Analysis of Parameter Estimation Algorithms in Nonlinear PDEs

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“Empty Hand” Data Assimilation

Fundamental Issues

1. **(Error)** in model and observations
2. **(High Dimensionality)** system dimension $\gg$ # of observations
3. **(Incompleteness)** initial data only known partially
4. **(Nonlinear)** problem is nonlinear (even when model is linear!)

Isolating Difficulties

(Highly) idealized scenario

1. ~~**(Error)** Model and Observations~~ Deterministic Problem!
2. **(High Dimensionality)** Model given by PDE
3. **(Incompleteness)** Only finite-rank projection of solution known
4. **(Nonlinear)** Parameters appear affinely in the system

Defining the Problem

Reality.

$$\partial_t u = F(u; \vec{\alpha}), \quad u = u(t, x). \qquad (Model)$$

where

$$\vec{\alpha} = (\alpha_1, \dots, \alpha_p) \sim \text{ unknown system parameters}$$

Observations.

$$\mathscr{O} = \{H_\delta u(t)\}_{t \geq 0}, \qquad (Obs)$$

where

$$\delta \sim \text{ spatial resolution}, \quad H_\delta \sim \text{ finite-rank projection}$$

Examples of H_δ

1. Projection onto Fourier modes up to wavenumbers $\leq \delta^{-1}$
2. Local spatial averages distributed domain of mesh size $\sim \delta$
3. Nodal values distributed across domain spaced $\sim \delta$ apart

Defining the Problem

$$\partial_t u = F(u; \vec{\alpha}) \qquad (\mathit{Model})$$

$$\mathscr{O} = \{H_\delta u(t)\}_{t \geq 0}, \qquad (\mathit{Obs})$$

Problem.

Given knowledge of (*Model*) and (*Obs*), define a mapping

$$\mathcal{A} : \mathscr{O} \mapsto \vec{\alpha}$$

Note that both $\underbrace{(I - H_\delta)u}_{\text{unobserved state}}$ and $\vec{\alpha}$ are **unknown**!

State Estimation

State Estimation via Dynamic Relaxation (Nudging)

Assume parameters are known...

Reality.

$$\partial_t u + Au = F(u)$$

Nudging equation.

$$\partial_t v + Av = F(v) - \underbrace{\mu(H_\delta v - H_\delta u)}_{nudging},$$

where

$$\mu \sim \text{ nudging parameter}$$

Azouani-Olson-Titi

2D Navier-Stokes Equations

$$\partial_t u + \underbrace{\nu(-\Delta)u}_{Au} = \underbrace{-u\cdot\nabla u - \nabla p + f}_{F(u)}, \quad \nabla\cdot u = 0, \qquad (NSE)$$

where $\nu > 0$ kinematic viscosity, p scalar pressure field, f external force

Nudged NSE

$$\partial_t v - \nu\Delta v = -v\cdot\nabla v - \nabla q + f - \mu(H_\delta v - H_\delta u), \quad \nabla\cdot v = 0 \qquad (NSE_\mu)$$

Theorem (Azouani-Olson-Titi, 2013)

There exists $\mu_0 = \mu_0(\nu, f)$ such that if

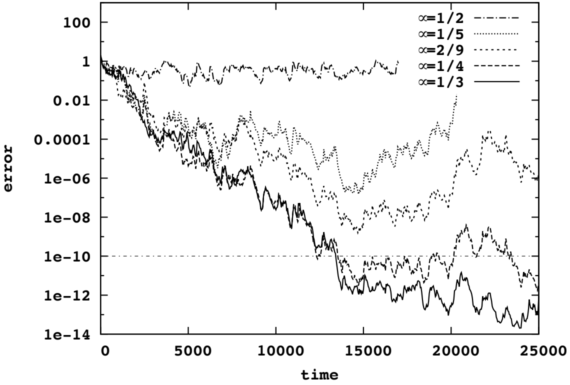
$$\mu > \mu_0 \quad \textit{and} \quad \mu\delta^2 < \nu$$

