Differentiable Stable Fluid Solver using TensorFlow

PRIM Project

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Introduction

Navier-Stokes equations

A fluid whose density ρ and temperature are nearly constant is described by a velocity field $u : \mathbb{R}^N \longrightarrow \mathbb{R}^N$ and a pressure field $p : \mathbb{R}^N \longrightarrow \mathbb{R}$.

Navier-Stokes equations

$$\nabla \cdot u = 0$$

$$\frac{\partial u}{\partial t} = -(u \cdot \nabla)u - \frac{1}{\rho}\nabla p + \nu \nabla^2 u + f$$

Resolution method

Too hard to analytcally solve...

Marching through each step

$$\nabla \cdot u_3 = 0$$

$$\frac{\partial u_4}{\partial t} = -(u_1 \cdot \nabla) u_1 - \frac{1}{\rho} \nabla p + \nu \nabla^2 u_2 + f$$

Problem: how to ensure $\nabla \cdot u_3 = 0$ ... ?

Projection operator

$$\nabla \cdot u_3 = 0 \text{ and } \frac{\partial u_4}{\partial t} = -(u_1 \cdot \nabla)u_1 - \frac{1}{\rho}\nabla p + \nu \nabla^2 u_2 + f$$

Problem: how to ensure $\nabla \cdot u_3 = 0$ ... ?

Helmholtz-Hodge Decomposition

Any vector field $w : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ can be decomposed into

$$w = u + \nabla q$$

where $u : \mathbb{R}^3 \longrightarrow \mathbb{R}^3, \nabla \cdot u = 0$ and $q : \mathbb{R}^3 \longrightarrow \mathbb{R}$

Projection operator

Any vector field w can be decomposed into a divergence-free field and a gradient

$$w = u + \nabla q$$

Define a projection operator and apply it to Navier-Stokes

$$\mathbb{P} : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$$

$$w = u + \nabla q \longmapsto \mathbb{P}(w) = u = w - \nabla q$$

q can be recovered with a Poisson equation

$$\nabla \cdot w = \underbrace{\nabla \cdot u}_{0} + \nabla \cdot \nabla q \iff \nabla \cdot w = \nabla^2 q$$

Projection operator

By applying $\mathbb{P}$ to Navier-Stokes, we keep $\nabla \cdot u = 0$ implicit.

$$\mathbb{P}\left(\frac{\partial u}{\partial t}\right) = \mathbb{P}\left(-(u \cdot \nabla)u - \frac{1}{\rho}\nabla p + \nu \nabla^2 u + f\right)$$

$$\frac{\partial u}{\partial t} = \mathbb{P}\left(-(u \cdot \nabla)u\right) - \underbrace{\mathbb{P}\left(\frac{1}{\rho}\nabla p\right)}_{0} + \mathbb{P}\left(\nu \nabla^2 u\right) + \mathbb{P}\left(f\right)$$

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

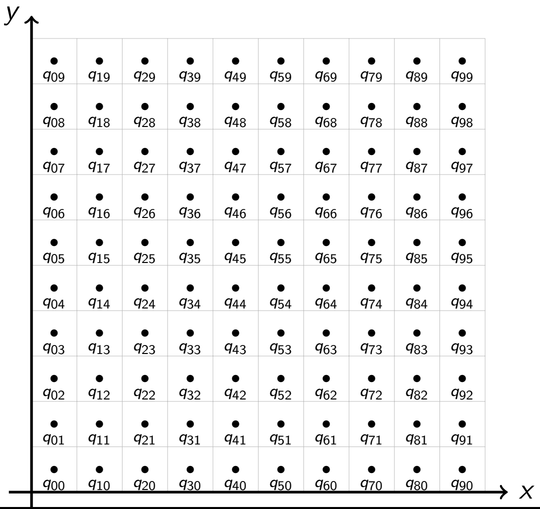
Roadmap

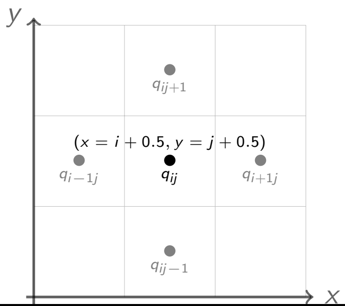
Goals of the project

- Implement a 2D stable fluid solver in Python
- Making it differentiable using TensorFlow library

