Data-Assimilation for Orszag-Tang Magnetohydrodynamic Vortex Problem

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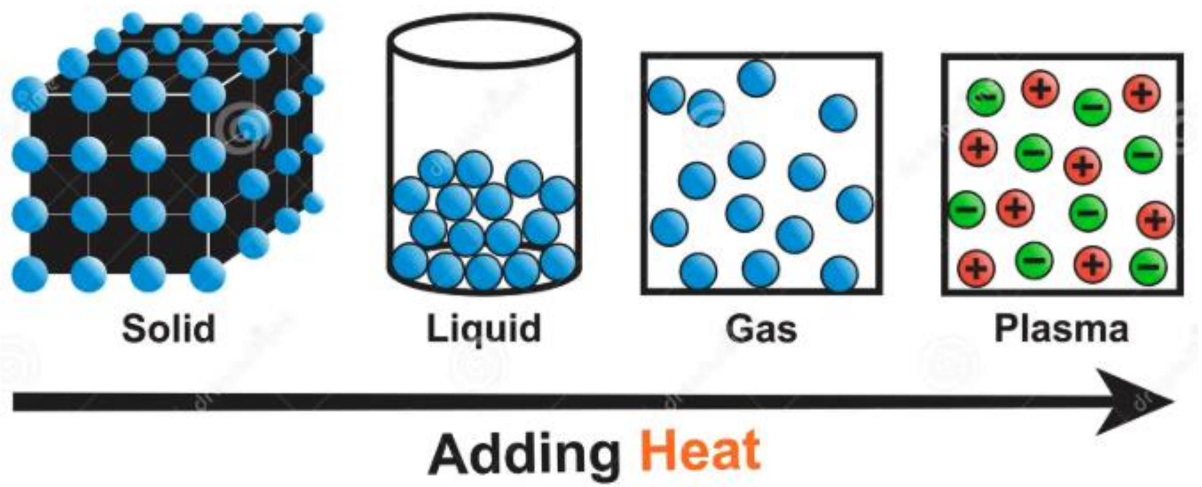
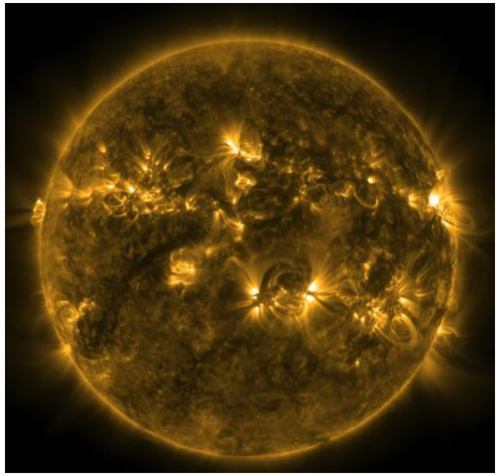
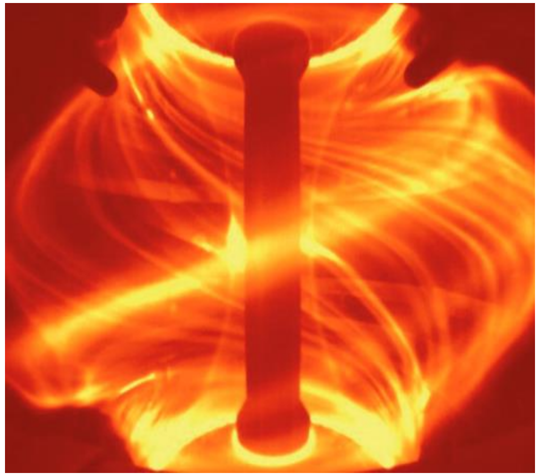
Plasma - Ionized gas with quasi-neutrality







- A combination of ions, electrons, and neutrals
- Types of interactions
  - Collisions: Particle-Particle
  - Coulomb force: Particle-Field
  - Electromagnetic coupling: Field-Field
- Complex nonlinear dynamics
  - Governed by Maxwell's equation (field) and fluid equation (particle)

Fluid approach for plasma dynamics

- Electromagnetic fluid: Interaction between field-particles + particles-particles (collision)
- E and B fields: governed by Maxwell equations
- Particle density and current density: governed by fluid equation

Maxwell's equation

$$\nabla \cdot E(x,t) = \sum \frac{q_s n_s}{\epsilon_0} \qquad (1)$$

$$\nabla \times E(x,t) = -\frac{\partial B(x,t)}{\partial t} \qquad (2)$$

$$\nabla \cdot B(x,t) = 0 \qquad (3)$$

$$\nabla \times B(x,t) = \sum \mu_0 J_S + \mu_0 \epsilon_0 \frac{\partial E(x,t)}{\partial t} \qquad (4)$$

$$\Longleftrightarrow$$

Fluid equation

$$\frac{\partial n_s}{\partial t} + \nabla \cdot (n_s v) = 0 \qquad (5)$$

$$m_s n_s \frac{dv}{dt} = q_s n_s (E + v \times B) - \nabla P \qquad (6)$$

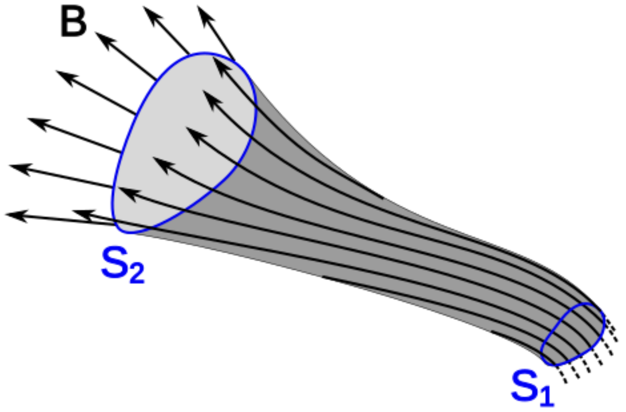
$$\frac{d}{dt}\left(\frac{P}{\rho^\gamma}\right) = 0 \qquad (7)$$