Then

$$\underbrace{RMS = \|v(t) - u(t)\|_{L^2} \leq O(e^{-\mu t})}_{\textit{asymptotic synchronization}}$$

Computational results with 2D Navier-Stokes

Gesho-Olson-Titi, 2016 (512^2, $f = P_{110 \le |k| \le 132} f, \nu = 10^{-4}, G = 2.5 \times 10^6$)



Proof of Azouani-Olson-Titi Theorem

Form the difference between (Model)

$$\partial_t u + Au = F(u),$$

and (Model)$_\mu$

$$\partial_t v + Av = F(v) - \mu(H_\delta v - H_\delta u)$$

Call $w = v - u$. Then

$$\partial_t w + Aw + \mu w = F(v) - F(u) + \mu(I - H_\delta)w$$

Proof of Azouani-Olson-Titi Theorem

Morally

$$\partial_t w + \underbrace{Aw}_{dissipation} + \underbrace{\mu w}_{damping} \sim \underbrace{(DF(u))w}_{nonlinear\ source} + \underbrace{\mu(I - H_\delta)w}_{interpolation\ error}$$

Want to balance

dissipation $\sim$ interpolation error & *damping* $\sim$ nonlinear source

Choose

$\mu \gtrsim$ maximal Lyapunov exponent

$\mu\delta^2 \lesssim$ dissipative length scale

Then

$$\partial_t w + \mu w \approx 0$$

"Done!"

Literature (of nudging-based DA (a lá Azouani, Olson, Titi) in the context of PDEs)

Computational Studies

2016, Gesho-Olson-Titi (2D NSE, nudging with general observables)
2016, Altaf-Titi-Knio-Zhao-McCabe-Hoteit (2D Bénard convection, low Rayleigh)
2017, Farhat-Jolly-Johnston-Titi (2D Bènard convection, large Rayleigh)
2017, Lunasin-Titi (stabilization, Kuramoto-Sivashinsky, Chafee-Infante)
2017, Larios-Pei (nonlinear CDA, 1D KSE)
2018, DiLeoni-Mazzino-Biferale (3D NSE, spectral nudging)
2018, Blocher-M-Olson (Lorenz equations, time-averaged obs.)
2018, Larios-Victor (Reaction-Diffusion, moving cluster observations)
2019, Celik-Olson-Titi (2D NSE, spectral filtering)
2019, Desamsetti-Dasari-Langodan-Titi-Knio-Hoteit (real atmospheric data)
2019, Hudson-Jolly (2D MHD equations)
2018, DiLeoni-Mazzino-Biferale (3D NSE, parameter estimation)
2020, Carlson-Hudson-Larios (2D NSE, parameter estimation)
2020, Buzzicotti-Bonaccorso-DiLeoni-Biferale (3D NSE, nudging vs. ML)
2021, Chen-Li-Lunasin (Shell models)
2021, McQuarrie-Pachev-Whitehead (1D KSE, parameter estimation)
2022, Agasthya-DiLeoni-Biferale (3D Rayleigh-Benard convection, temperature only)
2021, M-Ng (Lorenz, parameter estimation)
2021, Carlson-Hudson-Larios-M-Ng-Whitehead (Lorenz, parameter estimation)
2023, Farhat-Larios-M-Whitehead (2D NSE, forcing estimation)

Literature (of nudging-based DA (a lá Azouani, Olson, Titi) in the context of PDEs)

Analytical Studies (no errors)