Stable fluid solver

Stable fluid solver: Model





Stable fluid solver: Data structure

y

u_{09}	u_{19}	u_{29}	u_{39}	u_{49}	u_{59}	u_{69}	u_{79}	u_{89}	u_{99}
u_{08}	u_{18}	u_{28}	u_{38}	u_{48}	u_{58}	u_{68}	u_{78}	u_{88}	u_{98}
u_{07}	u_{17}	u_{27}	u_{37}	u_{47}	u_{57}	u_{67}	u_{77}	u_{87}	u_{97}
u_{06}	u_{16}	u_{26}	u_{36}	u_{46}	u_{56}	u_{66}	u_{76}	u_{86}	u_{96}
u_{05}	u_{15}	u_{25}	u_{35}	u_{45}	u_{55}	u_{65}	u_{75}	u_{85}	u_{95}
u_{04}	u_{14}	u_{24}	u_{34}	u_{44}	u_{54}	u_{64}	u_{74}	u_{84}	u_{94}
u_{03}	u_{13}	u_{23}	u_{33}	u_{43}	u_{53}	u_{63}	u_{73}	u_{83}	u_{93}
u_{02}	u_{12}	u_{22}	u_{32}	u_{42}	u_{52}	u_{62}	u_{72}	u_{82}	u_{92}
u_{01}	u_{11}	u_{21}	u_{31}	u_{41}	u_{51}	u_{61}	u_{71}	u_{81}	u_{91}
u_{00}	u_{10}	u_{20}	u_{30}	u_{40}	u_{50}	u_{60}	u_{70}	u_{80}	u_{90}

x

$$u = \begin{pmatrix} u_{00} & u_{10} & \cdots & u_{n0} \\ u_{01} & u_{11} & \cdots & u_{n1} \\ \vdots & \vdots & \ddots & \vdots \\ u_{0n} & u_{1n} & \cdots & u_{nn} \end{pmatrix}$$

Data structure 1

$$u_x = \begin{pmatrix} u_{x,00} \\ u_{x,10} \\ \vdots \\ u_{x,n0} \\ u_{x,n1} \\ \vdots \\ u_{x,nn} \end{pmatrix}, u_y = \begin{pmatrix} u_{y,00} \\ u_{y,10} \\ \vdots \\ u_{y,n0} \\ u_{y,n1} \\ \vdots \\ u_{y,nn} \end{pmatrix}$$

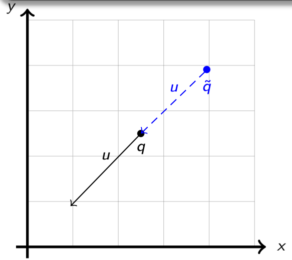
Data structure 2

Stable fluid solver: Advection

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

Backtracing - Method of characteristics

$$u(x, y, t + \Delta t) = u(x - \Delta t u_x(x, y, t), y - \Delta t u_y(x, y, t), t)$$



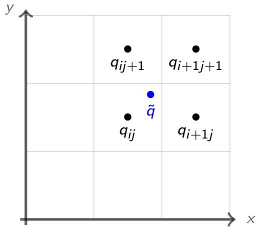

```python
def advectCentered(f,u,v,sizeX,sizeY,coords_x,coords_y,dt,offset,d):
    traced_x = np.clip(coords_x - dt*u, offset+0.5*d, offset+(sizeX-0.5)*d)
    traced_y = np.clip(coords_y - dt*v, offset+0.5*d, offset+(sizeY-0.5)*d)
    new_grid = []
    for it in range(len(traced_x)):
        new_grid.append(sampleAt(traced_x[it],traced_y[it],f,sizeX,sizeY,
                        offset,d))
    return np.array(new_grid)
```