$$J = \sum q_s n_s v_s (= J_s) \qquad (8)$$

Magnetohydrodynamics

- Single fluid approximation: Weighted average of multiple species' motions (Single fluid)
- MHD = Electrically conducting fluid system with self-consistent magnetic fields
- Charge-neutrality + Small gyro-radius approximation: $\nabla \cdot E = 0$ + $\nabla \times B = \frac{4\pi}{c} J$ (No displacement current)
- Appropriate for (1) low-frequency (2) large-scale system
- Example: Space plasma, Fusion plasma, Liquid metal

Frozeon-flux theorem



Different from the behavior of the general fluid model

Magnetic flux

Plasma flow

$$\frac{D\Phi}{Dt} = 0 \quad \Longleftrightarrow \quad \frac{\partial B}{\partial t} - \nabla \times (v \times B) = 0$$

MHD equations

$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$	Continuouity
$\rho \frac{dv}{dt} = \frac{1}{4\pi} (\nabla \times B) \times B - \nabla P$	Momentum
$\frac{d}{dt}\left(\frac{P}{\rho^\gamma}\right) = 0$	Adiabatic process
$\frac{\partial B}{\partial t} = \nabla \times (v \times B)$	Ohm's law
$\nabla \cdot B = 0$	Gauss' law (Divergence free condition)

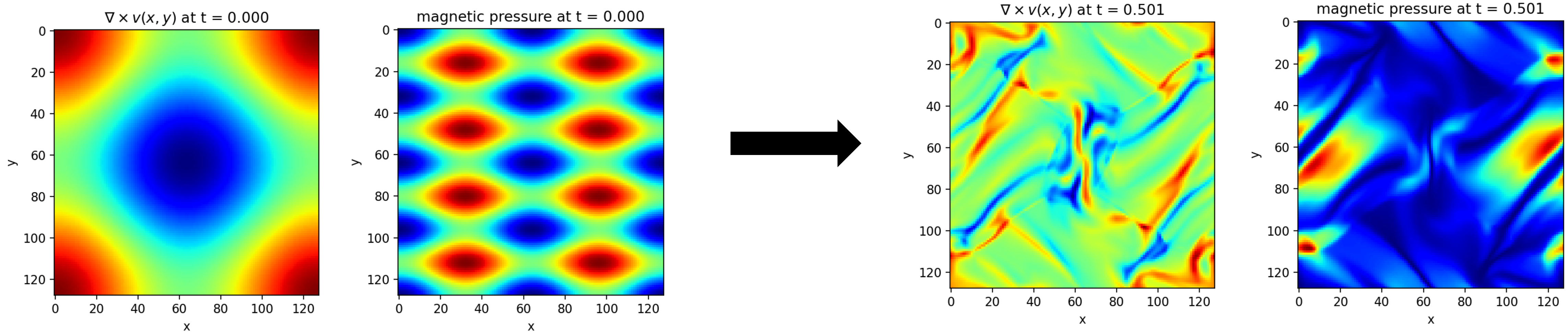
Orszag-Tang MHD vortex problem

- Small-scale MHD turbulence model observed from two-dimensional periodic system
- Formation of the MHD shocks: Alfven wave (transverse) + Magneto-sonic wave (compressional)
- Nonlinear plasma – wave interaction → Transition to MHD turbulent structure
- Initial conditions for turbulence observation

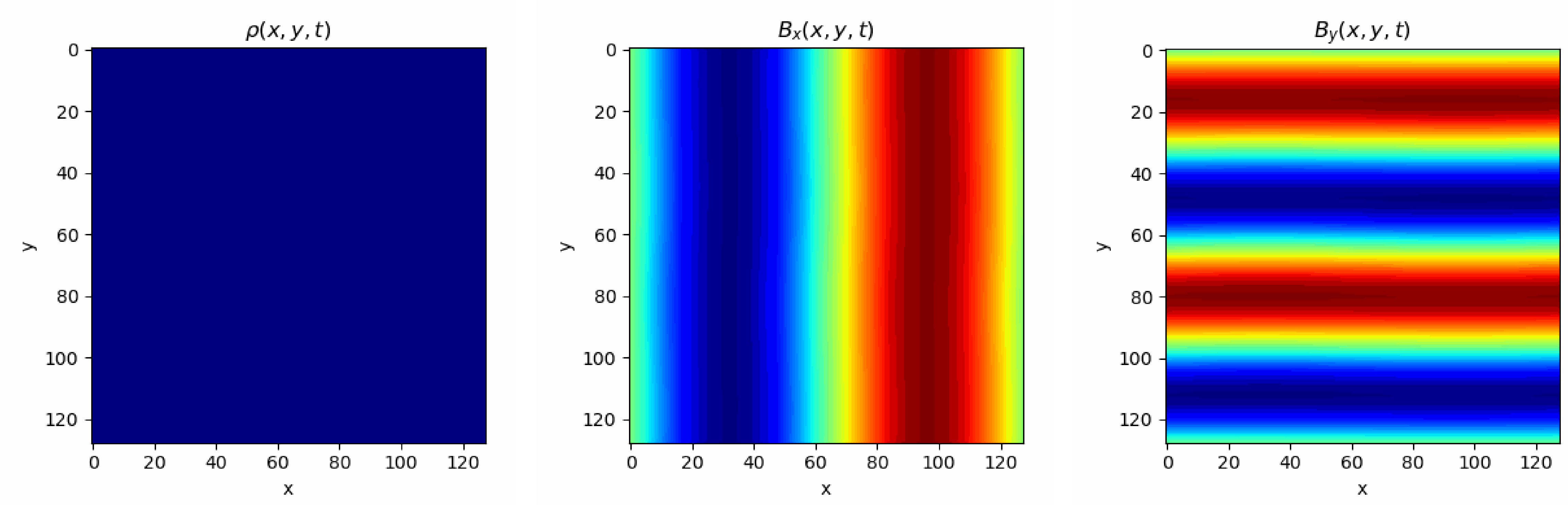
$$v = -\sin y\,\hat{\imath} + \sin x\,\hat{\jmath}$$