2013, Azouani-Olson-Titi (2D NSE, nudging, general observables)
2015, Kalantarov-Titi (stabilization of nonlinear wave equations)
2016, Farhat-Lunasin-Titi (2D NSE, horizontal velocity only)
2016, Farhat-Lunasin-Titi (3D RB convection in porous media, temp. only)
2016, Farhat-Lunasin-Titi (3D Planetary QG)
2016, Jolly-Sadigov-Titi (1D damped-driven NLS equation, spectral obs.)
2017, Farhat-Lunasin-Titi (2D RB convection, horizontal velocity only)
2017, Biswas-M (2D NSE, analytic convergence, spectral obs.)
2017, Biswas-Hudson-Larios-Pei (2D MHD, velocity only)
2017, Jolly-Sadigov-Titi (1D damped-driven KdV equation, spectral obs.)
2017, Jolly-M-Titi (2D SQG, surface observations)
2018, Larios-Rebholz-Zerfas (2D NSE, stability and accuracy of DA schemes)
2018, Kalantarov-Titi (stabilization of Navier-Stokes-Voight)
2020, Gardner-Larios-Rebholz-Vargun-Zerfas (CDA for Vel-Vort. form)
2020, Carlson-Larios (2D NSE, sensitivity analysis and CDA)
2020, Du-Shiue (Lorenz, nonlinear CDA)
2020, Biswas-Price (3D NSE)
2020, Balakrishna-Biswas (3D Boussinesq)
2021, Franz-Larios-Victor (2D NSE, dynamic observers)
2021, Chow-Leung-Pakzad (two-phase flow)
2021, Cao-Giorgini-Jolly-Pakzad (3D LES NSE)
2021, Biswas-Brown-M (2D NSE, higher-order convergence, mesh-free obs.)
2021, Carlson-Hudson-Larios-M-Ng-Whitehead (Lorenz, parameter estimation)
2022, M (2D NSE, parameter estimation)

Literature (of nudging-based DA (a lá Azouani, Olson, Titi) in the context of PDEs)

Analytical Studies (with errors)

2008, Apte-Jones-Stuart-Voss (2D linearized shallow water equations)
2013, Blömker-Law-Stuart-Zygalakis (2D NSE, noisy spectral obs., 3DVAR)
2014, Bessaih-Olson-Titi (2D NSE, noisy general obs.)
2014, Law-Shukla-Stuart (Lorenz equations, 3DVAR)
2016, Albanez-Lopes-Titi (3D NSE-α model)
2016, Foias-Mondaini-Titi (2D NSE, discrete-in-time obs.)
2016, Markowich-Titi-Trabelsi (3D Brinkman-Forchheimer-extended Darcy model)
2018, Albanez-Benvenutti (3D Bardina model)
2018, Blocher-M-Olson (Lorenz equations, time-averaged obs.)
2018, Jolly-M-Olson-Titi (2D SQG, time-averaged obs.)
2018, Larios-Pei (2D NSE via 2D NS-Voight)
2018, GarcíaArchilla-Novo-Titi (uniform-in-time error est. for finite elements)
2018, Mondaini-Titi (uniform-in-time error est. for post-proc. Galerkin)
2019, Ibdah-Mondaini-Titi (uniform-in-time error est. for fully discrete)
2019, Pei (3D Primitive Equations of the ocean)
2020, Farhat-GlattHoltz-M-McQuarrie-Whitehead (3D RB conv., large Pr, temp. only)
2020, Biswas-Bradshaw-Jolly (2D NSE, local-in-space, observations)
2021, Jolly-Pakzad (2D NSE, FEM interpolants)
2022, Biswas-Bradshaw-Jolly (2D NSE, moving observations)

Literature

And many, many others!

Studies on nudging or synchronization-based algorithms from greater DA community

1976, Hoke-Anthes (Nudging for DA introduced in context of ODEs)
2006, Duane-Tribbia-Weiss (DA via synchronization perspective: Lorenz, 2-layer QG)
2008, Auroux-Blum (BFN numerical implementation for Lorenz and 2-layer QG)
2011, Auroux-Blum-Nodet (Diffusive BFN: stabilizing diffusion in “back” step)
2013, Auroux-Bansart-Blum (BFN application to Burgers PDE)
2014, Rey, Eldridge, Kostuk, Abarbanel, Schumann-Bischoff, Parlitz (State & Parameter Estimation via delay synchronization: Lorenz 96)
2015, Pazó-Carrassi-López (Delay-coordinate nudging, relation to Takens: Lorenz 96)
2018, Carrassi-Bocquet-Bertino-Evensen (Overview of DA methods including nudging)
2018, Pinheiro-van Leeuwen, Partliz (Ensemble framework of delay synchronization)
2018, Pinheiro-van Leeuwen, Geppert (Particle filter via synch. framework for DA)
2021, Conti-Aydogdu-Gualdi-Navarra-Tribbia (“physical derivation" of nudging)

