Parallel spacetime approach to turbulence: computation of unstable periodic orbits and the dynamical zeta function

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1 – Navier-Stokes Equations

\[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla P + \nu \nabla^2 \mathbf{u} + \mathbf{F}(\mathbf{r}, t), \]

\[ \nabla \cdot \mathbf{u} = 0, \]

• nonlinearity arises directly from the kinematic aspects of the problem

• Typical control parameter, Reynolds number: \( \text{Re} = \frac{LU}{\nu} \)

• \( \text{Re} \approx 10^6 \) for many common situations; algorithmic complexity scales with \( \text{Re}^3 \)

• After the onset of turbulence, systems exhibit large fluctuations on many length and time scales

• Solution to the 3D NSE (proof of existence and smoothness) still an open problem (Temam, 1984)
1 – Navier-Stokes Equations

• Kolmogorov picture of turbulence: “Big whorls have little whorls
Which feed on their velocity
And little whorls have lesser whorls
And so on to viscosity”

- Lewis F. Richardson

• Kolmogorov length: \( l_0 \approx \frac{L}{\text{Re}^{3/4}} \)

• Dynamical systems approach: strange attractor is closure of the set of all the UPOs (in the neighbourhood of which the system will spend most of the time)

• For 2D NSE in the general case: finite-dimensional attracting set (scaling as a power of Re)

• For 3D NSE: proven with certain assumptions (Constantin, Foias, Temam, 1985)
Example of a strange attractor: Lorenz system

\[
\begin{align*}
\frac{dx}{dt} &= \sigma (y - x) \\
\frac{dy}{dt} &= x(\rho - z) - y \\
\frac{dz}{dt} &= xy - bz
\end{align*}
\]

- \( \sigma = \text{Rayleigh number} \)
- \( \rho = \text{Prandtl number} \)
- \( \beta = 8/3 \)
- \( \rho = 28 \)
- \( \sigma = 10 \)

\( x \): proportional to intensity of convection
\( y \): proportional to temperature difference

- 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 – 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.
2 – Unstable Periodic Orbits

• Abstract “dynamical landscape” with peaks representing the UPOs;

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

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

• Relative height of the peaks is related to the natural measure of the indicated UPOs (straight lines are just visual aids in identifying the corresponding cyclic pieces of the period-2 cycles in the diagram)

from: http://www.scholarpedia.org/article/Unstable_periodic_orbits
Curator: Dr. Paul So, George Mason University, Fairfax, VA
3 – 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 is using a generating function:

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

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

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

\[ \frac{\partial s}{\partial \beta} \bigg|_{\beta=0} = \langle A \rangle, \]

\[ \frac{\partial^2 s}{\partial \beta^2} \bigg|_{\beta=0} = \left\langle A^2 \right\rangle - \langle A \rangle^2. \]
3 – Dynamical Zeta function

• If a “sufficient” number of UPOs is known, the DZF can be calculated;

• DZF expression

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

  - product runs over all UPO’s with period \( T < T_{\text{max}} \)
  - \( T_p \) : period of the UPO.
  - \( A_p \) : average value of the observable on the UPO.
  - \( \Lambda_p \) : stability eigenvalue of the UPO.

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

• Computation of expectation value:

\[ \frac{\partial s}{\partial \beta} \bigg|_{\beta=0} = \langle A \rangle \]
3 – Dynamical Zeta function

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

B. M. Boghosian et al. Unstable Periodic Orbits in the Lorenz attractor, accepted for publication, *Phil. Trans. R. Soc. A*, 2011.
3 – 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
4 – HYPO4D

- Kawahara & Kida (2001) found two periodic solutions in plane Couette flow, using spectral methods;

- Novel efficient variational algorithm to locate UPOs\(^1\);

- Tested on Lorenz model and other low-dimensional systems; good convergence to the UPOs, including 2D fluid;

- Plot $\Delta(t,T)$: 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 (and $T$);

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\(^1\) B. M. Boghosian \textit{et al.} New Variational Principles for Locating Periodic Orbits of Differential Equations, accepted for publication, \textit{Phil. Trans. R. Soc. A}, 2011.
4 – HYPO4D (Lattice Boltzmann Method)

• Fluid flow (nearly incompressible NSE) is simulated using the Lattice Boltzmann Method\textsuperscript{1,2}

\[
f_i(\vec{r} + \vec{c}_i, t + 1) = f_i(\vec{r}, t) + \Omega_i(\vec{r}, t),
\]
\[
\rho = \sum_{i=1}^{b} f_i, \quad \rho \ddot{\vec{u}} = \sum_{i=1}^{b} \rho f_i \vec{c}_i.
\]
\[
\sum_{i=1}^{b} \Omega_i = 0, \quad \sum_{i=1}^{b} \Omega_i \vec{c}_i = \vec{0}.
\]
\[
f_i(\vec{r} + \vec{c}_i, t + 1) - f_i(\vec{r}, t) = S_{ij}(f_j(\vec{r}, t) - f_{ij}^{eq}(\vec{r})),
\]
\[
f_i(\vec{r} + \vec{c}_i, t + 1) - f_i(\vec{r}, t) = -\frac{1}{\tau}(f_i(\vec{r}, t) - f_{ij}^{eq}(\vec{r})).
\]

\[
f_i^{eq}(\rho, \ddot{\vec{u}}) = \rho[a + b \vec{c}_i \cdot \ddot{\vec{u}} + c(\vec{c}_i \cdot \ddot{\vec{u}})^2 + d\ddot{\vec{u}}^2],
\]
\[
\sum_{i=1}^{b} f_i^{eq} = \rho, \quad \sum_{i=1}^{b} f_i^{eq} \vec{c}_i = \rho \ddot{\vec{u}},
\]
\[
\nu = (\tau - \frac{1}{2})c_s^2 \Delta t,
\]