$$B = -\sin y\,\hat{\imath} + \sin 2x\,\hat{\jmath}$$

Shock – Shock interaction
(Small scale turbulent structure)



Orszag-Tang MHD vortex problem



Data assimilation for MHD systems

- In real systems, there are two limits on predicting the MHD phenomenon
- (1) Model error
  - Assumed (a) low-frequency wave (2) large-scale behavior : kinetic effect ignored
  - Ideal MHD: Magnetic diffusivity exists on the system + Lack of information
- (2) Measurement error
  - Inaccurate information about Initial / boundary conditions
  - External noise applied by radiations + electronic noise by thermal agitation
- Data assimilation techniques are required to compensate these errors

Kalman Filter

- Kalman filter: an approach to estimate the states variables based on Markov chain and Gaussian estimation
- Initial state and errors follow Gaussian + i.i.d

Linear discrete-time dynamic model

$$X_{k+1} = FX_k + \zeta_{k+1}$$
$$Y_{k+1} = HX_{k+1} + \eta_{k+1}$$

$$X_0 \sim N(\mu_0, \Sigma_0)$$
$$\zeta_k \sim N(0, \Sigma_x) \qquad (\zeta_k): i.i.d$$
$$\eta_k \sim N(0, \Sigma_y) \qquad (\eta_k): i.i.d$$

- Recursive process of Kalman Filter

New measurement data Y_{k+1}

Prediction step
(Priori state estimation + covariance)

$$\hat{\mu}_{k+1} = F\mu_k$$
$$\hat{\Sigma}_{k+1} = F\Sigma_k F^T + \Sigma_x$$

Find optimal Kalman gain

$$K_{k+1} = \hat{\Sigma}_{k+1}H^T\left(\Sigma_y + H\hat{\Sigma}_{k+1}H^T\right)^{-1}$$

Update step
(Posteriori state estimation)

$$\mu_{k+1} = \hat{\mu}_{k+1} + K_{k+1}(Y_{k+1} - H\hat{\mu}_{k+1})$$
$$\Sigma_{k+1} = (I - K_{k+1}H)\hat{\Sigma}_{k+1}$$

Ensemble Kalman Filter

- Monte-Carlo method based Kalman Filtering: Replace the posteriori estimation by ensemble samples
- Use ensemble to compute estimated mean and covariance: computational cost ↓ + Nonlinearity
- Kalman gain and posteriori state estimation can be obtained by sample covariance instead

Nonlinear discrete-time dynamic model

$$X_{k+1} = f(X_k) + \zeta_{k+1}$$
$$Y_{k+1} = HX_{k+1} + \eta_{k+1}$$

$$X_0 \sim N(\mu_0, \Sigma_0)$$
$$\zeta_k \sim N(0, \Sigma_x) \quad (\zeta_k): i.i.d$$
$$\eta_k \sim N(0, \Sigma_y) \quad (\eta_k): i.i.d$$

Define ensemble samples

$$X_k^e = [X_k^1, \dots, X_k^n] \quad X_0^i := X_0 + \zeta_0^i$$
$$Y_k^e = [Y_k^1, \dots, Y_k^n] \quad Y_k^i := Y_k + \eta_k^i$$

- Recursive process of Ensemble Kalman Filter

New measurement data Y_{k+1}

Prediction step
(Priori state estimation + covariance)

$$\hat{X}^e{}_{k+1} = f(X_k^e)$$
$$\hat{\Sigma}^e{}_{k+1} = cov[\hat{X}_{k+1}^e]$$

Find optimal Kalman gain

$$K_{k+1} = \hat{\Sigma}^e{}_{k+1} H^T \left(\Sigma_y + H\hat{\Sigma}^e{}_{k+1} H^T\right)^{-1}$$

Update step
(Posteriori state estimation)

$$Y_{k+1}^e = [Y_{k+1}^1, \dots, Y_{k+1}^n]$$
$$X_{k+1}^e = \hat{X}_{k+1}^e + K_{k+1}(Y_{k+1}^e - H\hat{X}^e{}_{k+1})$$

