Towards Multiscale Neural Operator Framework of Accretion and Feedback Applications

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Abstract

We present the method combining neural operator (NO) and direct [multi-level] numerical simulations for accretion and feedback problem, in both magnetohydrodynamic (MHD) and general relativistic magnetohydrodynamic (GRMHD) simulations. NO is trained to learn the semigroup of the numerical simulation at small scale and provide the boundary condition for the next level of simulation. As a first step towards multiscale simulations, we focus on black hole feeding and feedback problem. [Findings:] This method is generally applicable as the subgrid model of all the central accretor problems.

1 Introduction

[HYW: Multiscale problems.] Numerical simulations in astrophysics enables us to investigate a broad range of highly complex problems. Yet many longstanding questions persist because these systems are intrinsically multiscale in both space and time. Systems with a central accretor—such as the coevolution of supermassive black holes (SMBH) and their host galaxies, star and planet formation, and stellar-mass black holes or neutron stars in supernova remnants—are canonical examples of such multiscale phenomena.

Among all these multiscale problems, feeding and feedback of the SMBHs attracted a lot of attentions. The SMBHs harbored at the centers of most galaxy nuclei play a crucial role in the evolution of the galaxies, shown in various properties such as stellar and dark matter bulge masses [Needs citation]. Ideally one needs to resolve the small-scale dynamics near the event horizon (mpc size), while simultaneously resolving the large-scale dynamics of the host galaxy (kpc to Mpc size), making this a formidable task for direct numerical simulations. Consequently, the accretion flows around SMBHs and their feedbacks are modelled typically by a subgrid model in cosmological simulation [Needs citation]. And the accretion and outflow dynamics near the black hole are often modeled by general relativistic magnetohydrodynamis simulations (GRMHD). Due to the ignorance of accretion disk formation history, a torus in hydrodynamic equilibrium is usually adopted as the idealized initial condition [7]. Early attempt to bridge the feeding problem and construct a more realistic black hole accretion problem includes modelling infall and accretion from the Bondi radius [2].

[HYW: Relativistic outflows.] The feedback from low-Eddington accreting black holes are carried out mainly through relativistic outflows (winds and jets) [Needs citation]. Especially, the jets are observed from AU to Mpc scales, far beyond the range of host galaxies. These relativistic outflows can efficiently deposit energy and momentum into the interstellar medium (ISM) and intergalactic medium (IGM), triggering large-scale turbulence, and thus affect the star formation and galaxy evolution [Needs citation].

[HYW: Black hole feeding and feedback problem.] [HYW: And Computational advances.] A considerable amount of efforts adopting various techniqueshas been made to bridge different scales,

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which includes direct simulation assuming smaller scale separation [14, 15, 19, 16], "zoom-in" adopting nested mesh in grid codes [9, 10], and "Lagrangian hyper-refinement" in Lagrangian codes [12, 13], remapping between different simulations, and "multi-zone" [3, 5, 4] or "cyclic-zoom" [11] methods iteratively refining and de-refining the simulation domain near the central black hole. Earlier attempts on bridging scales adopting "two-zone" techniques have been made in the content of hydrodynamic accretion [23].

[HYW: Spatial-Temporal multiscale variability problem.] Except the direct simulation modifying the scale separation, only the "multi-zone" and "cyclic-zoom" methods are able to capture feedback from the small-scale and evolve the different domains to convergence. These two methods are very similar, but different in details, particularly the treatment on how to mask the inner levels when simulating the outer domains. "Multi-zone" "Cyclic-zoom" masked the inner levels by freezing the hydrodynamic variables while evolving the magnetic fields within the mask region using inductive electic fields, presering the divergence-free constraints on smaller scaler through constraint transport [1, 8].

[HYW: Temporal variability hierarchy.] Despite the huge success of these novel methods, they could still suffer from the temporal variability problem.

[HYW: Neural Operator] In this paper, we start

[HYW: Paper Structure.] The structure of the paper is as follows. [HYW: multiscal-NO?] In Section 4 and 5, we describe the numerical methods for direct simulations and algorithm of NO. In Section 7, we describe the problem setups and datasets used for training NOs. In Section 8, we present the results: comparing the long-term roll-out of NOs and the direct simulations, and showing the large-scale simulations with NOs as the inner boundary condition. We then conclude in Section 9.

2 Difficult of Capturing Variability in Multiscale Problems

3 Overview of Multiscale-NO Framework

3.1 Run Duration

4 Method-Simulation

We use a performance portable version of `Athena++` [21] based on `Kokkos` library [22]- `AthenaK` [20].

