Goal: Construction of a data-driven model (dynamical system) of a fluid flow

We have succeeded in constructing a closed form equation describing a macroscopic behavior of a fluid flow only from macroscopic data without prior knowledge of physical process.
Outline of this talk

1. Introduction to a fluid flow
2. Motivation
3. Reservoir computation
4. Partial-prediction of a microscopic variable
5. Full-prediction of a macroscopic variable (main topic)
6. Summary

1-1. Introduction to a fluid flow

- Fluid flow appears everywhere around us: from coffee cup to space.

Universality in turbulence

Energy spectrum for various types of fluid turbulence

Energy input

Energy dissipation

Energy cascade
1-2. Introduction to a fluid flow: high-dimensional chaos

- Fluid flow shows chaos in most cases.
  ➢ Deterministic
  ➢ Sensitivity for initial conditions

- Fluid flow shows a high-dimensional chaos in most cases.
  ➢ Coexistence of different number of unstable directions
  ➢ Intermittent behavior especially in higher wavenumbers (smaller scale)

![high-wavenumber variable E(9)](image)

4. Introduction to a fluid flow: Navier-Stokes equation

- Most fluid flow is known to be modeled by three dimensional incompressible Navier-Stokes equation:

\[
\begin{align*}
\partial_t v - \nu \Delta v + (v \cdot \nabla)v + \nabla \pi &= f, \\
\nabla \cdot v &= 0
\end{align*}
\]

\[v|_{t=0} = v_0 \quad \text{with} \quad \nabla \cdot v_0 = 0,\]

- ν: velocity
- π: pressure
- ν: viscosity (more turbulent for smaller ν)

- Lots of difficulties in this equation:
  ➢ nonlinear
  ➢ nonlocal interactions
  ➢ high-dimensional (especially for small ν)

We do not even know the existence of a “global solution”.
(One of the Millennium prize problems by Clay Mathematics Institute $1,000,000)
1-5. Introduction to a fluid flow: Mean flow
• There are lots more open problems in the area of fluid mechanics such as the analytical derivation of mean flow velocity profile (=macroscopic quantity) of turbulence due to the “closure problem”, that is, it is impossible to get a closed form equation of a mean flow (=1st order quantity) without knowing a higher order quantity.
[In order to write down the equation of the nth order quantity, we need the information of the n+1th order quantity for all n.]

2. Motivation and outline of our study
• Data-driven modeling of fluid flow: Based on the limited time-series data of a fluid flow, we would like to construct a model. Especially, we are interested in constructing a model for macroscopic variables.

• We employ reservoir computation technique, which is proved to be very powerful for constructing models from data.
  Lu et al. (2017), Pathak et al. (2017, 2018): Lorenz & Kuramoto-Sivashinsky systems
• Training data as well as a reference data are generated from the direct numerical simulation of the three dimensional incompressible Navier-Stokes equation with periodic-boundary conditions.
  ➢ Fourier variables of velocity: microscopic
  ➢ Energy functions: macroscopic
• We would like to construct a data-driven model which can predict future behaviors of both microscopic and macroscopic fluid variables without a prior knowledge of physical process in relatively small computational costs.
3-1. Reservoir computation

- Machine-learning technique that uses a neural-network composed of simple nonlinear dynamical systems.
- The framework was proposed as echo-state network (Jaeger 2001, 2004) and liquid-state machine (Maass et al. 2002).
- Effort in training is concentrated on the determination of output layer.

![Diagram of reservoir computation]

3-2. Reservoir computation

\[ r(t) = (1 - \alpha) r(t) + \alpha \tanh(A r(t) + W_{in} E(t)) \]

\( A, W_{in} \): sparse random matrix, whose maximal eigenvalue is controlled
\( \alpha \): nonlinearity parameter (\( \alpha = 0.3 \)).

We determine \( W_{out} \) and \( c \) s.t.

\[ \hat{s}(t+\Delta t) < T \quad W_{out} r(t+\Delta t) + c \approx s(t+\Delta t). \]
3-3. Reservoir computation: How to determine $W_{\text{out}}$ and $c$?

