Hidden Fluid Mechanics

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Overview

- Motivation of HFM
- Navier Stokes Equations
- Deep Learning Method
- Examples & Results
- Feedback

Motivation

Fluid Dynamics & “Inverse” Problem

HFM Experiment

Fluid Dynamics

- Kinematic flow of fluid substances:
  - gases (aerodynamics), liquids (hydrodynamics)
- Fluid flow can be described by Navier Stokes Equations

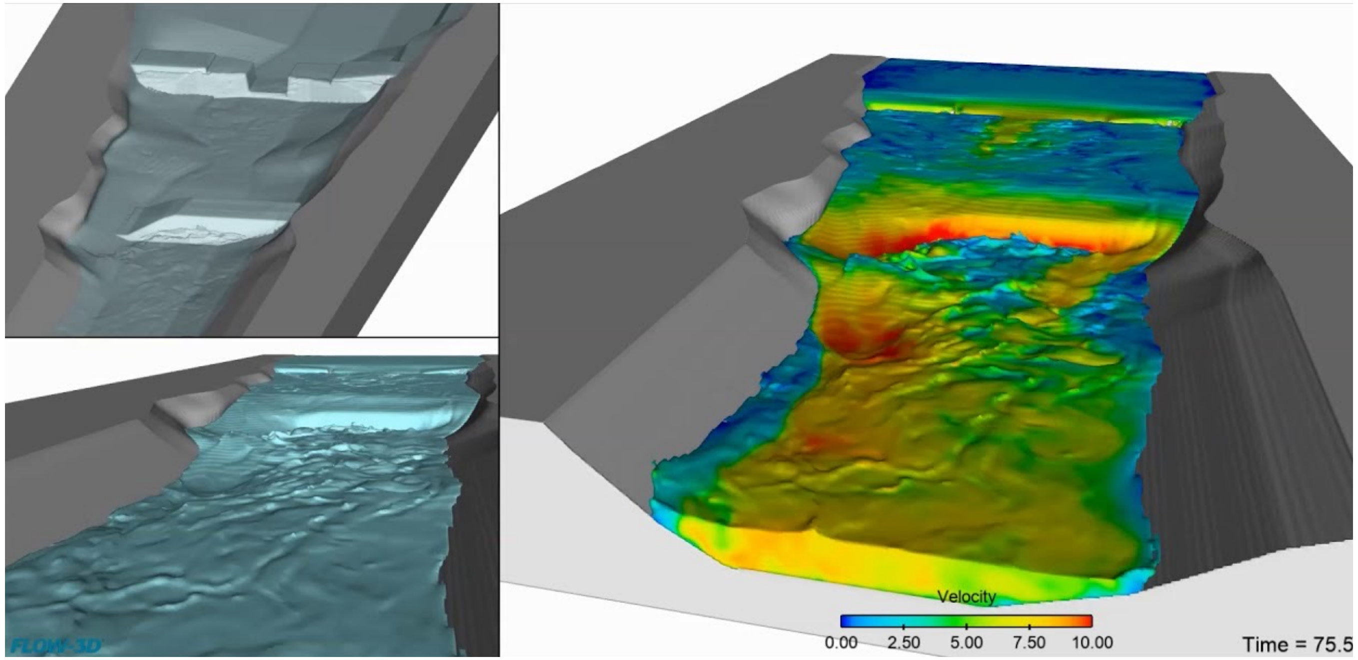
$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{\nabla P}{\rho} + \nu \cdot \nabla^2 \boldsymbol{u} + f$$

- No general solution in 3D! (Millenium prize problem)

Fluid Dynamics

Two main goals:

1. Simulate flows, modelling physical systems (forward)



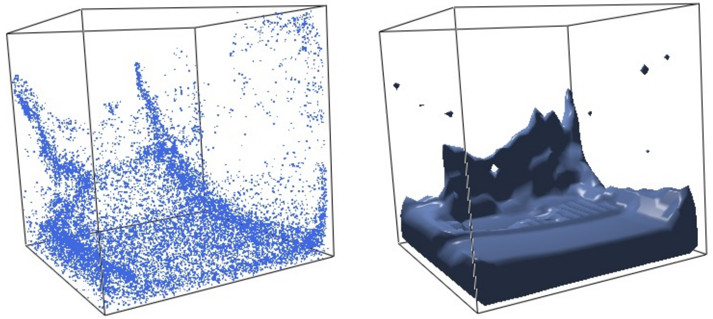
2. Inference of flow properties in given system

Velocity at given points?
Pressure?
Viscosity?

Inverse Problem

- “Forward” simulation possible (1)
  - direct numerical simulation of NSE, approximation

Initial / Boundary conditions
Domain definition
Fluid properties



- “Backward” solution computationally infeasible and complex (2)
  - Ill posed problem (high sensitivity)
  - Turbulence and chaos

Inverse Problem

How do we solve the “backward” problem?

We want to find:

Velocity fields,
Pressure gradient,
Viscosity,
Etc.

Given

Spatiotemporal data points

i.e. coordinates of particles
as time series

Inverse Problem

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{\nabla P}{\rho} + \nu \cdot \nabla^2 \boldsymbol{u} + f$$

We want to find:

Velocity fields,
Pressure gradient,
Viscosity,
Etc.

Given

How do we get data?

Spatiotemporal data points

i.e. coordinates of particles as time series

Hidden Fluid Mechanics Experiment

1. Introduce "passive scalar" into fluid system
   - Transported by fluid but no influence on flow
   - Smoke, dye

2. Sample **concentration** of passive scalar at various times, locations
   - image velocimetry, MRI
   - simulation

Idea: use concentration changes to learn velocity (unobservable)

Intracranial Aneurysm

- Ballooning of blood vessels in the brain
- Direct measurements of pressure, stress are invasive
- No access to boundary conditions (plaque from lipid accumulation)
- Application of HFM

Why is HFM desirable?

- Agnostic to initial/boundary conditions
  - Only need coordinates in time
  - Zero slip, zero concentration conditions implicitly inferred
- Computationally efficient after training
- Robust against low resolution sampling and noise
- Can infer: velocity, pressure, shear stress, drag, lift, viscosity
- Broad applications: Engineering, Health care, Geophysics…

Navier Stokes Equations

What is Navier Stokes?

How do we utilize knowledge of NSE to construct our neural network?