4 – HYPO4D (LBM)

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

Main advantages of LBM:

- local collision operator + linear streaming operator (nearly “embarrassingly” parallel);
- minimal set of velocities;
- no need for extra term for extra eq. for pressure term;

• HYPO4D: Linear scaling up to 16K on Ranger (TACC), TG08 scalability award;
4 – HYPO4D

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 (seamlessly) deployed on a great number of platforms;

Linear scaling up to 131K on JUGENE (IBM BlueGene/P), after slight optimization in communication pattern;
4 – HYPO4D

• Current approach: fluid starts from rest, periodic boundary conditions in all directions (isotropic, homogeneous turbulence), ABC (Arnold-Beltrami-Childress) type force\(^1\) applied:

\[
\begin{align*}
\nabla \cdot \vec{F} &= 0 \\
\nabla \times \vec{F} &= \vec{F}
\end{align*}
\]

• 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 the Reynolds number, inertia overcomes acceleration and (steady) turbulent behaviour sets in;

\(^{1}\)L. Fazendeiro et al. Unstable Periodic Orbits in Weak Turbulence, JOCS, 1, 13-23, 2010.
4 - HYPO4D: Convergence test

Convergence test for the velocity field, taken between consecutive time steps. Notice sharp increase after inertia of the fluid becomes predominant (vertical axis scale is logarithmic). (L. Fazendeiro et al. Unstable Periodic Orbits in Weak Turbulence, JOCS, 1, 13-23, 2010).

- Cubic lattice, $64^3$, varying LB relaxation time;
- Maximum Re ~ 500, taking velocity averaged over many time, steps, but DNS, no modeling included;
4- HYPO4D: Energy spectrum $E(q)$

Kolmogorov picture of turbulent flow divides it into 3 different scales: kinetic, inertial, dissipative.

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

Right plot shows spectrum for two different time snapshots after the transition, with Kolmogorov fitting for visual aid.
4 - HYPO4D: locating candidate orbits

- System is $64^3$, with $\epsilon=0.53$, Re=371
- Vertical axis is $T$, horizontal axis is $t$, color code gives:

$$\Delta(t, T) \equiv \sqrt{\sum_r \sum_{i=1}^{l} (f_i(r, t + T) - f_i(r, t))^2},$$
4 - HYPO4D: locating candidate orbits

- Detail of previous plot, showing several (purplish) minima/areas of interest; Sampling rate = 500 (.xdr format for I/O)
4 - HYPO4D: locating candidate orbits (now at fixed t)

- Same as before, but this time fixed t, in order to determine optimal T; sampling rate = 1;
4 - HYPO4D: spacetime relaxation

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

- For T=24.5K, we have to keep in memory at least $64^3 \times 19$ (number of LB velocities) $\times 8$ (double precision) $\times 2.45 \times 10^4$ variables $\sim 1$ TB; Then SD=5 copies and CG=8!!!!!!

- Minimization algorithm:

  - define functional

  
  \[
  \mathcal{F} \equiv \frac{1}{2} \sum_{t=0}^{T-1} \sum_{\vec{r}} \sum_{i=1}^{b} |\phi_i(\vec{r}, t)|^2 \quad \text{with}
  \]

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

  - compute gradient

  \[
  \frac{\delta \mathcal{F}}{\delta f_k(\vec{s}, q)}
  \]
4 - HYPO4D: spacetime relaxation

- Fill (4D) lattice with $f_i(\vec{r}, t)$ from $t = t_0, T - 1$
- 4D collide and stream (periodic time BC)
- Compute $\phi$ and initial $\mathcal{F}$
- Combination of SD and/or CG until $\mathcal{F}$ no longer varies
- SD algorithm:
  $$f_i(\vec{r}, t) = \alpha \times \frac{\partial \mathcal{F}}{\partial f_i(\vec{r}, t)}$$
- $\alpha$ found through golden mean search procedure, done at every step
4 - HYPO4D: spacetime relaxation

- Left: t=177K, T=26864 orbit, RMS value of F per lattice site = 1.7504e-05, after 340 SD iterations;
- Right: t=637K, T=24594 orbit, RMS value of F per lattice site = 1.4076e-05 after 300 SD iterations;
4 - HYPO4D: vorticity field

- Magnitude of the vorticity field, thresholded, for the $t=177K$, $T=26864$ UPO, displaying very structured patterns (perhaps smaller UPOs may be escaping detection....)
5 – Computational aspects

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

- For the minima shown previously, assuming $T = 3 \times 10^4$ time steps, we have to load memory $64^3 \times 19$ (number of velocities) $\times 8$ (double precision) $\times 3 \times 10^4$ variables $\sim 1.2$ TB;

- One single minimization run can take $\sim 1$M SUs and more ($\sim 24$h wall clock time);

- On JUGE NE: 17M core hours, with 7 new UPOs (largest so far) - post-processing work still ongoing;

- About 15TBytes of data, shipped back to UCL (and US storage facilities) via globus-url-copy;
6 - Prospects

• Further characterization of the turbulent state (energy dissipation rate, vorticity, enstrophy, etc);

• Relaxation procedure in order to identify prime (smaller period) UPOs in 3D NSE (and make sure we identify all the smallest ones);

• Implementation of more sophisticated minimization algorithms, using Newton-Krylov solvers and GMRES (maintaining spacetime variational principle);
6 - Prospects

- Long-term goal: Compare averages from several UPOs (via DZF) with time forward averaging;

- Classification of the (prime) UPOs identified + creation and maintenance of a digital library of such orbits;

- Compute dynamical zeta function for turbulent hydrodynamics!
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