- Minimizing the quadratic form with respect to $W_{\text{out}}$ and $c$:
  \[
  \sum_{l=1}^{L} \| (W_{\text{out}} r(l\Delta t) + c) - s(l\Delta t) \|^{2} + \beta [Tr(W_{\text{out}} W_{\text{out}}^{T})]
  \]
  regularization term to avoid overfitting

- Solution: 
  \[
  \ddot{s}(t) = W_{\text{out}}^{*} r(t) + c^{*}
  \]
  \[
  W_{\text{out}}^{*} = \delta S \delta R^{T} (\delta R \delta R^{T} + \beta I)^{-1}
  \]
  \[
  c^{*} = -[W_{\text{out}}^{*} \bar{r} - \bar{s}]
  \]
  where $\bar{r} = \sum_{l=1}^{L} r(l\Delta t)/L$, $\bar{s} = \sum_{l=1}^{L} s(l\Delta t)/L$, and $I$ is the $N \times N$ identity matrix, $\delta R$ (respectively, $\delta S$) is the matrix whose $l$-th column is $r(l\Delta t) - \bar{r}$ (respectively, $s(l\Delta t) - \bar{s}$).

4-1. Partial-prediction of a microscopic variable:

Generation of learning data using direct numerical simulation of the Navier-Stokes equation

\[
\begin{cases}
\partial_{t} v - \nu \Delta v + (v \cdot \nabla)v + \nabla \pi = f, \quad \nabla \cdot v = 0, \quad \mathbb{T}^{3} \times (0, \infty) \\
v|_{t=0} = v_{0} \quad \text{with} \quad \nabla \cdot v_{0} = 0,
\end{cases}
\]

- We employ Fourier spectral method with $N_{0}=9$ modes, meaning that the system is approximated by $2(2N_{0}+1)^{3}=13718$ dimensional ODE.
- We focus on time-series data of 270 variables

\[
\alpha_{\eta} = |F_{\zeta}(\kappa)| := \left| \frac{1}{(2\pi)^{3}} \int_{\mathbb{T}^{3}} v_{\zeta}(x,t) e^{-i(\kappa \cdot x)} dx \right|
\]

and predict another variable.
4-2. Partial-prediction of a microscopic variable: Fourier variable of a velocity

Partial-prediction of a microscopic variable from a measurement $u(t)$ of dimension 270 is quite successful.

5-1. Full-prediction

For the full-prediction we do not have measurements $u(t)$ for $t > T$, and use predicted value of $\hat{s}(t)$ for $u(t)$. 

Training phase ($t < T$)

Prediction phase ($t > T$)
5-2. Full-prediction of a macroscopic variable

The energy function $E_0(k, t)$ for wavenumber $k \in \mathbb{N}$ is defined by

$$E_0(k, t) := \frac{1}{2} \int_{D_k} \sum_{\zeta=1}^{3} |F[v_\zeta](\kappa, t)|^2 d\kappa,$$

where $D_k := \{ \kappa \in \mathbb{Z}^3 | k - 0.5 \leq |\kappa| < k + 0.5 \}$.

Short-time average of the energy function will be used later

$$E(k, t) = \sum_{s=t-49\Delta t}^{t+50\Delta t} E_0(k, s)/100$$

• By learning 9 time-series data of $E(k, t)$ ($k=1, \cdots, 9$) for $t \leq T$, we predict $E(k, t)$ ($k=1, \cdots, 9$) for $t > T$. We do not learn any data during the prediction time for $t > T$.

5-3. Full-prediction of a macroscopic variable: Energy function

• When $t < T + 100$, predicted time-series data obtained from our reservoir system almost coincides with that of a reference data obtained from the DNS of the Navier-Stokes equation.
• The increase in the prediction error is due to the chaotic property of the fluid flow, which is inevitable.
5-4. Full-prediction of a macroscopic variable: Reproducing energy spectrum by the reservoir model

- The energy spectrum obtained from the full-prediction procedure of $E(k,t)$ for $t>T+100$ (after the time-series prediction fails) coincides with that from a reference data obtained from the direct numerical simulation of the Navier-Stokes equation.

