An efficient 2nd order scheme for the long time statistical behavior of the 2D Navier-Stokes equations

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Outline

Statistical Approach
- Examples
- Definitions

Temporal Approximation
- Possible deficiency of classical schemes
- First order scheme
- 2nd order scheme

Fully discretized scheme

Summary

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Logistic map

$$x^{n+1} = T(x^n), \quad T(x) = 4x(1-x), x \in [0,1]$$

Figure: Sensitive dependence

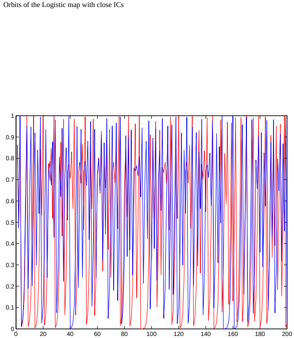
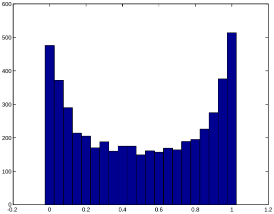


Figure: Statistical coherence



Lorenz 96 model (Majda-Abramov version)

Edward Norton Lorenz, 1917-2008

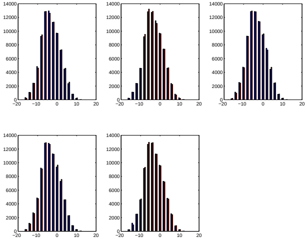
$$\textcolor{red}{Lorenz96}: \frac{du_j}{dt} = (u_{j+1} - u_{j-2})u_{j-1} - u_j + F$$

$$j = 0, 1, \cdots, J; \qquad J = 5, F = -12$$

Figure: Sensitive dependence

(Sensitive dependence)

Figure: Statistical coherence



Energy dissipation rate per unit mass

- $$\begin{aligned} \mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \nu\Delta\mathbf{u} + \mathbf{F}, \nabla\cdot\mathbf{u} = 0, \\ \varepsilon &= \nu < \|\nabla\mathbf{u}\|^2 >, \end{aligned}$$

  Energy injected at large scale, cascaded down in the inertial range, dissipated at small scale

Figure: Andrey Kolmogorov, 1903-1987

- $$\begin{aligned} U_e &= \sqrt{2e}, \quad e = \frac{1}{2} < |\mathbf{u}|^2 >, \\ t_e &= \frac{e}{\varepsilon} = \frac{L_e}{U_e}, \\ &\Rightarrow \quad \varepsilon \approx \frac{U^3}{L} \end{aligned}$$

- Kolmogorov dissipation length

$$l_d = (\frac{\nu^3}{\varepsilon})^{\frac{1}{4}}$$

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Statistical Approaches

$$\frac{d\mathbf{u}}{dt} = \mathbf{F}(\mathbf{u}), \quad \mathbf{u} \in H$$

- Long time average

$$< \Phi >= \lim_{T\to\infty} \frac{1}{T} \int_0^T \Phi(\mathbf{v}(t))\, dt$$

- Spatial averages

$$< \Phi >_t = \int_H \Phi(\mathbf{v})\, d\mu_t(\mathbf{v})$$

$\{\mu_t, t \geq 0\}$ statistical solutions

Statistical Solutions

$$\{\mu_t, t \geq 0\}, \quad \frac{d\mathbf{v}}{dt} = \mathbf{F}(\mathbf{v}), \quad \{S(t), t \geq 0\}$$

- Pull-back

$$\mu_0(S^{-1}(t)(E)) = \mu_t(E)$$

- Push-forward (Φ: suitable test functional)

$$\int_H \Phi(\mathbf{v})\, d\mu_t(\mathbf{v}) = \int_H \Phi(S(t)\mathbf{v})\, d\mu_0(\mathbf{v})$$

- Finite ensemble example

$$\mu_0 = \sum_{j=1}^{N} p_j \delta_{\mathbf{v}_{0j}}(\mathbf{v}), \mu_t = \sum_{j=1}^{N} p_j \delta_{\mathbf{v}_j(t)}(\mathbf{v}), \mathbf{v}_j(t) = S(t)\mathbf{v}_{0j}$$

$$\mu_t(E) = \sum_{\mathbf{v}_j(t)\in E} p_j = \sum_{\mathbf{v}_{0j}\in S^{-1}(E)} p_j = \mu_0(S^{-1}(E))$$