Foundations

Velocity field

$$\boldsymbol{u}: \mathbb{R}^4 \to \mathbb{R}^3$$

$$\boldsymbol{u}(x, y, z, t) = (u, v, w)$$

Unit volume: $V = 1$

$$\text{Mass} = V \cdot \rho = \rho = \text{Density}$$

Incompressible Navier Stokes

Continuity Equation

Conservation of Mass

$$\nabla \cdot \boldsymbol{u} = 0$$

Momentum Equation

Newton's Second Law: F=ma

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{\nabla P}{\rho} + \nu \nabla^2 \boldsymbol{u} + f$$

Incompressible Navier Stokes

Continuity Equation

Divergence Operator

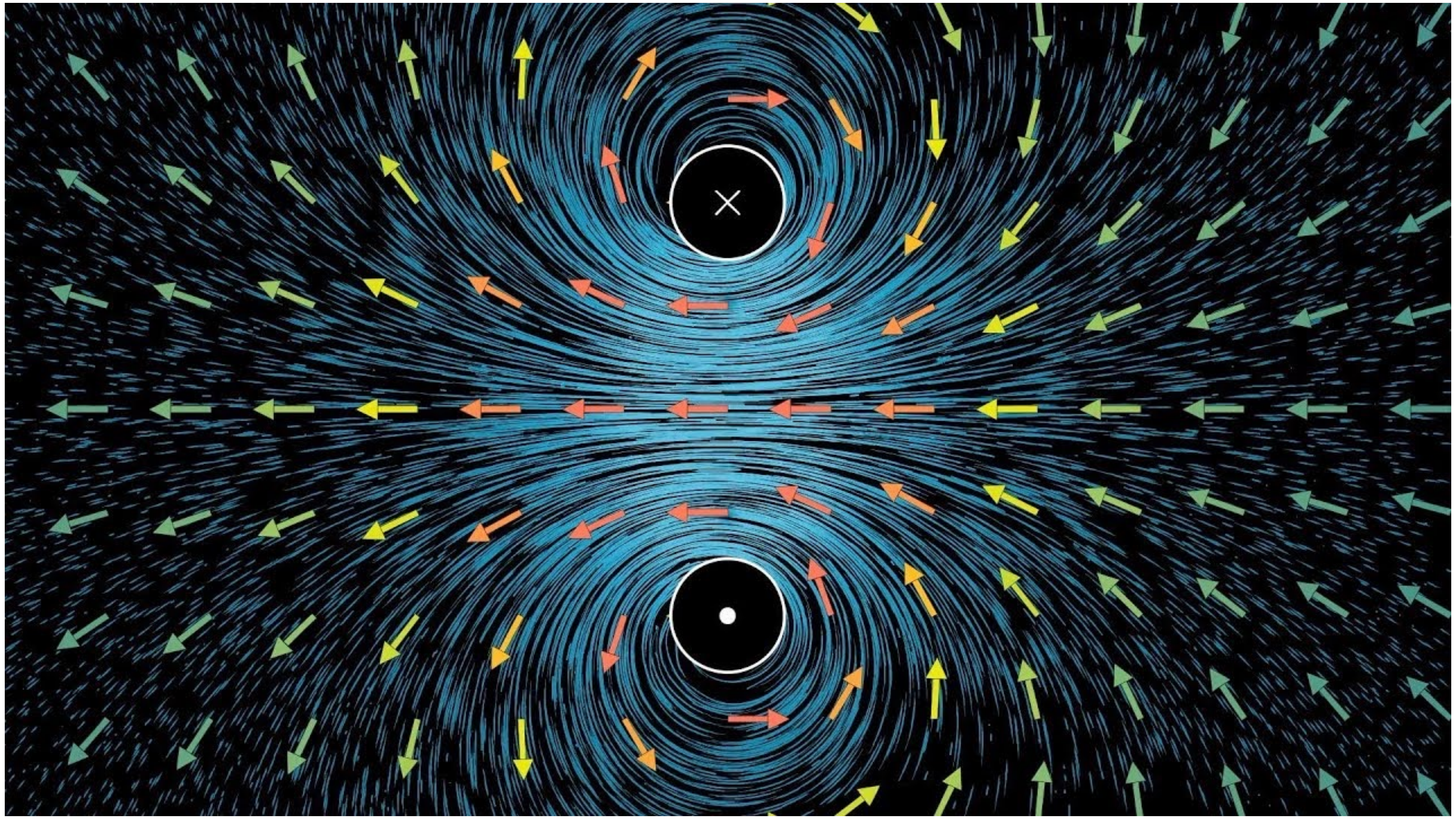
$$\boxed{\nabla \cdot} \boldsymbol{u} = 0$$

$$\nabla \cdot \boldsymbol{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$

$$\nabla = \left[\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right] \rightarrow \nabla \cdot \boldsymbol{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

Incompressible Navier Stokes

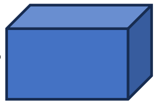
Intuition divergence free: inflow = outflow

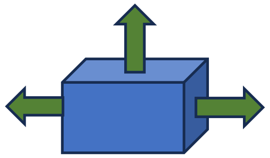


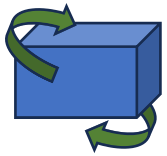
Incompressible Navier Stokes

How is the **Continuity Equation** related to **Conservation of Mass**?

In simple terms: CE = CoM + Gauss Divergence

$\frac{dM}{dt}$ 



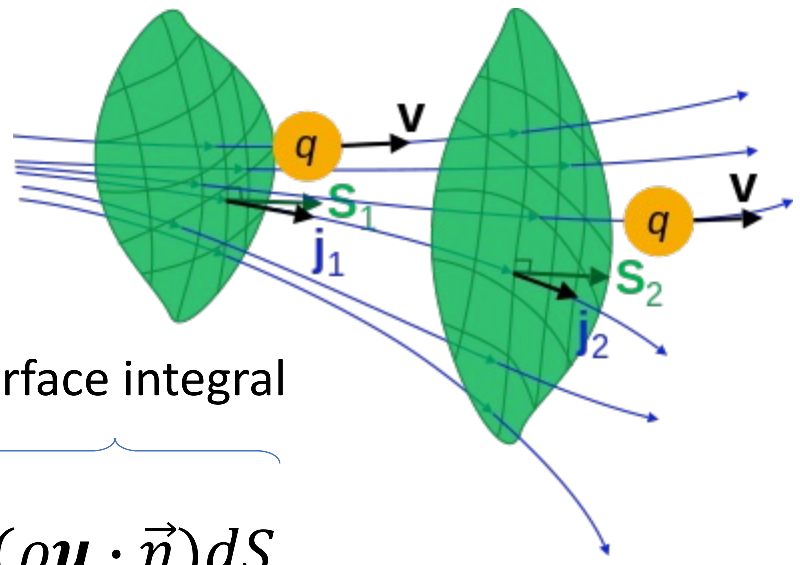


Change of mass of an object = Mass leaving the surface of the object = Divergence of mass in the object

Conservation of Mass

Gauss Divergence Theorem

Continuity Equation



Conservation of Mass:

Volume integral　Surface integral

$$\frac{d}{dt}Mass = \frac{d}{dt}\int \rho\, dV = \overbrace{\int \frac{d\rho}{dt} dV}^{\text{Volume integral}} = \overbrace{-\int (\rho \boldsymbol{u} \cdot \vec{n}) dS}^{\text{Surface integral}}$$