*Many thanks to Alberto Carrassi and Peter Jan van Leeuwen for the additional references

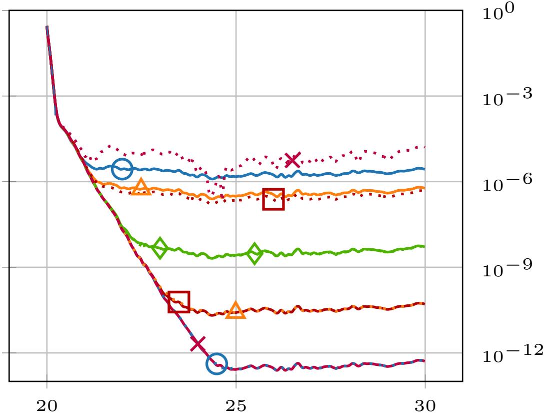
Nota bene. The above references encompass rigorous theoretical and numerical results in the *finite-dimensional setting of ODEs*, or numerical tests in PDE settings, but *do not* cover rigorous theoretical results in infinite-dimensional PDE settings. This talk discusses **rigorous theoretical results in the PDE setting**.

Parameter (& State) Estimation

Carlson-Hudson-Larios

Sensitivity Analysis of ν in 2D NSE

$$\partial_t u + \nu_1(-\Delta)u = -u\cdot\nabla u - \nabla p + f, \quad \nabla\cdot u = 0,$$
$$\partial_t v + \nu_2(-\Delta)v = -v\cdot\nabla v - \nabla q + f - \mu(H_\delta v - H_\delta u), \quad \nabla\cdot v = 0.$$



Carlson-Hudson-Larios

Studied Sensitivity of Nudging to ν in 2D NSE

$$\partial_t u + \nu_1(-\Delta)u = -u\cdot\nabla u - \nabla p + f, \quad \nabla\cdot u = 0,$$
$$\partial_t v + \nu_2(-\Delta)v = -v\cdot\nabla v - \nabla q + f - \mu(H_\delta v - H_\delta u), \quad \nabla\cdot v = 0.$$

Energy balance for $H_\delta w = H_\delta v - H_\delta u$.

$$\frac{1}{2}\frac{d}{dt}\|H_\delta w\|_{L^2}^2 + (\nu_1 - \nu_2)\langle H_\delta(-\Delta)v, H_\delta w\rangle + \mu\|H_\delta w\|_{L^2}^2$$
$$= -\langle H_\delta(\nu_1(-\Delta)w + u\cdot\nabla v + u\cdot\nabla w), H_\delta w\rangle.$$

Hence

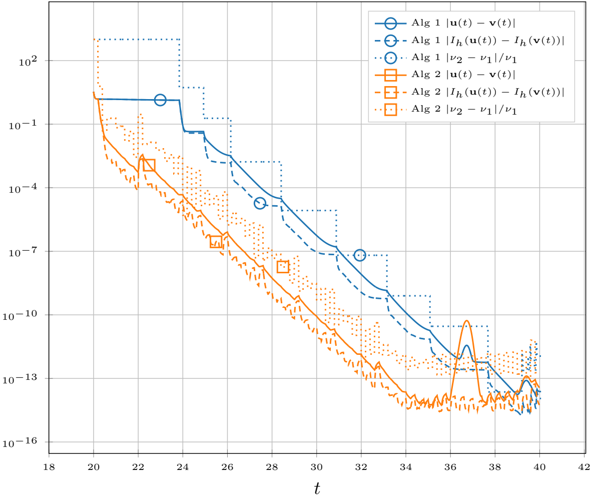
$$\nu_1 \approx \nu_2 + \frac{\mu\|H_\delta w\|_{L^2}^2}{\langle H_\delta \Delta v, H_\delta w\rangle}$$