Liouville's equations

Figure: Joseph Liouville, 1809-1882

- Liouville type equation (Foias)

$$\frac{d}{dt}\int_H \Phi(\mathbf{v})\, d\mu_t(\mathbf{v}) = \int_H < \Phi'(\mathbf{v}), \mathbf{F}(\mathbf{v}) > \, d\mu_t(\mathbf{v})$$

Φ good test functionals e.g.

$$\Phi(\mathbf{v}) = \phi((\mathbf{v}, \mathbf{v}_1), \cdots, (\mathbf{v}, \mathbf{v}_N))$$

- Liouville equation (finite d)

$$\frac{\partial}{\partial t} p(\mathbf{v}, t) + \nabla \cdot (p(\mathbf{v}, t)\mathbf{F}(\mathbf{v})) = 0$$

Hopf's equations

Figure: Eberhard Hopf, 1902-1983

Hopf's equation (special case of Liouville type)

$$\frac{d}{dt}\int_H e^{i(\mathbf{v},\mathbf{g})}\, d\mu_t(\mathbf{v})$$

$$= \int_H i < \mathbf{F}(\mathbf{v}), \mathbf{g} > e^{i(\mathbf{v},\mathbf{g})}\, d\mu_t(\mathbf{v})$$

Stationary Statistical Solutions (IM)

- Invariant measure (IM) $\mu \in \mathcal{PM}(H)$

$$\mu(S^{-1}(t)(E)) = \mu(E), \forall t \geq 0$$

- Stationary statistical solutions: essentially

$$\int_H < F(\mathbf{v}), \Phi'(\mathbf{v}) > \, d\mu(\mathbf{v}) = 0, \forall \Phi$$

- Example:

$$\frac{dr}{dt} = r(1 - r^2), \frac{d\theta}{dt} = 1$$

$$\mu_0 = \delta_0, d\mu_1 = \frac{1}{2\pi} d\theta$$

Figure: George David Birkhoff, 1884-1944

Definition

μ is ergodic if $\mu(E) = 0,$ or 1 for all invariant sets E.

Theorem (Birkhoff's Ergodic Theorem)

If μ is invariant and ergodic, the temporal and spatial averages are equivalent, i.e.

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \varphi(S(t)\mathbf{u})\, dt = \int_H \varphi(\mathbf{u})\, d\mu(\mathbf{u}),\ a$$

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$$\frac{d\mathbf{u}}{dt} = \mathbf{F}(\mathbf{u}), \quad \mathbf{u} \in H$$

- classical scheme of order m

$$\|\mathbf{u}(n\Delta t) - \mathbf{u}^n\| \leq C(n\Delta t)\Delta t^m, \quad C(T) = \exp(\alpha T)$$

- Error in approximation of long time averages

$$\begin{aligned} & |\limsup_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} (\Phi(\mathbf{u}(n\Delta t)) - \Phi(\mathbf{u}^n))| \\ \leq \quad & c \limsup_{N\to\infty} \Delta t^m \frac{\exp((N+1)\alpha\Delta t) - \exp(\alpha\Delta t)}{\exp(\alpha\Delta t) - 1} \\ = \quad & \infty. \end{aligned}$$

- Classical schemes may not be suitable for approximating the climate although they may work well for weather.
- Preliminary numerics on Lorenz 96 (Majda-Abramov version) indicates various regimes with forward Euler: blow-up, severe numerical artifacts in pdf with relatively small time step
- similar issue with SDE (Majda, E, Liu)
- What schemes ensure the convergence of stationary (long time) statistical properties?

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Dissipative system

Definition

A dynamical system $\{S(t), t \geq 0\}$ on a phase space H is called dissipative if there exists a global attractor $\mathcal{A}$ such that

- $\mathcal{A}$ is invariant under $S(t)$
- $\mathcal{A}$ is compact.
- $\mathcal{A}$ attracts all bounded set B in H, i.e.,

$$\lim_{t \to \infty} \text{dist}(S(t)B, \mathcal{A}) = 0.$$

- $\mathcal{IM}$ (the set of all invariant measures) is a convex compact set (with respect to the weak topology)
- supp$\mu \subset \mathcal{A}, \forall \mu \in \mathcal{IM}$

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Discrete dynamical system S_k approximate dissipative dynamical system $S(t), t \geq 0$.