Application to MHD transport simulation

- Nonlinear dynamics $f(x)$: Constrained Transport Method to predict next state with primitive variables
- EnKF: State estimation
- N_m: Number of the datapoints (measurement points) = 100 (Default)
- N_g: Number of the mesh grid = 50 (Default)
- $\Sigma_{x,y}$: 0.1 / 0.01 (default) / 0.001 / 0.0001

Model error

$$X_{k+1} = f(X_k) + \zeta_{k+1}$$

$$Y_{k+1} = HX_{k+1} + \eta_{k+1}$$

Measurement error

State variables: Primitive variables for MHD

$$X_k = \left[\rho_k, u_{x,k}, u_{y,k}, P_k, B_{x,k}, B_{y,k}\right] \in R^{N_g^2}$$

$$\rho_k, u_{x,k}, u_{y,k}, P_k, B_{x,k}, B_{y,k} \in R^{N_g \times N_g}$$

2D vectors to 1D arrays

$$\zeta_k \in R^{N_g^2} \quad \eta_k \in R^{N_m}$$

$$\zeta_k \sim N(0, \Sigma_x)$$

$$\eta_k \sim N(0, \Sigma_y)$$

$f(X)$:

$$\frac{\partial U}{\partial t} + \nabla \cdot F(U) = 0$$

$$U_{k+1} = U_k - \frac{\Delta t}{\Delta x}(F_R - F_L)$$

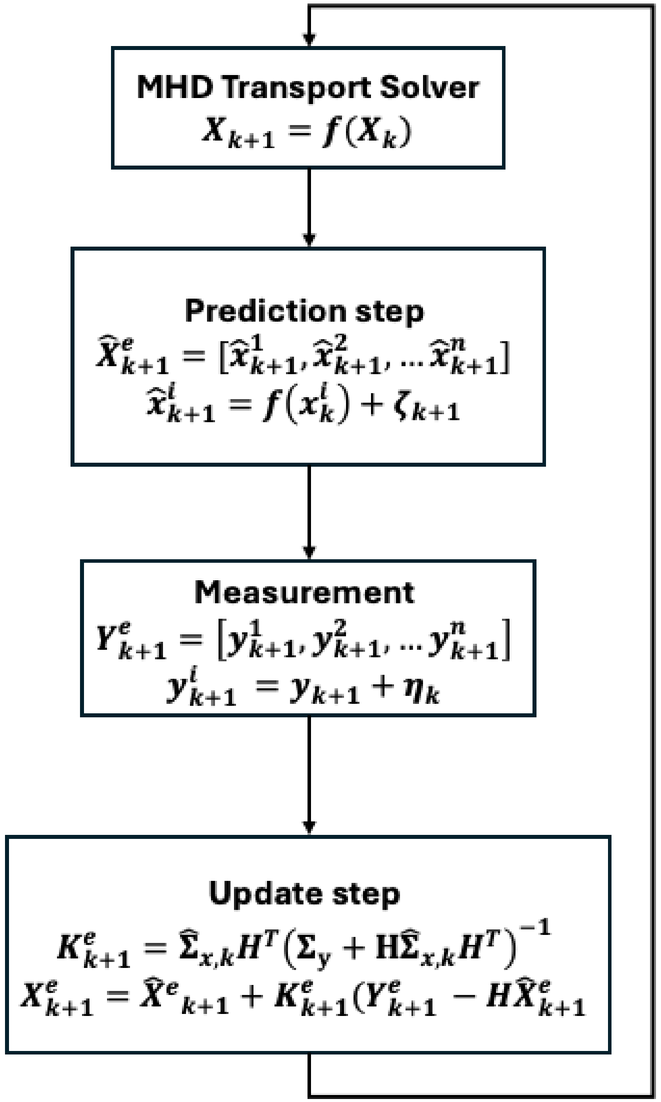
$F_{R,L}$: Rusanov flux

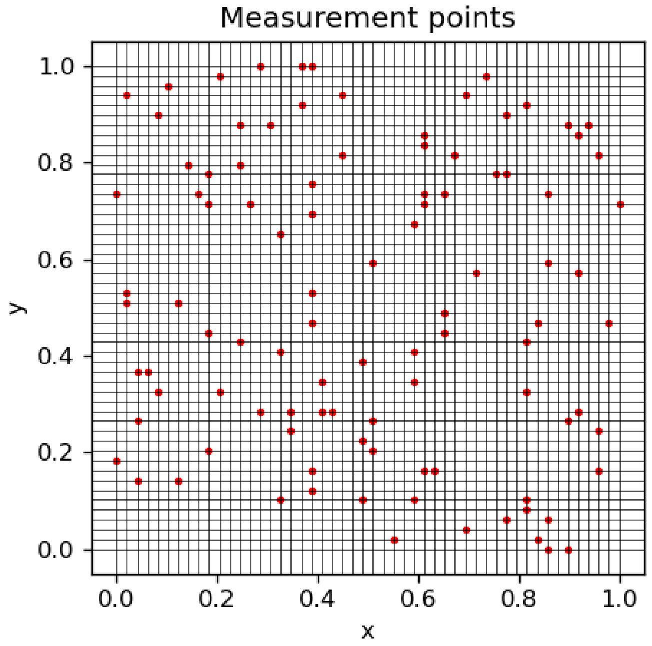
$$E_z = \frac{1}{4}\sum F_{i,j}^{B_{i,j}}$$