Gauss Theorem: $\int (\nabla \cdot F)\, dV = \int (F \cdot \vec{n}) dS$

$$\int (\nabla \cdot \rho \boldsymbol{u})\, dV = \int (\rho \boldsymbol{u} \cdot \vec{n}) dS = -\int \frac{d\rho}{dt} dV$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

Continuity Equation

Incompressible ⇔ density is constant

Compressible

$$\boxed{\frac{\partial \rho}{\partial t}} + \nabla \cdot (\boxed{\rho} \boldsymbol{u}) = 0$$

= 0 Constant

Incompressible

$$\frac{\partial \rho}{\partial t} = 0 \Rightarrow \nabla \cdot \boldsymbol{u} = 0$$

Incompressible Navier Stokes

Continuity Equation

Conservation of Mass

Divergence Theorem

$$\nabla \cdot \boldsymbol{u} = 0$$

Momentum Equation

Newton's Second Law: F=ma

Pressure forces

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{\nabla P}{\rho} + \nu \cdot \nabla^2 \boldsymbol{u} + f$$

Other forces

Acceleration

Viscous forces

Incompressible Navier Stokes

Momentum Equation

Multiply to obtain m*a on LHS

Newton's Second Law: F=ma

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{\nabla P}{\rho} + \nu \cdot \nabla^2 \boldsymbol{u} + f$$

- Acceleration of infinitesimal volume (particle) at (x, y, z, t)
- Acceleration wrt. time & position
- Chain rule

Incompressible Navier Stokes

$$\frac{d\boldsymbol{u}(x,y,z,t)}{dt} = \frac{\partial \boldsymbol{u}}{\partial t}\frac{dt}{dt} + \frac{\partial \boldsymbol{u}}{\partial x}\frac{dx}{dt} + \frac{\partial \boldsymbol{u}}{\partial y}\frac{dy}{dt} + \frac{\partial \boldsymbol{u}}{\partial z}\frac{dz}{dt}$$

$$\frac{d\boldsymbol{u}}{dt} = \frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{u}}{\partial x}u + \frac{\partial \boldsymbol{u}}{\partial y}v + \frac{\partial \boldsymbol{u}}{\partial z}w$$

$$\frac{d\boldsymbol{u}}{dt} = \frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u}$$

Incompressible Navier Stokes

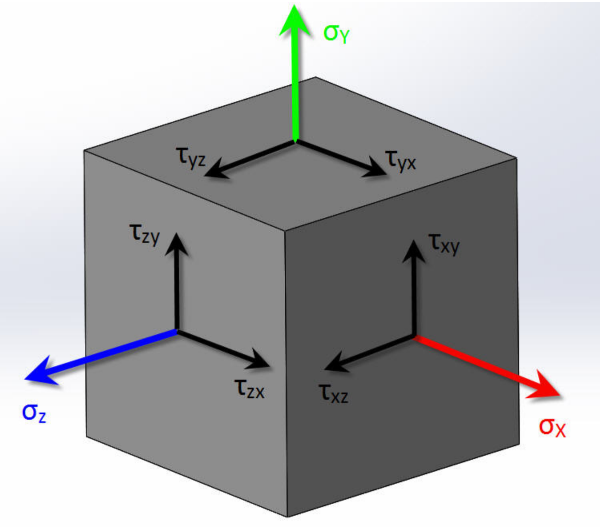
Momentum Equation

Newton's Second Law: F=ma

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \boxed{-\frac{\nabla P}{\rho} + \nu \cdot \nabla^2 \boldsymbol{u} + f}$$

- $\nu = \frac{\mu}{\rho}$ kinematic viscosity coefficient
- Shear stress from Laplacian operator:

$$\nabla^2 \boldsymbol{u} = \frac{\partial^2 \boldsymbol{u}}{\partial x^2} + \frac{\partial^2 \boldsymbol{u}}{\partial y^2} + \frac{\partial^2 \boldsymbol{u}}{\partial z^2} = \nabla \cdot \nabla \boldsymbol{u}$$



Incompressible Navier Stokes

Continuity Equation

Conservation of Mass

Divergence Theorem

$$\nabla \cdot \boldsymbol{u} = 0$$

Momentum Equation

Newton's Second Law: F=ma

Pressure forces

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{\nabla P}{\rho} + \nu \cdot \nabla^2 \boldsymbol{u} + f$$

Other forces

Viscous forces

Acceleration

Non-dimensionalized Navier Stokes

- Scale the momentum equation to remove physical units
- Analogous to vector normalization

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla P + \frac{1}{Re}\nabla^2 \boldsymbol{u} + f$$

Reynolds number: $Re = \frac{\text{inertia}}{\text{viscosity}}$ (fluid particle)

Method

Neural Network with Regularization based on NSE

Model Architecture & Training

Recall: Hidden Fluid Mechanics Experiment

1. Introduce “passive scalar” into fluid system

2. Sample **concentration** of passive scalar
at various times, locations

This means our training data will map from (t, x, y, z) to **concentration** c
But c is not part of Navier-Stokes!
We need something to link it back to other variables in Navier-Stokes…

Transport Equation

https://www.istockphoto.com/de/foto/holzstamm-der-auf-dem-flusswasser-schwimmt-gm1214359156-353280776

Diffusion coefficient

$$\frac{\partial c}{\partial t} = \nabla \cdot (\underbrace{-\vec{\boldsymbol{u}}c}_{\text{Advection}} + \underbrace{D\nabla c}_{\text{Diffusion}})$$

https://www.thoughtco.com/definition-of-diffusion-604430

Divergence operator reminder: $\nabla \cdot (u, v, w)^T = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$

Transport Equation

Diffusion coefficient

$$\frac{\partial c}{\partial t} = \nabla \cdot (\underbrace{-\vec{\boldsymbol{u}}c}_{\text{Advection}} + \underbrace{D\nabla c}_{\text{Diffusion}})$$

$\nabla \cdot (\vec{\boldsymbol{u}}c)$ can be simplified with Navier Stokes!

$\vec{\boldsymbol{u}} := (u, v, w)^{\boldsymbol{T}}$

Simplifying Transport Equation

$$\nabla \cdot (\vec{\boldsymbol{u}} c)$$

$$= \frac{\partial(uc)}{\partial(x)} + \frac{\partial(vc)}{\partial(y)} + \frac{\partial(wc)}{\partial(z)}$$

$$= (u_x c + u c_x) + (v_y c + v c_y) + (w_z c + w c_z)$$

$$= c\,\underbrace{(u_x + v_y + w_z)} + \underbrace{(u c_x + v c_y + w c_z)}$$

$= \nabla \cdot \vec{\boldsymbol{u}} = \boldsymbol{0}$ due to Incompressible Navier Stokes (continuity eq)

$(\vec{\boldsymbol{u}} \cdot \nabla c)$

$$= (\vec{\boldsymbol{u}} \cdot \nabla c)$$

Simplified Transport Equation

$$\frac{\partial c}{\partial t} = \underbrace{-(\vec{\boldsymbol{u}} \cdot \nabla c)}_{\text{Advection}} + \underbrace{D\nabla^2 c}_{\text{Diffusion}}$$

Non-dimensionalized Transport Eq.