Theorem (Abstract result, W. (Math. Comp. 2010))

Assume

1. *(Uniform dissipativity)* $K = \bigcup_{0<k\leq k_0} \mathcal{A}_k$*: pre-compact*
2. *(Finite time uniform convergence)* $\sup_{\mathbf{u}\in\mathcal{A}_k, nk\in[t_0,1]} \|S_k^n\mathbf{u} - S(nk)\mathbf{u}\| \to 0,$ *as* $k \to 0$.
3. *(Uniform continuity of the continuous system)* $\lim_{t\to T^*} \sup_{\mathbf{u}\in K} \|S(t)\mathbf{u} - S(T^*)\mathbf{u}\| = 0$.

Then

1. *(Conv. of stationary stat. prop.)*

$$\mu_k \rightharpoonup \mu, \ \mu_k \in \mathcal{IM}_k, \mu \in \mathcal{IM}.$$

2. *(Conv. of attractors)*

$$\lim_{k\to 0} dist(\mathcal{A}_k, \mathcal{A}) = 0.$$

Remark 1. Possible deficiency with fully explicit (stability) or fully implicit (unique solvability). 2. Classical energy stability is insufficient

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The infinite Prandtl number model

- $$\begin{aligned} \frac{1}{Pr}\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) + \nabla p &= \Delta \mathbf{u} + Ra\,\mathbf{k}T, \quad \nabla\cdot\mathbf{u} = 0, \quad \mathbf{u}|_{z=0,1} = 0, \\ \frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T &= \Delta T. \end{aligned}$$
- $$\begin{aligned} \nabla p &= \Delta \mathbf{u} + Ra\,\mathbf{k}T, \quad \nabla\cdot\mathbf{u} = 0, \quad \mathbf{u}|_{z=0,1} = 0, \\ \frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T &= \Delta T. \end{aligned}$$
- Alternative form (large Peclét number)
$$\frac{\partial T}{\partial t} + Ra\,A^{-1}(\mathbf{k}T)\cdot\nabla T = \Delta T$$
- Fast advection time formulation $\tau = Ra\,t$ (multiple time scale, optimal transport)
$$\frac{\partial T}{\partial \tau} + A^{-1}(\mathbf{k}T)\cdot\nabla T = \frac{1}{Ra}\Delta T$$

Application to ∞ Pr. model, Cheng&W. SINUM2008, W.MathComp2010

∞ Prandtl number model (perturbative form)

$$\frac{\partial\theta}{\partial t} + Ra\, A^{-1}(\mathbf{k}\theta)\cdot\nabla\theta - Ra\, A^{-1}(\mathbf{k}\theta)_3\tau' = \Delta\theta + \tau'', \quad \theta|_{z=0,1} = 0.$$

$\tau(z) = \frac{1}{2}, cRa^{-1/3} \leq z \leq 1 - cRa^{-1/3}$, essentially piecewise linear

Linear implicit scheme

$$\begin{aligned} & \frac{\theta_k^{n+1} - \theta_k^n}{k} + Ra\, A^{-1}(\mathbf{k}\theta_k^n)\cdot\nabla\theta_k^{n+1} \\ & + Ra\,(A^{-1}(\mathbf{k}(\lambda\theta_k^{n+1} + (1-\lambda)\theta_k^n)))_3\tau'(z) \\ = \quad & \Delta\theta_k^{n+1} + \tau''(z), \quad \lambda \in [0,1] \end{aligned}$$

A linear symmetric implicit scheme(W.)

$$\frac{\theta_k^{n+1} - \theta_k^n}{k} + Ra\, A^{-1}(\mathbf{k}\theta_k^n) \cdot \nabla\theta_k^n + Ra\,(A^{-1}(\mathbf{k}(\theta_k^n)))_3\tau'(z)$$
$$= \quad \Delta\theta_k^{n+1} + \tau''(z),$$

- severe restriction on step size

Yet another linear scheme (Douglas-Dupont regularization)

$$\frac{\theta_k^{n+1} - \theta_k^n}{k} - \lambda\Delta(\theta_k^{n+1} - \theta_k^n) + Ra\, A^{-1}(\mathbf{k}\theta_k^n) \cdot \nabla\theta_k^n + Ra\,(A^{-1}(\mathbf{k}(\theta_k^n)))_3\tau'(z$$
$$= \quad \Delta\theta_k^{n+1} + \tau''(z),$$