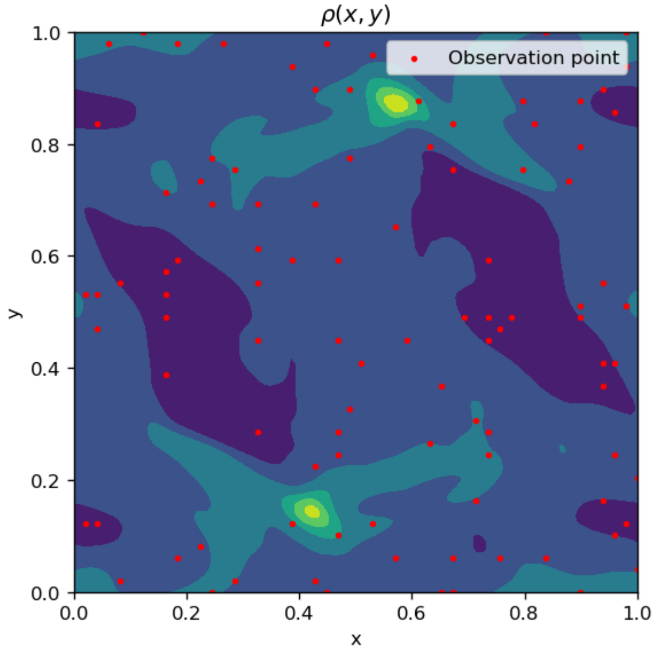
$$\nabla \cdot B = 0$$

Constrained Transport Method

Application to MHD transport simulation







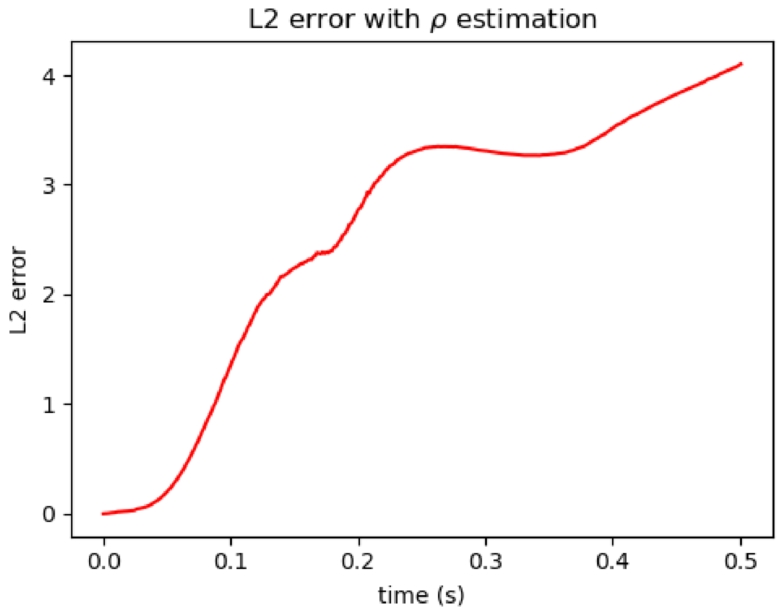
$$\rho^{measure}_{k+1} = H\rho^{state}_{k+1}$$