Algorithm. When ν is **unknown**, consider update scheme given by

$$\nu_{n+1} = \nu_n + \left.\frac{\mu\|H_\delta w\|_{L^2}^2}{\langle H_\delta \Delta v, H_\delta w\rangle}\right|_{t=t_{n+1}}$$

Carlson-Hudson-Larios

Numerical experiments demonstrate convergence



Proof?

Lorenz equations

Lorenz equations.

$$\begin{aligned} \frac{dx}{dt} &= -\sigma x + \sigma y, \quad x(0) = x_0 \\ \frac{dy}{dt} &= -y - \sigma x - xz, \\ \frac{dz}{dt} &= -\beta z + xy - \beta(\rho + \sigma) \end{aligned} \qquad (Lor)$$

Suppose $\mathscr{O} = \{x(t)\}_{t \geq 0}$ is **known**.

Nudging equation.

$$\begin{aligned} \frac{d\widetilde{x}}{dt} &= -\widetilde{\sigma}\widetilde{x} + \widetilde{\sigma}\widetilde{y} - \mu(\widetilde{x} - x), \quad \widetilde{x}(0) = \widetilde{x}_0 \\ \frac{d\widetilde{y}}{dt} &= -\widetilde{y} - \widetilde{\sigma}\widetilde{x} - \widetilde{x}\widetilde{z}, \quad \widetilde{y}(0) = \widetilde{y}_0 \\ \frac{d\widetilde{z}}{dt} &= -\beta\widetilde{z} + \widetilde{x}\widetilde{y} - \beta(\rho + \widetilde{\sigma}), \quad \widetilde{z}(0) = \widetilde{z}_0 \end{aligned} \qquad (\widetilde{Lor})$$

Note. (Lor) is a toy model for Rayleigh-Bénard Convection.

Parameter update via nudging

Following (Carlson-Hudson-Larios, 2020)

Lorenz equations.

Let $u = \widetilde{x} - x$. Observe

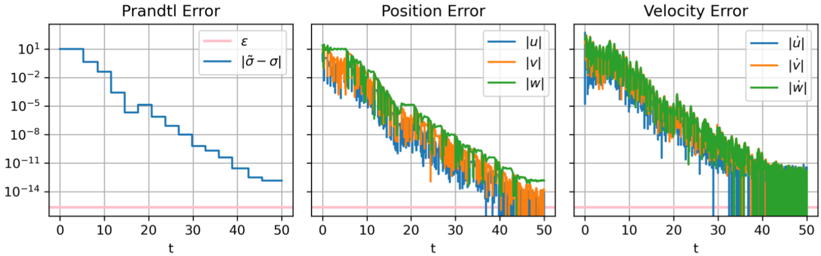
$$\frac{du}{dt} = -\widetilde{\sigma}(\widetilde{x} - \widetilde{y}) - \mu(\widetilde{x} - x) + \sigma(x - y).$$

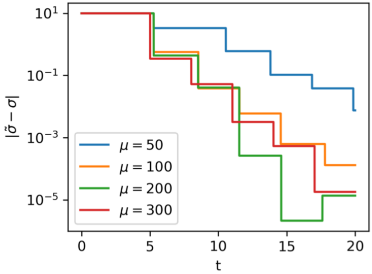
Suppose $du/dt \approx 0$. Then

$$\sigma \approx \widetilde{\sigma} - \frac{\mu u}{\widetilde{y} - \widetilde{x}}$$

M-Ng, 2021

Numerical Results





Convergence in Lorenz

Theorem (Carlson-Hudson-Larios-M-Ng-Whitehead, 2021)