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=\ &\Delta\theta_k^{n+1} + \tau''(z),
\end{aligned}
$$

NSE 1st order scheme

- 2D NSE in a periodic box in streamfunction-vorticity formulation

$$\frac{\partial \omega}{\partial t} + \nabla^{\perp}\psi \cdot \nabla\omega - \nu\Delta\omega = f, \ -\Delta\psi = \omega$$

- an efficient classical 1st order scheme

$$\omega^{n+1} = \omega^{n} + k(\Delta\omega^{n+1} - \nabla^{\perp}\psi^{n} \cdot \omega^{n} + f^{n})$$

- Main result (Gottlieb-Tone-Wang-W.-Wirosoetisno 2011) Long time statistical properties of the scheme converge to that of the 2D NSE.
- Alternative schemes exist

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Second order scheme

- BDF2AB2 scheme

$$\frac{3\omega^{n+1} - 4\omega^n + \omega^{n-1}}{2k} + \nabla^\perp(2\psi^n - \psi^{n-1}) \cdot \nabla(2\omega^n - \omega^{n-1}) - \nu\Delta\omega^{n+1} = f^{n+1}.$$

- Dynamical system formulation

$$\mathbb{S}_k \begin{bmatrix} \omega^n \\ \omega^{n-1} \end{bmatrix} = \begin{bmatrix} \omega^{n+1} \\ \omega^n \end{bmatrix}$$

Theorem (convergence of stationary statistical properties)

Let $f \in \dot{H}^1_{per}$ be a time-independent function. Then the discrete dynamical systems defined via the scheme is autonomous and dissipative with non-empty set of invariant measures $\mathcal{IM}_k$. Denote $\mathcal{P}_j, j = 1, 2$ the projection from $(\dot{L}^2)^2$ onto its j^{th} coordinate. Let $\{\mu_k, k \in (0, k_0]\}$ with $\mu_k \in \mathcal{IM}_k, \forall k$, be an arbitrary invariant measure of the numerical scheme . Then each subsequence of $\{\mu_k\}$ must contain a subsubsequence (still denoted $\{\mu_k\}$) and two invariant measure μ_j of the NSE so that $\mathcal{P}_j \mu_k$ weakly converges to μ_j, i.e.,

$$\mathcal{P}_j^* \mu_k \rightharpoonup \mu_j, k \to 0,$$

where $\mathcal{P}_j^* \mu_k(S) = \mu_k(\mathcal{P}_j^{-1}(S)), \forall S \in \mathcal{B}(\dot{L}^2)$.

- Dynamical system approach is not directly applicable.
- Dissipation from the BDF2 is crucial

$$(\frac{3}{2}v_2 - 2v_1 + \frac{1}{2}v_0)v_2 = \frac{1}{2}\left(|\mathbf{V}_1|_G^2 - |\mathbf{V}_0|_G^2\right) + \frac{(v_2 - 2v_1 + v_0)^2}{4}$$

$$\|\mathbf{V}\|_G = \mathbf{V} \cdot G\mathbf{V}, G = ([\frac{1}{2}, -1]^T, [-1, \frac{5}{2}]^T)$$

- Choice of AB2 is important
- New estimate on the nonlinear term via Wente type approach
- new two step Gronwall type approach
- Advection term treatment in the collocation Fourier is important in fully discretized case
- Appropriate projection (combination) ($\mathbf{V} \cdot [-\frac{1}{2}, \frac{3}{2}]^T$) is also critical