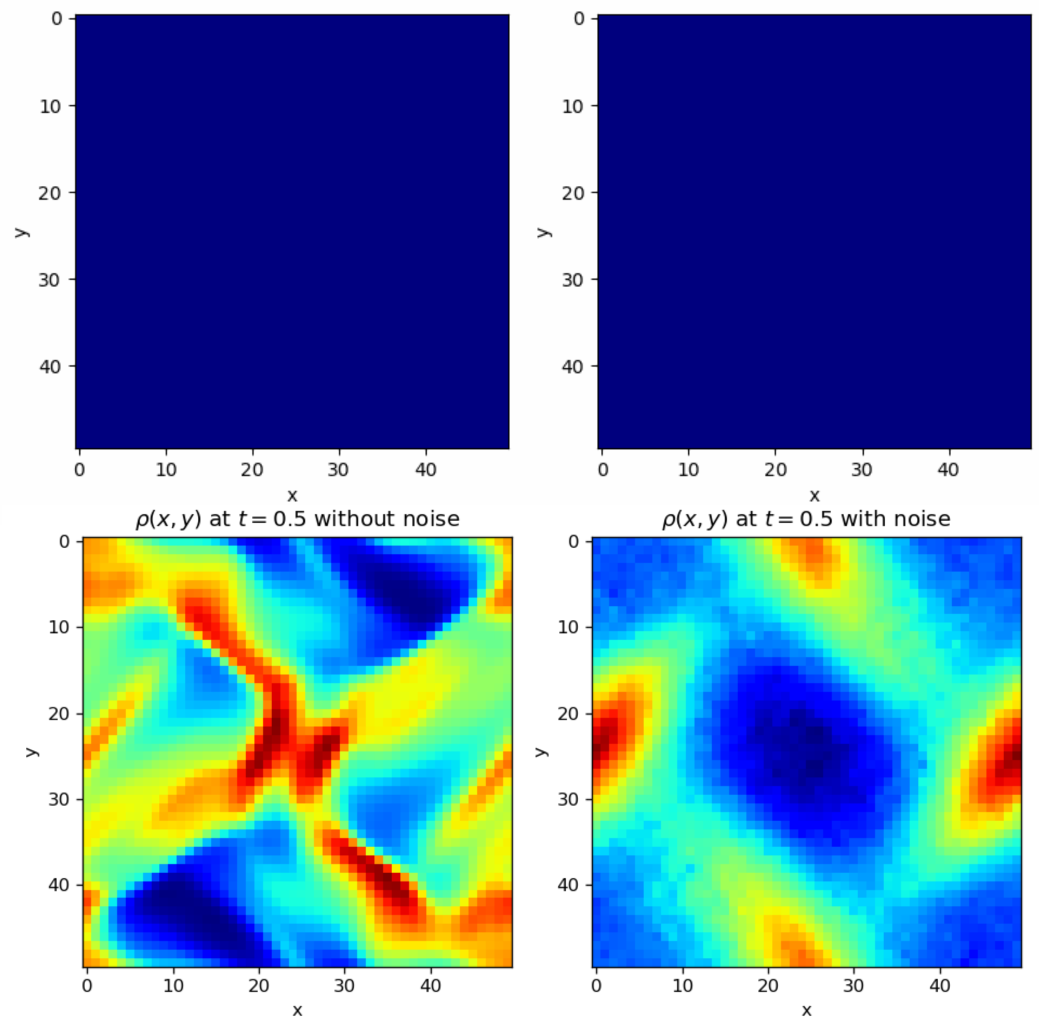
$$H \in R^{N_m \times N_g^2}$$

$$H_{ij} = \begin{cases} 1\ if\ (i,j) \in M \\ 0\ otherwise \end{cases}$$

Numerical results

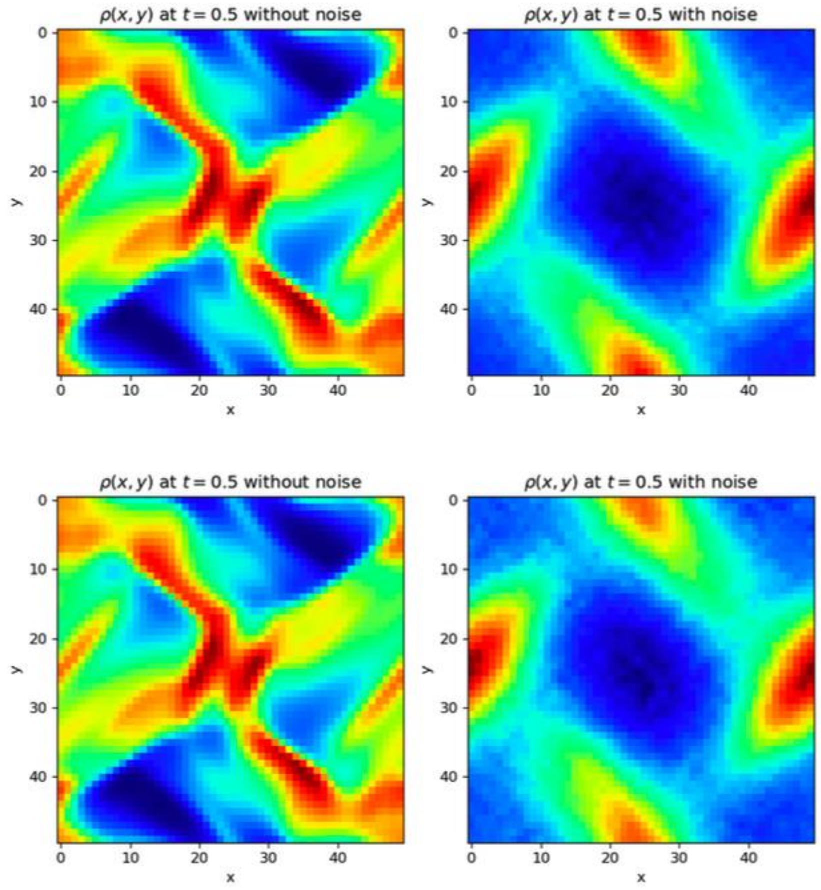
- Plasma density estimation with measurement noise + model error
- $\Sigma_x = \Sigma_y = 0.01, N_m = 100\ , N_g = 50, N_e = 100$
- Noise directly added to the plasma density
- Turbulence structure cannot be observed





Numerical results

- Divergence of the magnetic field abruptly increases during simulation
- Scale of the covariance does not affect the formation of the shock wave