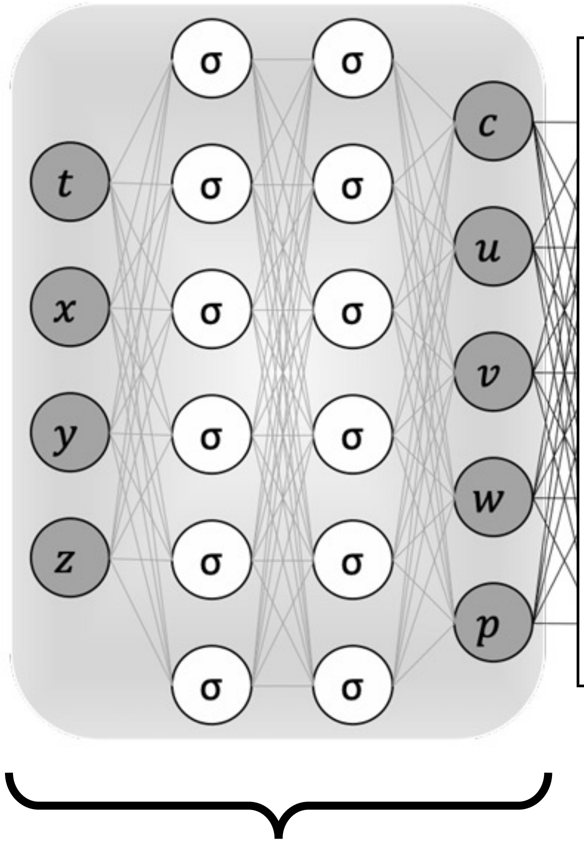
$$c_t = -\underbrace{(u\, c_x + \ v\, c_y + \ w\, c_z)}_{\text{Advection}} + \underbrace{\frac{1}{Pec}\left(c_{xx} + c_{yy} + c_{zz}\right)}_{\text{Diffusion}}$$

High Péclet number: Advection dominates

Low Péclet number: Diffusion dominates

NN: (t, x, y, z) –> (c, u, v, w, p)

Model Introduction



Physics-uninformed NN

Physics-informed regularization

How should c, u, v, w, p behave,
According to Navier-Stokes & Transport equations?

From Navier Stokes to Regularization Terms

Continuity Equation:

$$\nabla \cdot \vec{\boldsymbol{u}} = 0$$

Equivalent regularization:

$$e_5 = u_x + v_y + w_z$$

Note that $\vec{\boldsymbol{u}} := (u, v, w)^{\boldsymbol{T}}$!

$\vec{\boldsymbol{u}} \coloneqq (u, v, w)^{\boldsymbol{T}}$

From Navier Stokes to Regularization Terms

Momentum Equation (Non-dimensionalized with f set to 0):

$$\frac{\partial \vec{\boldsymbol{u}}}{\partial t} + (\vec{\boldsymbol{u}} \cdot \nabla)\vec{\boldsymbol{u}} = -\nabla P + \frac{1}{Re}\nabla^2 \vec{\boldsymbol{u}}$$

Let's bring everything to LHS.

$\boldsymbol{u} := (u, v, w)^{\boldsymbol{T}}$

From Navier Stokes to Regularization Terms

Momentum Equation (Non-dimensionalized with f set to 0):

Linear differential operator

$$\frac{\partial \vec{\boldsymbol{u}}}{\partial t} + (\vec{\boldsymbol{u}} \cdot \nabla)\vec{\boldsymbol{u}} + \nabla P - \frac{1}{Re}\nabla^2\vec{\boldsymbol{u}} = \boldsymbol{0}$$

$= u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z}$

Laplacian operator
(scalar -> scalar)
Applied component-wise to $\boldsymbol{u}$

Equivalent regularization:

$$e_2 = u_t + uu_x + vu_y + wu_z + p_x - Re^{-1}(u_{xx} + u_{yy} + u_{zz})$$

$$e_3 = v_t + uv_x + vv_y + wv_z + p_y - Re^{-1}(v_{xx} + v_{yy} + v_{zz})$$

$$e_4 = w_t + uw_x + vw_y + ww_z + p_z - Re^{-1}(w_{xx} + w_{yy} + w_{zz})$$

From Transport Eq. to Regularization Terms

Transport equation (non-dimensionalized):

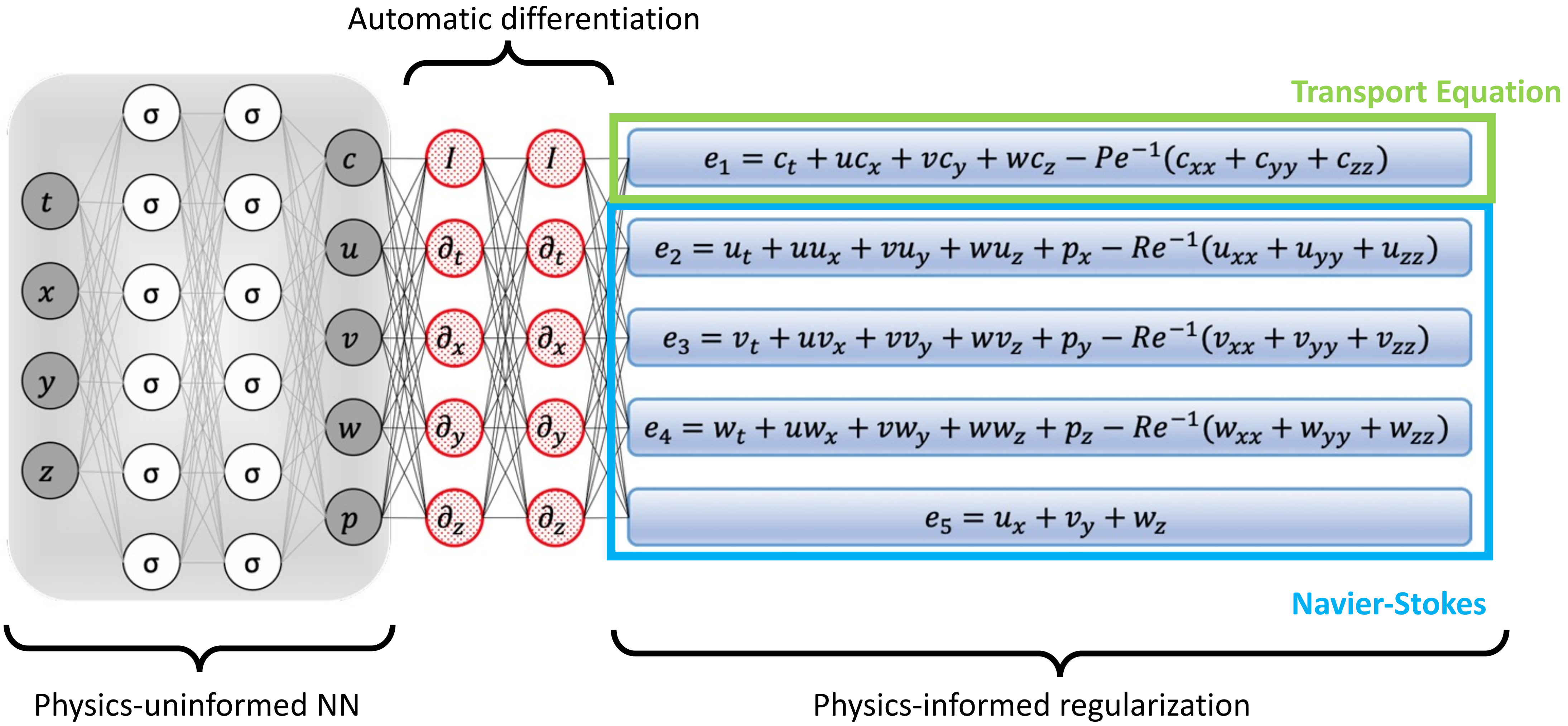
$$c_t = -(u\, c_x + \ v\, c_y + \ w\, c_z) + \frac{1}{Pec}\left(c_{xx} + c_{yy} + c_{zz}\right)$$