Stable fluid solver: Advection

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

$\tilde{q}$ is not necessarely centered

Backtraced value is bilinearly interpolated using the stencil.




```python
def sampleAt(x,y,data,sizeX, sizeY, offset,d):
    _x = (x-offset)/d - 0.5
    _y = (y-offset)/d - 0.5
    i0 = np.clip(np.floor(_x),0,sizeX-1)
    j0 = np.clip(np.floor(_y),0,sizeY-1)
    i1 = np.clip(i0+1,0,sizeY-1)
    j1 = np.clip(j0+1,0,sizeY-1)

    p00 = data[ int(indexTo1D(i0,j0,sizeX))]
    p01 = data[ int(indexTo1D(i0,j1,sizeX))]
    p10 = data[ int(indexTo1D(i1,j0,sizeX))]
    p11 = data[ int(indexTo1D(i1,j1,sizeX))]

    t_i0 = (offset + (i1+0.5)*d -x)/d
    t_j0 = (offset + (j1+0.5)*d -y)/d
    t_i1 = (x - (offset + (i0+0.5)*d))/d
    t_j1 = (y - (offset + (j0+0.5)*d))/d

    return t_i0*t_j0*p00 + t_i0*t_j1*p01 + t_i1*t_j0*p10 + t_i1*t_j1*p11
```

Stable fluid solver: Poisson equation

Problem: how to solve $\nabla^2 q = w$?

Discretize using forward and backward derivatives

$$w_{ij} = \frac{q_{i+1j} + q_{i-1j} + q_{ij+1} + q_{ij-1} - 4q_{ij}}{h^2} \text{ by taking } dx = dy = h$$

Two possibilities: Gauss-Seidel updates or Laplacian matrix

```python
def gauss_seidel_solver(w,q,a,b,n_iter):
    dim_x, dim_y = u1.shape
    for it in range(n_iter):
        for i in range(1,dim_x-1):
            for j in range(1,dim_y-1):
                q[i,j] = (w[i,j] + a*(w[i+1, j] + q[i, j+1] + q[i
                        -1, j] + q[i,j-1]))/b
        u1 = set_solid_boundary(u1, 0)
    return u1
```

$$\begin{matrix}
-4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1
\end{matrix}$$

Stable fluid solver: Diffusion

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

Implicit method: find $\tilde{u}$ such that $(I - \Delta t \nu \nabla^2)\tilde{u} = u$.

It is possible to use the Poisson solver

Apply the following transformations: $\frac{-4}{h^2} \longrightarrow \frac{1 + 4\nu\Delta t}{h^2}$ and $\frac{1}{h^2} \longrightarrow \frac{-\nu\Delta t}{h^2}$.

Stable fluid solver: Projection

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

1. Find q such that $\nabla^2 q = \nabla \cdot u$ (Poisson equation)
2. $u \longleftarrow u - \nabla q$

```python
def project(u,v,sizeX,sizeY,mat,h,boundary_func):
    _u,_v = set_boundary(u,v, sizeX, sizeY,boundary_func)
    p = solvePressure(_u,_v,sizeX,sizeY,h, mat)
    gradP_u = []
    gradP_v = []
    for j in range(sizeY):
        for i in range(sizeX):
            if (i>1) and (i < sizeX-1):
                gradP_u.append(p[indexTo1D(i+1,j,sizeX)] - p [indexTo1D(i
                    -1, j, sizeX)])
            else:
                gradP_u.append(0)
            if (j>1) and (j < sizeY-1):
                gradP_v.append(p[indexTo1D(i,j+1,sizeX)] - p[indexTo1D(i,j
                    -1,sizeX)])
            else:
                gradP_v.append(0)

    gradP_u = (0.5/h)*np.array(gradP_u)
    gradP_v = (0.5/h)*np.array(gradP_v)
    new_u = _u - gradP_u
    new_v = _v - gradP_v
    new_u, new_v = set_boundary(new_u, new_v, sizeX, sizeY, boundary_func)
    return new_u, new_v
```

Stable fluid solver: Moving a substance through the fluid

A substance $s : \mathbb{R}^N \longrightarrow \mathbb{R}$ moving through the field