Wente type estimates

Let $\dot{H}^m_{per}(\Omega)$ be the periodic Sobolev space of order m with zero average. There exists an absolute constant $C_w \geq 1$ such that

$$\begin{aligned}
\|\nabla^\perp\psi\cdot\nabla\phi\|_{H^{-1}} &\leq C_w\|\psi\|_{H^1}\|\phi\|_{H^1}, \quad \forall\psi\in\dot{H}^1_{per}, \phi\in\dot{H}^1_{per}(\Omega),\\
\|\nabla^\perp\psi\cdot\nabla\phi\|_{H^{-1}} &\leq C_w\|\psi\|_{H^2}\|\phi\|_{L^2}, \quad \forall\psi\in\dot{H}^2_{per}, \phi\in\dot{L}^2(\Omega),\\
\|\nabla^\perp\psi\cdot\nabla\phi\|_{L^2} &\leq C_w\|\psi\|_{H^2}\|\phi\|_{H^1}, \quad \forall\psi\in\dot{H}^2_{per}, \phi\in\dot{H}^1_{per}(\Omega),\\
\|\nabla^\perp\psi\cdot\nabla\phi\|_{L^2} &\leq C_w\|\psi\|_{H^1}\|\phi\|_{H^2}, \quad \forall\psi\in\dot{H}^1_{per}, \phi\in\dot{H}^2_{per}(\Omega),\\
\|\nabla^\perp\psi\cdot\nabla\phi\|_{H^1} &\leq C_w\|\psi\|_{H^2}\|\phi\|_{H^2}, \quad \forall\psi,\phi\in\dot{H}^2_{per}(\Omega).
\end{aligned}$$

2 step discrete Gronwall

Let $\{g^n\}$ be a non-negative sequence. Suppose there exist constants $\varepsilon > 0, \beta > 0, \lambda \in (0,1)$ such that

$$g^{n+1} \leq \frac{\lambda}{1+\varepsilon} g^n + \frac{1-\lambda}{1+\varepsilon} g^{n-1} + \frac{\beta\varepsilon}{1+\varepsilon}, \forall n \geq 1.$$

Then we have, for $\gamma = \frac{1+\varepsilon/2}{1+\varepsilon} < 1$, and $n \geq 2$,

$$\begin{aligned} g^{n+1} &\leq \gamma \max\{g^n, g^{n-1}, 2\beta\}, \\ g^{n+1} &\leq \gamma \max\{\gamma^{\lfloor \frac{n-1}{2} \rfloor} g^2, \gamma^{\lfloor \frac{n-1}{2} \rfloor} g^1, 2\beta\}. \end{aligned}$$

where $\lfloor \cdot \rfloor$ denotes the floor function (the biggest integer bounded by $\cdot$).
($g \approx \|\mathbf{V}\|^2_{\mathbf{G}}$)

fully discrete scheme

- Galerkin Fourier

$$\frac{3\omega_N^{n+1} - 4\omega_N^n + \omega_N^{n-1}}{2k} + P_N(\nabla^\perp(2\psi_N^n - \psi_N^{n-1}) \cdot \nabla(2\omega_N^n - \omega_N^{n-1})) - \nu\Delta\omega_N^{n+1} = F$$

- Collocation Fourier

$$\begin{aligned} & \frac{3\omega_N^{n+1} - 4\omega_N^n + \omega_N^{n-1}}{2k} - \nu\Delta\omega_N^{n+1} - f_N^{n+1} \\ = \quad & -\frac{1}{2}(\nabla_N^\perp(2\psi_N^n - \psi_N^{n-1}) \cdot \nabla(2\omega_N^n - \omega_N^{n-1}) \\ & +\nabla_N \cdot (\nabla_N^\perp(2\psi_N^n - \psi_N^{n-1})(2\omega_N^n - \omega^{n-1}))) \\ & -\Delta_n\psi^j = \omega_N^j, j = n-1, n. \end{aligned}$$

Summary

- Statistical approach is necessary for chaotic/turbulent system
- Classical schemes may not be good for climate simulation
- Preserving dissipativity is crucial (Hale, Gunzburger, Shen, Foias, Temam, Jolly, Titi, Stuart, Suli, Ju, Tone, Yan,...)
- Similar idea exist for Hamiltonian system (symplectic integrator), hyperbolic conservation law (SSP, or TVD), dispersive wave (DRP scheme), ...
- There exist "efficient" 1st and 2nd order numerical schemes
- Long way to go to reach our goal

Questions

- Is 2nd order really better than 1st order?
- What happens if we are interested in a few simple observables only?
- Selection of physical invariant measure? Noise effect? Mixing rate and noise?
- Multi-scale schemes?
- Partially/weakly dissipative systems?
- Generalized dynamical systems?
- Non-autonomous system, seasonal effect?
- Model error and uncertainty?
- Linear response? Climate change?

Happy 60th Birthday!