Equivalent regularization:

$$e_1 = c_t + uc_x + vc_y + wc_z - Pe^{-1}(c_{xx} + c_{yy} + c_{zz})$$

NN: $(t, x, y, z) \rightarrow (c, u, v, w, p)$

Full Model Overview



Loss Function

MSE for Physics-uninformed NN

$$\frac{1}{N}\sum_{n=1}^{N}\left(\left| c(t^n, x^n, y^n, z^n) - c^n \right|^2 \right)$$

$$+$$

Physics-informed regularization

$$\sum_{i=1}^{5} \frac{1}{M}\sum_{m=1}^{M}\left(\left| e_{\mathrm{i}}(t^{\mathrm{m}}, x^{\mathrm{m}}, y^{\mathrm{m}}, z^{\mathrm{m}}) \right|^2 \right)$$

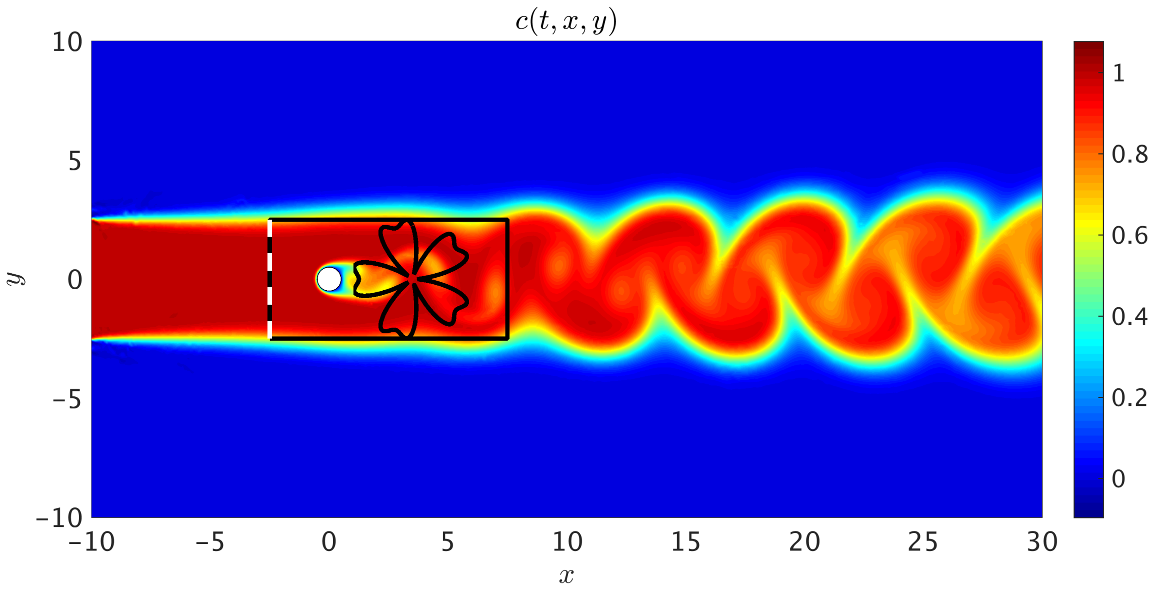
Experiment Results

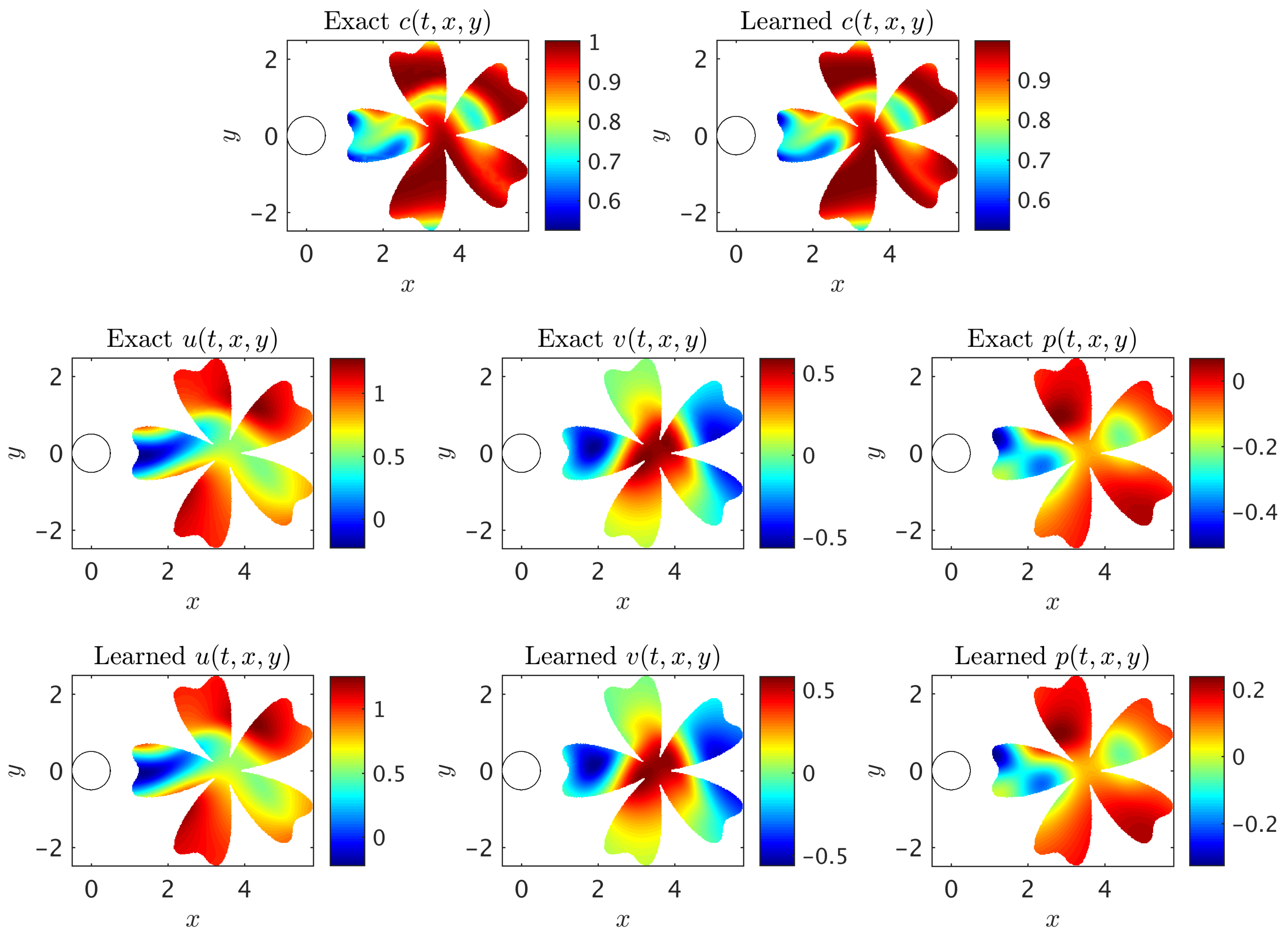
Case studies: External vs. Internal flow in 2D/3D