- This implies that the obtained reservoir system constructed without the knowledge of microscopic variables is equivalent to the dynamical system describing a macroscopic behavior of energy functions.

6-1. Summary

- We can predict time-series of both microscopic and macroscopic variables of fluid flow by machine-learning technique using reservoir computation without a prior knowledge of a physical process.

- In order to generate a time-series data of a macroscopic variable of a fluid flow, we do not need to go back to the microscopic dynamics.

  We have especially succeeded in constructing a closed form equation of a fluid flow describing macroscopic behavior only from data.

- The method is shown to be especially useful in generating a macroscopic time-series data with small computational costs.
6-2. Comparison about computational costs

\[ \text{Training phase (} t \leq T \text{)} \]

\[ \text{Prediction phase (} t > T \text{)} \]

\[ \text{Microscopic } v = 0.05862 \]

\[ M=270, M'=2, N=6400 \]

\[ \Delta t=0.25 \text{ [1/10 times]} \]

\[ \text{Macroscopic } v = 0.058 \]

\[ M=M'=9, N=3200 \]

\[ \Delta t=0.25 \text{ [1/80 times]} \]

DNS of Navier-Stokes eqns

13718-dim ODE, 4stage-RK4, \( \Delta t=0.05 \)

6-3. Remarks on the choice of parameters

- As \( N(\gg M) \) increases, the error tends to decrease. Especially for the full prediction, \( N \) should be significantly larger than \( M \) to get an accurate prediction.

- As \( T \) increases, the error tends to decrease, but \( N \) should also be increased for getting a better result.

- If we choose measurements independently with each other, we can use smaller \( \beta (\geq 0) \). On the other hand, when we have a better set of measurements, smaller \( \beta \) is better.

- In order to obtain a “nonhomogeneous” behavior, the parameters \( D_1 \) and \( D_2 \) should be relatively small and avoid strong coupling among \( r \). They should be proportional to \( N \).

<table>
<thead>
<tr>
<th>parameter</th>
<th>( (a) )</th>
<th>( (b) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \tau ) transient time</td>
<td>1000</td>
<td>2500</td>
</tr>
<tr>
<td>( T ) learning time</td>
<td>10000</td>
<td>20000</td>
</tr>
<tr>
<td>( M ) dimension of measurements</td>
<td>270</td>
<td>9</td>
</tr>
<tr>
<td>( P ) dimension of predicted variables</td>
<td>2</td>
<td>9</td>
</tr>
<tr>
<td>( N ) number of reservoir nodes</td>
<td>6400</td>
<td>3200</td>
</tr>
<tr>
<td>( D_1 ) parameter of determining elements of ( A )</td>
<td>60</td>
<td>320</td>
</tr>
<tr>
<td>( D_2 ) parameter of determining elements of ( A )</td>
<td>60</td>
<td>0</td>
</tr>
<tr>
<td>( \gamma ) scale of input weights in ( A )</td>
<td>0.1</td>
<td>0</td>
</tr>
<tr>
<td>( \rho ) maximal eigenvalue of ( A )</td>
<td>1.0</td>
<td>0.5</td>
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<tr>
<td>( \sigma ) scale of input weights in ( W_{in} )</td>
<td>0.4</td>
<td>0.3</td>
</tr>
<tr>
<td>( \alpha ) nonlinearity degree of reservoir dynamics</td>
<td>0.7</td>
<td>0.3</td>
</tr>
<tr>
<td>( \Delta t ) time step for reservoir dynamics</td>
<td>0.1</td>
<td>0.25</td>
</tr>
<tr>
<td>( \beta ) regularization parameter</td>
<td>0</td>
<td>0.01</td>
</tr>
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</table>

TABLE I. Sets of parameters for the reservoir computations. The set \((a)\) is used for the partial-prediction of microscopic Fourier variables, whereas the set \((b)\) is for the full-prediction of macroscopic variables of Energy function and Energy spectrum.
6-4. References