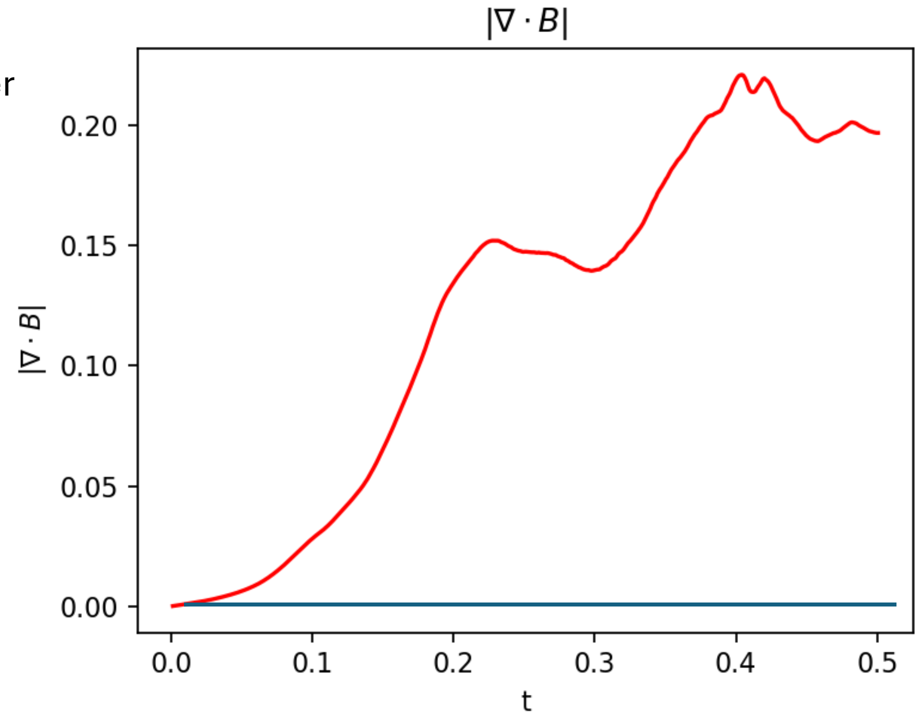


Scale of the noise doesn't matter

$$\Sigma_x = \Sigma_y = 0.1$$

$$\Sigma_x = \Sigma_y = 0.0001$$

Shock formulation cannot be observed



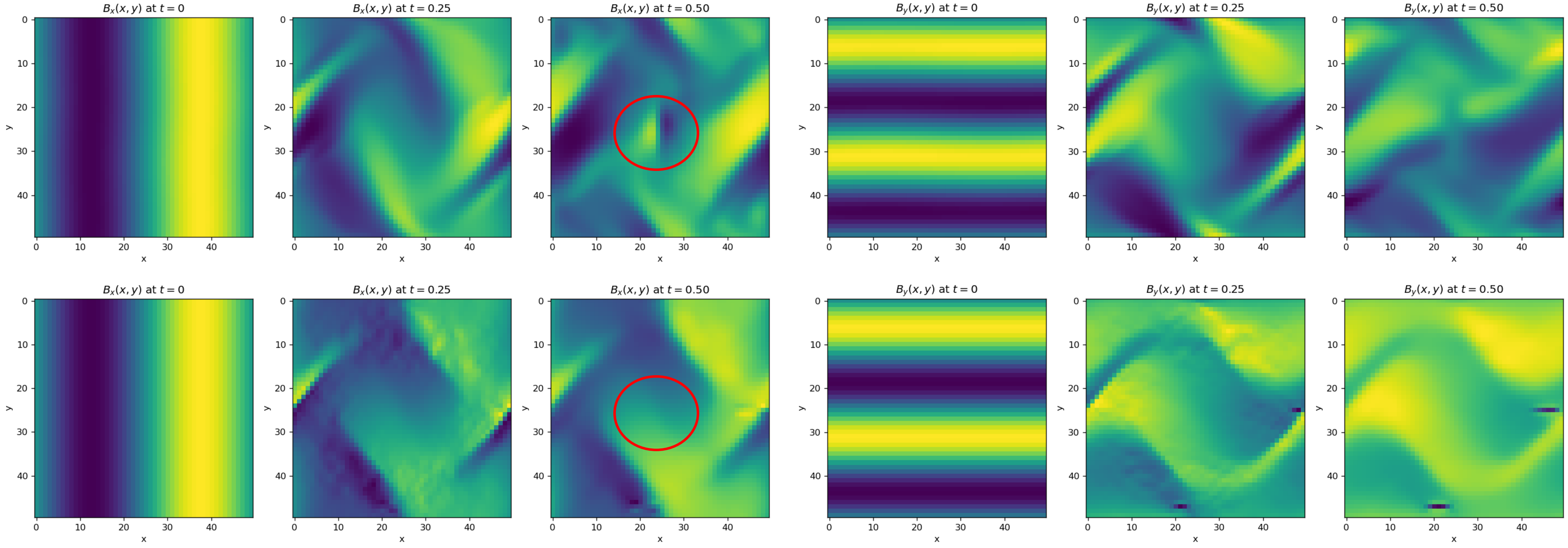
Divergence-free condition violated

Numerical results

- Violation of the divergence-free condition on magnetic field: Different B structure shown in the simulation