Suppose that there exists $\varepsilon > 0$ *such that*

$$\inf_{k=1,\ldots,n+1} |\widetilde{y}(t_k) - \widetilde{x}(t_k)| \geq \varepsilon.$$

Then for μ *appropriately tuned, depending on* ε*, one has*

$$|\sigma_{k+1} - \sigma| \leq \frac{1}{2}|\sigma_k - \sigma|,$$

for all $k = 1, \ldots, n$*.*

Convergence in 2D NSE

Theorem (M, 2021)

Suppose there exists $\varepsilon > 0$ *such that*

$$\inf_{k=1,\dots,n+1} |\langle H_\delta \Delta v, H_\delta w\rangle| \Big|_{t=t_{n+1}} \geq \varepsilon.$$

Then for μ *appropriately tuned, depending on* ε*, one has*

$$|\nu_{k+1} - \nu| \leq \frac{1}{2}|\nu_k - \nu|,$$

for all $k = 1, \dots, n$.

Unknown Sources

Can one reconstruct unknown external sources?

2D NSE.

$$\partial_t u + \nu(-\Delta)u = -(u\cdot\nabla)u - \nabla p + f, \quad \nabla\cdot u = 0. \tag{NSE}$$

Now f is **unknown**.

Issues at play.
Consider heat equation

$$\partial_t u + \nu(-\Delta u) = f. \tag{Heat}$$

If $f = H_\delta f$. Then $\mathscr{O}$ determines f **trivially**:

$$\partial_t H_\delta u + \nu(-\Delta)H_\delta u = H_\delta f$$

However in (NSE)

$$\partial_t H_\delta u + \nu(-\Delta)H_\delta u + P(H_\delta u\cdot\nabla)H_\delta u = H_\delta f - \underbrace{P\left(H_\delta(u\cdot\nabla)u - (H_\delta u\cdot\nabla)H_\delta u\right)}_{\text{Reynolds stress!}}$$

Note. P is projection onto divergence-free vector field

Unknown Sources

Can one reconstruct unknown external sources?

2D NSE.

$$\partial_t u + \nu(-\Delta)u = -(u\cdot\nabla)u - \nabla p + f, \quad \nabla\cdot u = 0. \qquad (NSE)$$

Now f is **unknown**.

Nudging equation.

$$\partial_t v - \nu\Delta v = -(v\cdot\nabla)v - \nabla q + g - \mu(H_\delta v - H_\delta u), \quad \nabla\cdot v = 0, \qquad (NSE_{\mu,g})$$

where g is some **guess** for f.

Observe that $(NSE_{\mu,g})$ provides a reconstruction of small scales. Then

$$u \approx \underbrace{H_\delta u}_{observed} + \underbrace{(I - H_\delta)v}_{reconstructed}$$

Algorithm for Reconstructing f

Nonlinear filtering.

Let

$$\widetilde{u} = H_\delta u + (I - H_\delta)v$$

Recall $v = v(\mathscr{O}, g)$. Then define

$$\widetilde{g} := \partial_t \widetilde{u} + \nu(-\Delta)\widetilde{u} + P(\widetilde{u} \cdot \nabla)\widetilde{u}.$$

After a transient period (allowing $(NSE_{\mu,g})$) to relax, solve for v:

$$\partial_t v - \nu\Delta v = -(v \cdot \nabla)v - \nabla q + \widetilde{g} - \mu(H_\delta v - H_\delta u), \quad \nabla \cdot v = 0. \qquad (NSE_{\mu,\widetilde{g}})$$

Observe that $v = v(\mathscr{O}, \widetilde{g})$.

Rinse and Repeat.

Convergence in 2D NSE

Theorem (M, 2022)

Suppose $f = H_\delta f$. Consider any f_0 such that $f_0 = H_\delta f_0$ over $[t_0, \infty)$, $t_0 = 0$.