Comparison of Learned Solution vs Ground truth

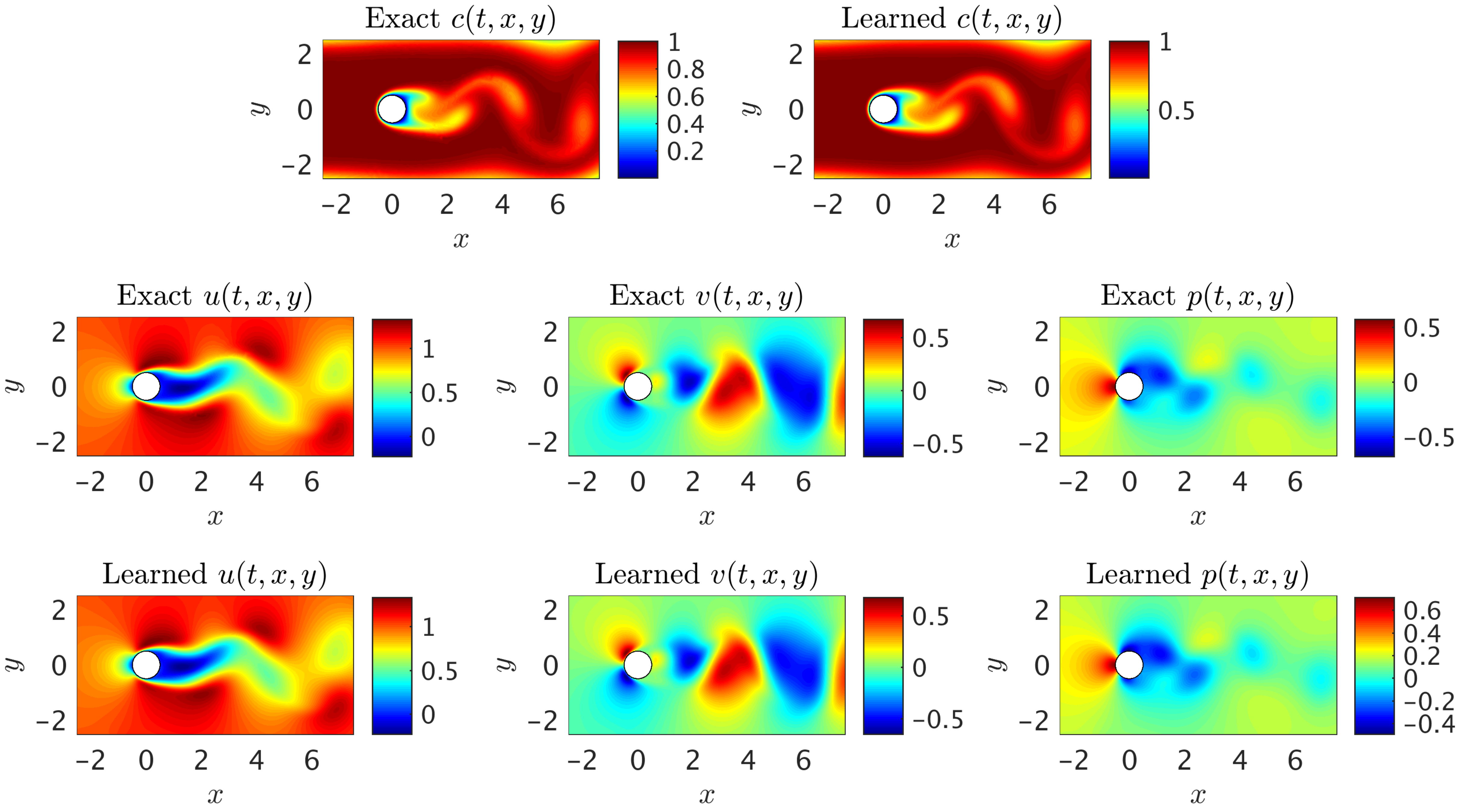
External Flow

- 2D flow past a cylinder (simulation)
- Passive scalar injected from left inlet
- Sample area for training data can be arbitrary





Exact $c(t,x,y)$
Learned $c(t,x,y)$
Exact $u(t,x,y)$
Exact $v(t,x,y)$
Exact $p(t,x,y)$
Learned $u(t,x,y)$
Learned $v(t,x,y)$
Learned $p(t,x,y)$
x
y



Exact $c(t, x, y)$
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Exact $v(t, x, y)$
Exact $p(t, x, y)$
Learned $u(t, x, y)$
Learned $v(t, x, y)$
Learned $p(t, x, y)$
x
y

