluing tiles
- bye bye, dynamics
- theory of turbulence ?

are d-tori

a theory of turbulence?

part 9

- (semi-)classical field theories
- state space
- symbolic dynamics

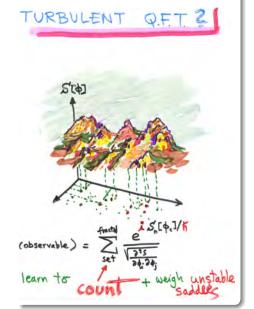
Dreams of Grand Schemes: solve

Yang-Mills

QFT path integrals : semi-classical quantization

a local unstable extremum

a fractal set of saddles

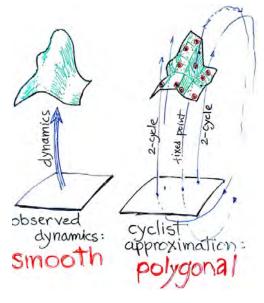


the very short answer: POT



if you win: I teach you how

(for details, see ChaosBook.org)



tessellate the state space by recurrent flows

classical trace formula for continuous time flows

$$\sum_{\alpha=0}^{\infty} \frac{1}{s - s_{\alpha}} = \sum_{p} T_{p} \sum_{r=1}^{\infty} \frac{e^{r(\beta A_{p} - sT_{p})}}{\left| \det \left(\mathbf{1} - M_{p}^{r} \right) \right|}$$

relates the spectrum of the evolution operator

$$\mathcal{L}(x',x) = \delta(x'-f^t(x)) e^{\beta A(x,t)}$$

to the unstable periodic orbits p of the flow $f^t(x)$.

classical trace formula for averaging over 2-tori

something like

$$\sum_{\alpha=0}^{\infty} \frac{1}{s - s_{\alpha}} = \sum_{p} V_{p} \sum_{r=1}^{\infty} \frac{e^{r(\beta A_{p} - sV_{p})}}{|\det \mathcal{J}_{p^{r}}|}$$

weighs the unstable relative prime (all symmetries quotiented) d-torus p by the inverse of its Hill determinant, the determinant (state space volume) of its orbit Jacobian matrix \mathcal{J}_p

$$\det \mathcal{J}_p$$

and V_p is the volume

$$V_p = T_p L_p$$

of the prime spacetime tile p

extras

speculation: code discrete Lagrangian methods?

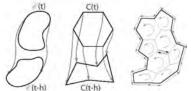
the idea : construct a discrete counterpart to the considered system

variational integrator : evolution map that corresponds to the discrete Euler–Lagrange equations

Discrete Lagrangian methods

action
$$S(q)=\int_0^T\!dt\,L(q,\dot q)$$
 + Hamilton's principle $\delta S(q)=0$ discretize $\int_{t_k}^{t_{k+1}}L(q,\dot q)\,dtpprox \Delta t L(q_k,q_{k+1})\,.$

symplectic methods preserve phase-space areas¹³



(left) Kelvin's circulation advected by the flow is constant (middle) the discrete version, on a Voronoi loop (right) circulation is constant on any discrete loop.

¹³J. E. Marsden and M. West, Acta Numerica **10**, 357–514 (2001).

Discrete Lagrangian codes?

so far, no codes for discretized spatiotemporal action / Lagrangian density

$$S = \int dq^d \, \mathcal{L}(q)$$

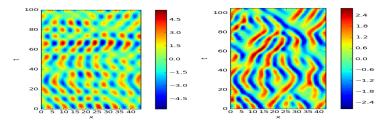
symplectic Euler incompressible fluid dynamics time-evolution codes exist¹⁴

claim: can apply to non-conservative system

Navier-Stokes?

¹⁴D. Pavlov et al., Physica D **240**, 443–458 (2011).

an intermediate spacetime domain

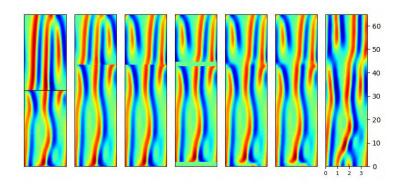


(left)
$$\bar{L}=2\pi\sqrt{2}$$
 modulated initial random guess $(L_0,T_0)=(5\bar{L},100)=(44.4,100)$

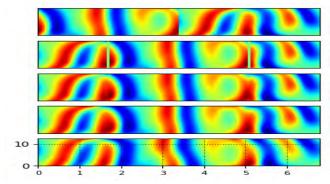
(right) Resulting invariant 2-torus
$$(L_f, T_f) = (43.066, 105.08) = (L_0 - 1.363, T_0 + 5.08)$$

Adjoint descent took only 7 laptop CPU seconds

temporally glued Frankenstein

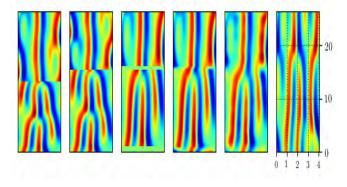


spatial gluing of two invariant 2-tori



- 1) two invariant 2-tori side by side
- 2) initial invariant 2-tori split into smaller tiles
- 3) a guess invariant 2-torus obtained by gluing / smoothing
- 4) converges to a larger invariant 2-torus

temporal gluing of two invariant 2-tori



- 1) an invariant 2-torus atop another invariant 2-torus
- 2) initial invariant 2-tori split into smaller tiles
- 3) a guess invariant 2-torus obtained by gluing / smoothing
- 4) converges to a larger invariant 2-torus

KS invariant 2-tori found by rocket science

the initial guess the converged solution u(x, t)

¹⁵Q. Wang et al., Phys. Fluids **25**, 110818 (2013).