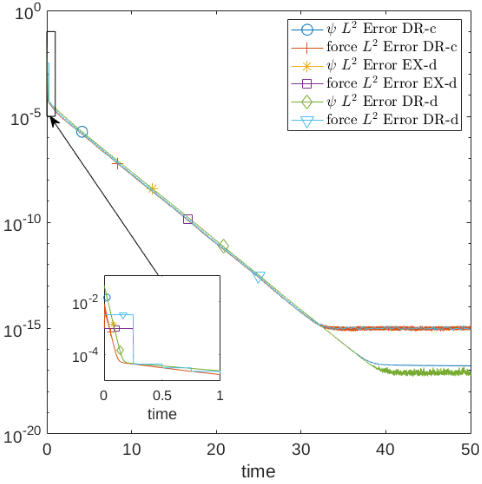
There exists $\delta = \delta(\nu, f)$ so that for μ appropriately tuned the sequence $f_1|_{t \geq t_1}, f_2|_{t \geq t_2}, \ldots$ generated as above satisfies

$$\sup_{t \geq t_{k+1}} \|f_{k+1}(t) - f(t)\|_{L^2} \leq \frac{1}{2} \sup_{t \geq t_k} \|f_k(t) - f(t)\|_{L^2}$$

for all $k \geq 0$.

Farhat-Larios-M-Whitehead, 2022

2048^2, $f = P_{16\leq|k|\leq 64} f$, $\nu = 10^{-4}$, $G = 2.5 \times 10^6$



Lessons

Equation possesses its own mechanism for filtering errors!

Mechanism for recovering unobserved state is *nonlinear*

Works *in conjunction* with observations

Same mechanism *enables* parameter recovery

Current & Future Directions

Theoretical results in the PDE setting

State Estimation.

- justification of $\mu \longrightarrow \infty$ limit? with E. Carlson (Caltech), A. Farhat (Florida State University), C. Victor (Texas A&M)
- effects of rotation and stratification? with A. Farhat (FSU) and A. Kumar (FSU)

Parameter Estimation.

- recovering several parameters? with J. Murri (UCLA) and J. Whitehead (Brigham Young Unviersity)
- recovering anisotropic viscosities? with Q. Lin (Clemson University)
- force reconstruction beyond obs. scale with J. Broecker (University of Reading), G. Carigi (University of L'Aquila), and T. Kuna (University of L'Aquila)

Future.

- non-spectral observations?
- state-dependent parameters?
- observational errors?

Thank you!

Support is provided by the National Science Foundation through NSF-DMS 2213363, 2206491

Proof

Viscosity reconstruction.

Model error

$$
\begin{aligned}
&\nu_{k+1} - \nu \\
&= \frac{\frac{d}{dt}\frac{1}{2}\|H_\delta w\|_{L^2}^2 - \nu\|H_\delta \nabla w\|_{L^2} + \langle P(w\cdot\nabla)H_\delta w, (I - H_\delta)w\rangle - \langle PH_\delta(u\cdot\nabla)w + (w\cdot\nabla), H_\delta w\rangle}{\langle H_\delta \Delta v, H_\delta w\rangle}
\end{aligned}
$$

Synchronization error

$$
\|w(t)\|_{L^2} + \|\nabla w(t)\|_{L^2} + \|\Delta w(t)\|_{L^2} \le O\left(\frac{|\nu_k - \nu|}{\mu^{1/2}}\right)
$$

Forcing reconstruction.

Model error

$$
\begin{aligned}
&f_{k+1} - f \\
&= H_\delta((I - H_\delta)w\cdot\nabla)(I - H_\delta)w + H_\delta(u\cdot\nabla)(I - H_\delta)w + H_\delta((I - H_\delta)w\cdot\nabla)u
\end{aligned}
$$

Synchronization error

$$
\|w(t)\|_{L^2} \le O\left(\frac{\|f_k - f\|_{L^2}}{\mu}\right), \quad \|\nabla w(t)\|_{L^2} \le O\left(\frac{\|f_k - f\|_{L^2}}{\mu^{1/2}}\right)
$$