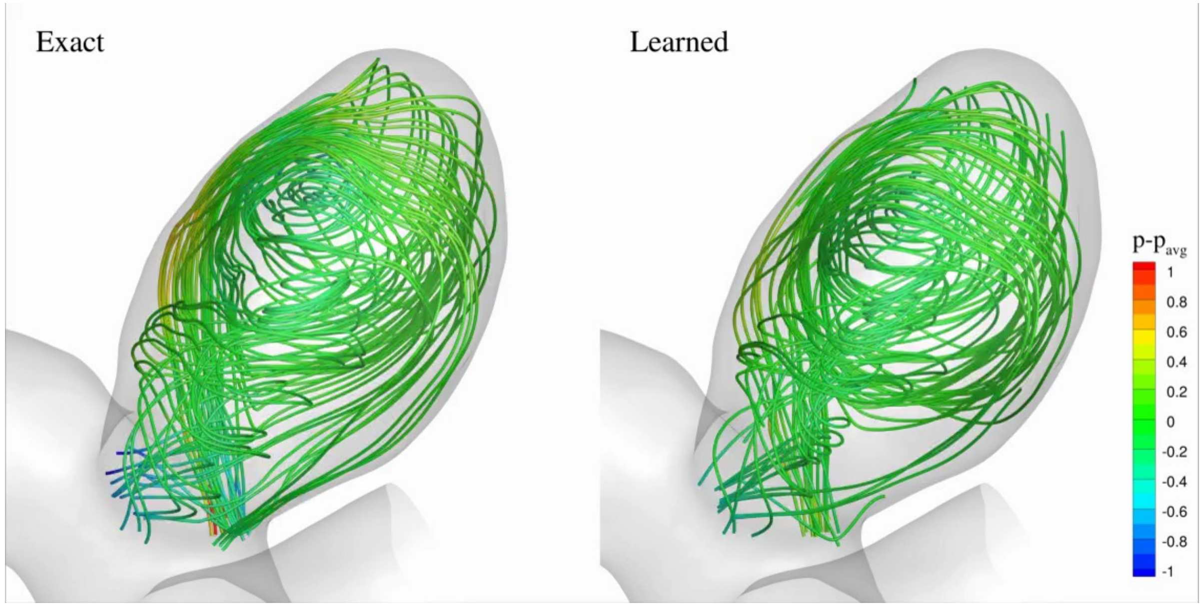
Learning Reynold & Péclet numbers

- In both experiments, Re and Pec are prescribed (both set to 100)
- But we can also modify the model slightly to learn them

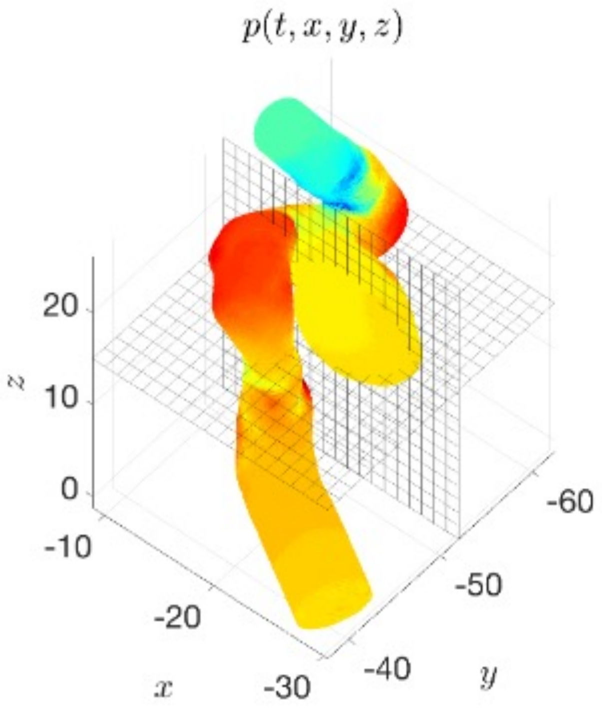
	Exact	Learned	Rel. Error
Pec	100	92.39	7.60%
Re	100	92.47	7.52%

Internal Flow: Intracranial Aneurysm (ICA)

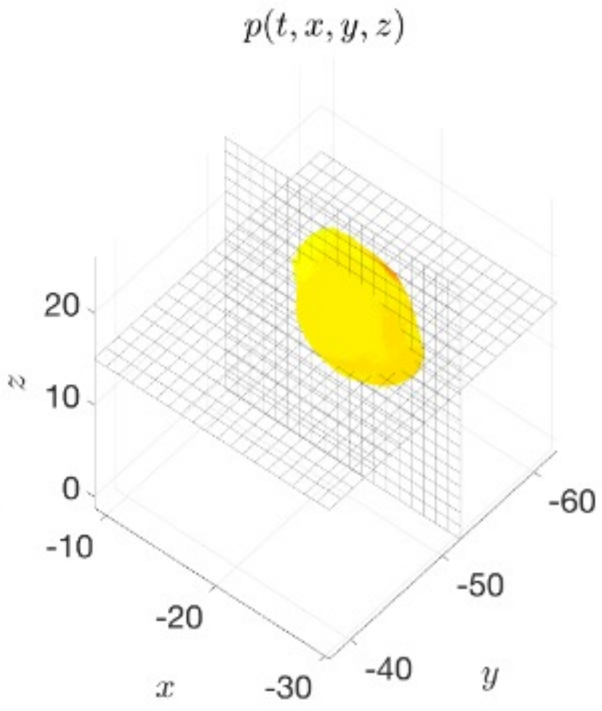
- No boundary conditions except for at outlet (velocity & concentration)
- Use only sac for training