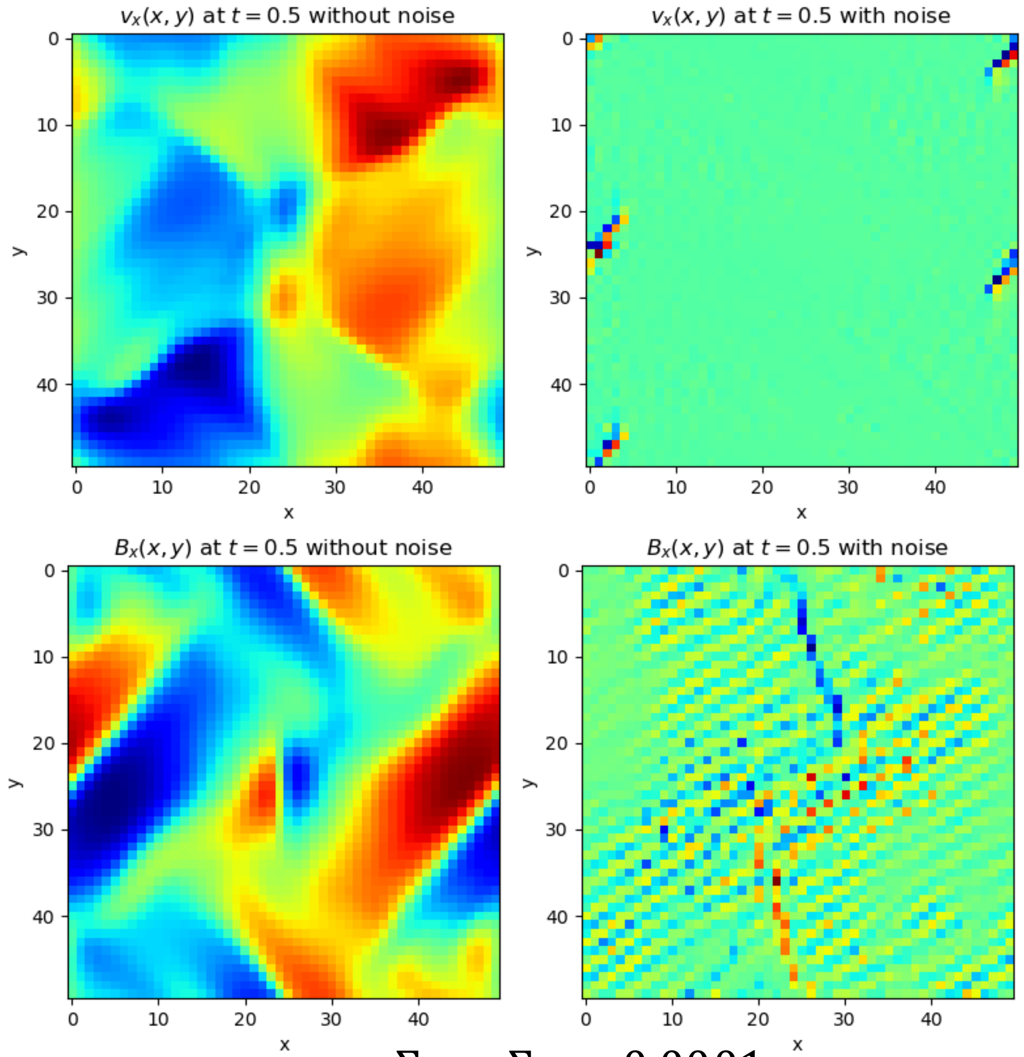
Shock formulation disappers

B_y cannot be estimated at all



Numerical results

- The L2 error of the magnetic field abruptly increases during simulation if adding noise directly into v and B

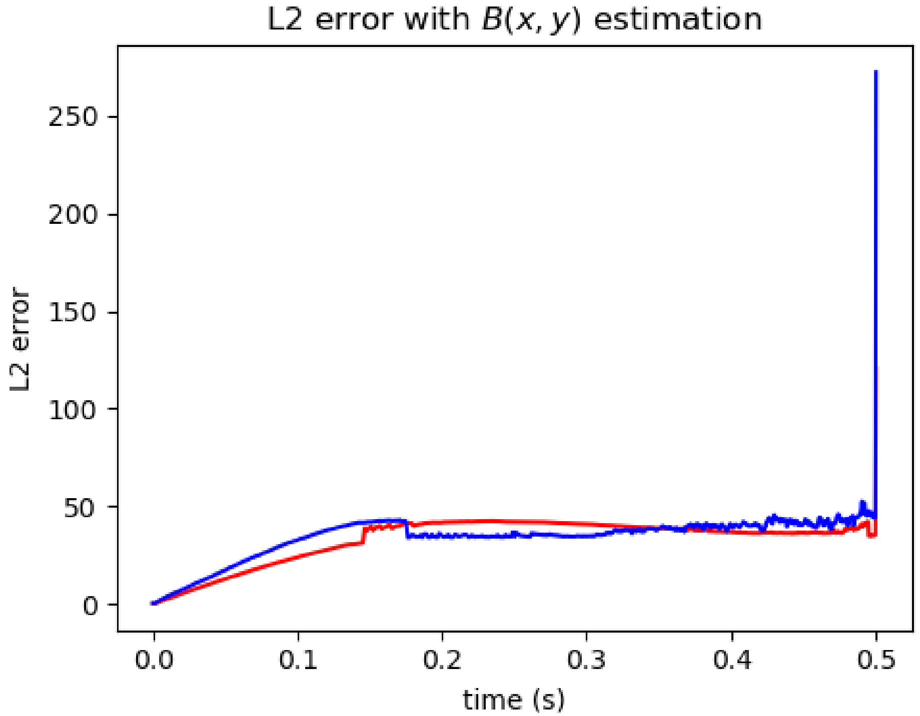


$$\Sigma_x = \Sigma_y = 0.0001$$

Ohm's law for time integration of B

$$\frac{\partial B}{\partial t} = \nabla \times (v \times B)$$

Constrained Transport Method doesn't work



Conclusion

- We integrated the MHD transport simulator with EnKF to estimate the dynamics under the uncertainties
- The violation of the divergence-free condition is issued
- The prediction of the state based on the nonlinear dynamic simulator doesn't work due to violation of the B-divergence free condition.
- EnKF with physics-informed constraints for MHD dynamics is required*: Localized Equality-Constrained Unscent Kalman Filter (LECUKF)* for MHD systems

$$X_k = [\rho_k, u_{x,k}, u_{y,k}, P_k, B_{x,k}, B_{y,k}] \in R^{N_g^2}$$

$$\nabla \cdot B = 0$$

$$DX_k = 0$$

$\Rightarrow$

Linear dynamics / Linearlized case

$$K_{k+1} = \hat{\Sigma}_{k+1} H^T D^T [D(\Sigma_y + H\hat{\Sigma}_{k+1} H^T) D^T]^{-1}$$