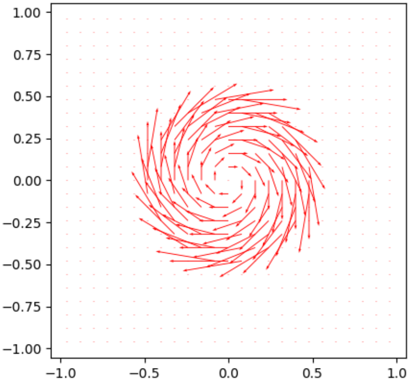
Navier-Stokes for a scalar field

$$\frac{\partial s}{\partial t} = -u \cdot \nabla s + \kappa \nabla^2 s - \alpha s + f_s$$

Similar to what we explained before ! $\Longrightarrow$ same resolution method

Results

Vortex

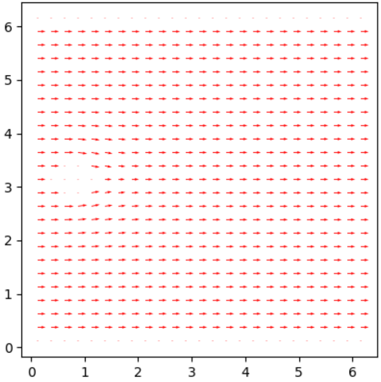


Initial velocity field (grid $[-1, 1]$ of size 25×25)

Initial density field (grid $[-1, 1]$ of size 99×99)

Vortex

Karman vortex



Initial velocity field (grid $[-1, 1]$ of size 25×25)

Initial vorticity field (grid $[-1, 1]$ of size 90×90)

About the two data structures

Using matrix data structure

Using tensor data structure

Roadmap

Goals of the project

- ✓ Implement a 2D stable fluid solver in Python
- Making it differentiable using TensorFlow library

Differentiable physics in TensorFlow

TensorFlow

TensorFlow

- open-source software library for ML and AI applications
- developed by Google Brain Team
- could be used to train a neural network to predict the behavior of a physical system based on a set of inputs
- uses backpropagation

$$\begin{tikzcd}
u \arrow[r, "\texttt{addForce()}"] & u \arrow[r, "\texttt{advect()}"] & u \arrow[r, "\texttt{diffuse()}"] & u \arrow[r, "\texttt{project()}"] & u \arrow[d, "\texttt{advect()}"] & & \\
 & & & s \arrow[r, "\texttt{addForce()}"'] & s \arrow[r, "\texttt{diffuse()}"'] & s \arrow[r, "\texttt{dissipate()}"'] & s
\end{tikzcd}$$

```python
import tensorflow as tf
u_init = ...#Initialize u_init
density_init = ...#Initialize density_init
u_init = tf.convert_to_tensor(u_init)
density_init = tf.convert_to_tensor(density_init)
with tf.GradientTape() as tape:
    velocity_field = tf.Variable(u_init)
    density_field = solveDens(density_init, solveVel(velocity_field))
grad = tape.gradient([density_field], [velocity_field])
```

Every operation must be differentiable $\implies$ is currently slow

An application to a matching shape problem

Starting density s_0

$\Longrightarrow$

Target density field t

An application to a matching shape problem

Goal: Minimize $\mathcal{L}(s_0, u) = ||\mathbb{F}_2(s_0, \mathbb{F}_1(u)) - t||^2$

Use the gradient to perform a gradient descent

$$u_{n+1} = u_n - \alpha_n \left. \frac{\partial \mathcal{L}(s_0, u_n)}{\partial u} \right|_{u_n}$$

Every operation must be differentiable $\Longrightarrow$ is currently slow

Different learning rate α_n possible

An application to a matching shape problem

Density obtained with the trained velocity

Target density field at frame 20

An application to a matching shape problem

Density obtained at frame 20 with the trained velocity

Target density field t at frame 20

Discussions and Future work

Discussions and Future work

- different grid model (velocity stored at the edges, ...)
- explore parallelization to reduce execution time
- extension in 3D

Conclusion

Goals of the project

- ✔ Implement a 2D stable fluid solver in Python
- ✔ Making it differentiable using TensorFlow library
- Testing on training problems
- Applying it to constraint-based physical problems

Thank You

Questions?