Visualized blood flow paths within the aneurysm



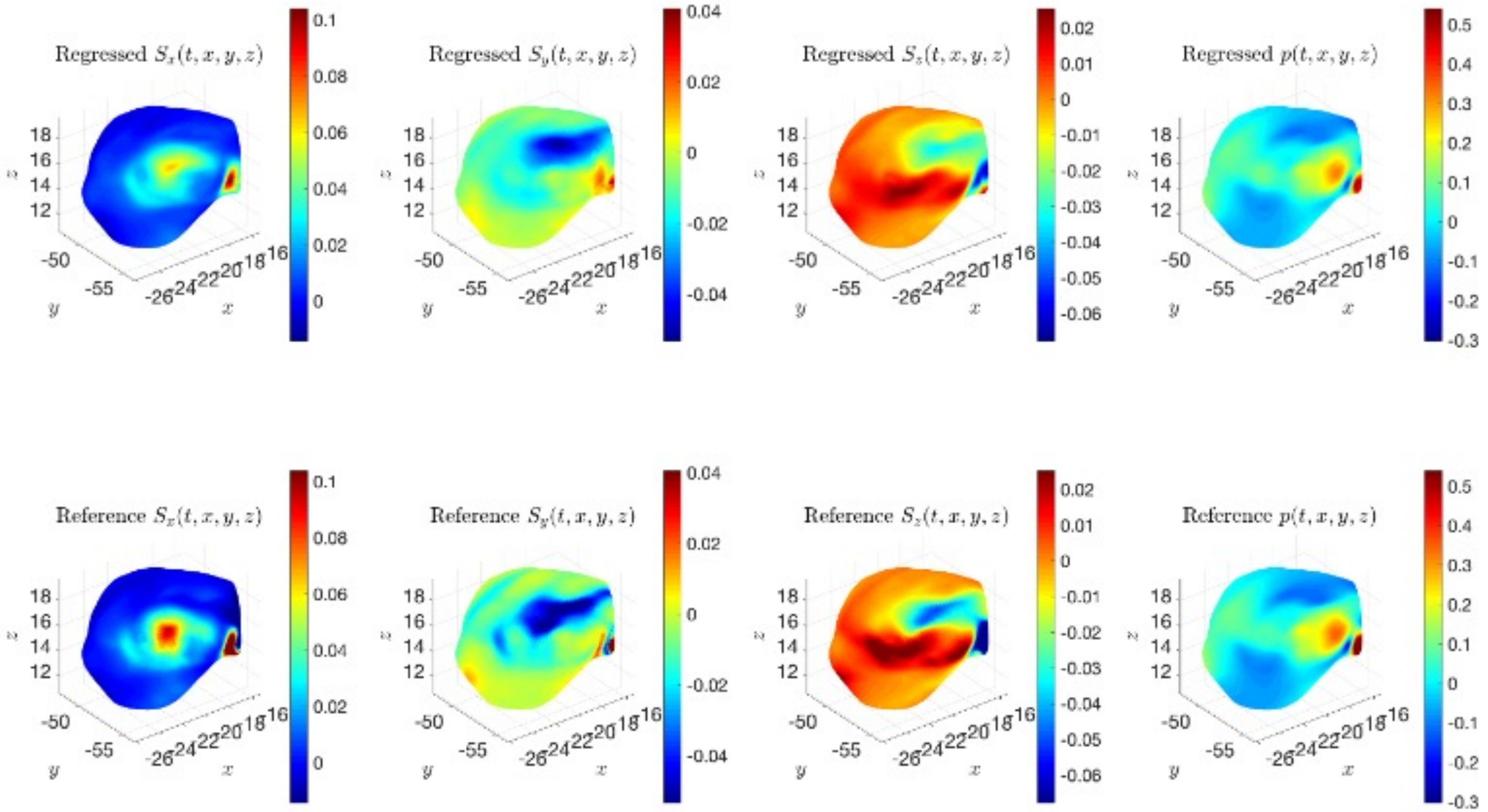
Simulation domain



Training domain

Intracranial Aneurysm (ICA)

- Wall shear stress



Feedback

What are some problems with the paper?

What was done well?

Our takeaways

Negative:

- Only simulation data
- Overfitting / Generalizability?
- Short overview of NS would have been nice
- “Agnostic to initial/boundary conditions” shown but not explained

Positive:

- Easy to follow
- Good separation of main paper and additional material
- Descriptive diagrams
- Interesting experiments (ICA)

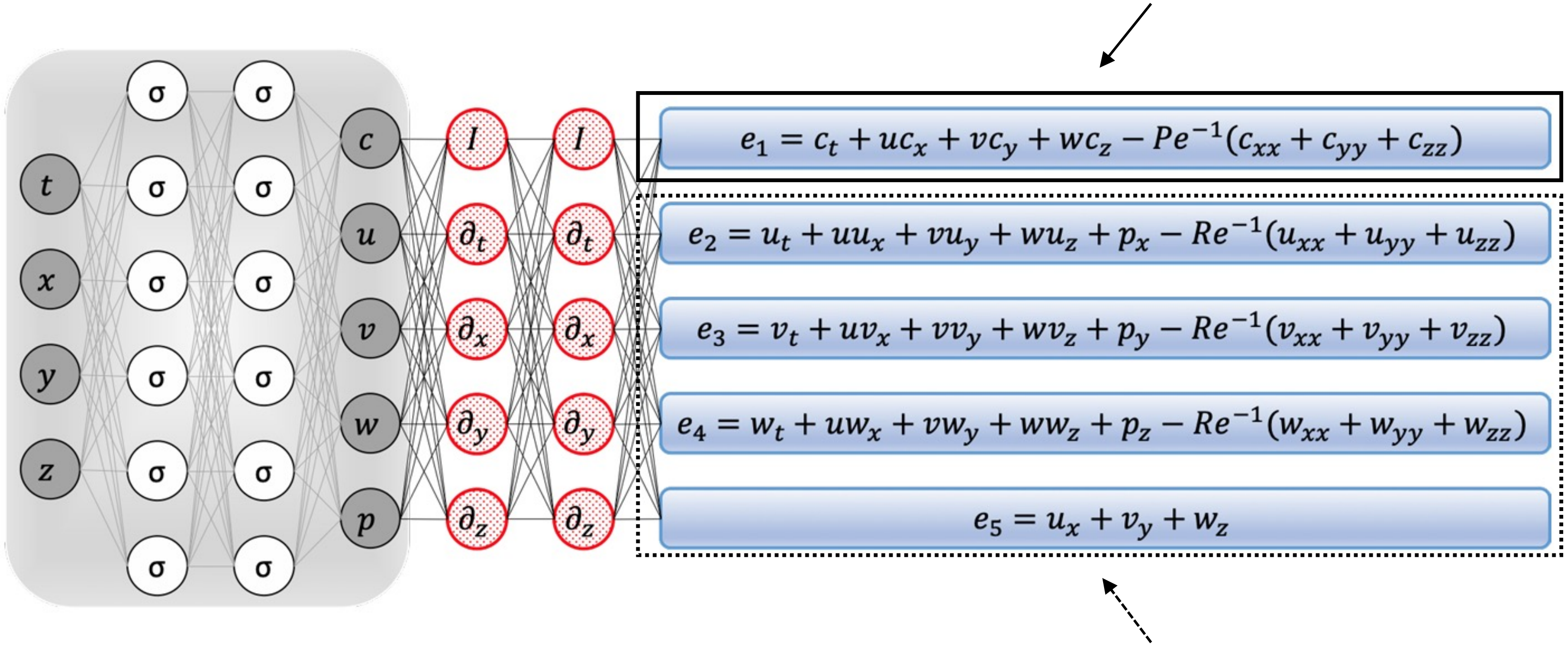
Thank you for listening!

We will gladly answer any further questions

Hidden Fluid Mechanics

Transport Equation

$$c_t = -(u\,c_x + v\,c_y + w\,c_z) + \frac{1}{Pec}(c_{xx} + c_{yy} + c_{zz})$$



Reynolds number: $Re = \frac{inertia}{viscosity}$ (fluid particle)

Péclet number: $Pec = \frac{advection}{diffusion}$ (transported particle)

Navier-Stokes Equations

$$\frac{\partial \vec{\boldsymbol{u}}}{\partial t} + (\vec{\boldsymbol{u}} \cdot \nabla)\vec{\boldsymbol{u}} = -\nabla P + \frac{1}{Re}\nabla^2 \vec{\boldsymbol{u}}$$

$$\nabla \cdot \vec{\boldsymbol{u}} = 0$$

Notation	
$\boldsymbol{u}, \vec{\boldsymbol{u}}$	velocity (vector)
u, v, w	velocity (scalar)
u_x	$\partial u / \partial x$
t	time
ρ	density
ν	viscosity
P	pressure
V	volume
∇	gradient
$\nabla \cdot$	divergence, e.g. $\nabla \cdot (u, v, w)^T = \partial u / \partial x + \partial v / \partial y + \partial w / \partial z$
∇^2	laplacian, e.g. $\nabla^2 c = c_{xx} + c_{yy} + c_{zz}$