4.1 Magneto-hydrodynamics Simulations: Magnetized SCAF

The setup we use in this work is a magnetized version of SCAF [10], without cooling and heating terms. In this case, we solve the Newtonian magnetohydrodynamics equations in conservative form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = s_\rho \,, \tag{1}$$

$$\frac{\partial (\rho \boldsymbol{v})}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} + P\boldsymbol{I} - \boldsymbol{B}\boldsymbol{B}) = \boldsymbol{s_p} - \rho \nabla \Phi \,, \tag{2}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E+P)\boldsymbol{v} - (\boldsymbol{B}\cdot\boldsymbol{v})\,\boldsymbol{B}] = s_E - \rho \boldsymbol{v} \cdot \nabla \Phi, \tag{3}$$

$$\frac{\partial \boldsymbol{B}}{\partial t} - \nabla \times [\boldsymbol{v} \times \boldsymbol{B}] = 0 \,, \tag{4}$$

where $\rho : \mathbb{R}^3 \to \mathbb{R}$ is the gas density, $\boldsymbol{v} : \mathbb{R}^3 \to \mathbb{R}^3$ is the velocity, $P : \mathbb{R}^3 \to \mathbb{R}$ is the pressure, $E = P/(\gamma-1) + \rho|v|^2/2$ is the total energy density, and $-\nabla\Phi$ is the gravitational acceleration due to the central accretor. The flow evolved following ideal gas law with adiabatic index $\gamma = 5/3$.

In code unit, $GM = r_0 = \rho_0 = 1$. The output quantities include $(\rho, P, \boldsymbol{v} = (v_x, v_y, v_z), \boldsymbol{B} = (B_x, B_y, B_z))$.

We use piecewise parabolic reconstruction [6], an HLLD Riemann solver [18], a constraint transport algorithm [8] for the divergence-free magnetic field evolution, and first-order flux correction [17].

4.2 GRMHD Simulations

The conservative Valencia formulations for solving GRMHD equations with induction equation

$$\partial_t \boldsymbol{U} + \partial_i \boldsymbol{F} = \boldsymbol{S} \tag{5}$$
$$\partial_t(\sqrt{-g}B^i) + \partial_j(\sqrt{-g}(b^i u^j - b^j u^i)) = 0 \tag{6}$$

where the conserved variables, fluxes, and source terms associated with the connection are

$$\mathbf{U} = \sqrt{-g}\begin{bmatrix} \rho u^t \\ T_i^t \\ T_t^t + \rho u^t \end{bmatrix},$$
$$\mathbf{F} = \sqrt{-g}\begin{bmatrix} \rho u^j \\ T_i^j \\ T_t^j + \rho u^j \end{bmatrix}, \tag{7}$$
$$\mathbf{S} = \sqrt{-g}\begin{bmatrix} 0 \\ \frac{1}{2}\left(\partial_i g_{\alpha\beta}\right) T^{\alpha\beta} \\ 0 \end{bmatrix}$$

respectively, where the metric is $\boldsymbol{g}$ and $g = \det \boldsymbol{g}$. The rest-mass density is ρ, the coordinate frame 4-velocity is u^μ and the stress-energy tensor is

$$T^\mu{}_\nu = w u^\mu u_\nu - b^\mu b_\nu + (p_g + p_m)\delta^\mu_\nu \tag{8}$$

where the magnetic field is b^μ, the magnetic pressure is $p_m = b_\mu b^\mu/2$, and the total enthalpy is w. The non-monopole constraint is preserved when evolving the 3-components B^i of the magnetic field:

$$\partial_j(\sqrt{-g}B^j) = 0 \tag{9}$$

where

$$b^t = u_i B^i \tag{10}$$
$$b^i = \frac{1}{u^t}(B^i + b^t u^i) \tag{11}$$

We solve the GRMHD equations in a Cartesian Kerr-Schild coordinate. We adopt piecewise parabolic spatial reconstruction, HLLE Riemann solver, RK2 time integrator, and first-order flux correction [17].

In all runs, we adopt $G = M = \rho_0 = 1$

5 Method-NO

5.1 Learning

Define the semigroup $\{S(h)\}_{h>0}$ as

$$\begin{aligned} S(h) :&(\rho(x,t), P(x,t), v(x,t)) \to \\ &(\rho(x,t+h), P(x,t+h), v(x,t+h)). \end{aligned} \tag{12}$$

Our target is to learn a neural surrogate G_θ that approximates $S(h)$ for a particular h.

Basic Method: Supervised Learning.

Use FNO as the ansatz of G_θ. Train the FNO by fitting data (input-output pairs) from numerical solvers.

In this project, we employed LocalNO to better capture small-scale (high-frequency) information.

5.1.1 Problem-Specific Methods

1. Logarithm transform for density and energy.

2. Position information. The center of the blackhole, though only taking up a tiny portion of the domain, plays a vital role in the simulation. We notice that the standard approach to doing position embedding fails to achieve satisfactory performance. We divide the domain into 8 (?) regions determined by the distance from the center and apply one-hot embedding, namely the grid points in the i- th region is equipped with a feature vector $e_i \in \mathbb{R}^8$. Further, we reweight the loss function, replacing vanilla L^2 norm $\int |u(x) - v(x)|^2 dx$ with $\int |u(x) - v(x)|^2 \lambda(x) dx$, forcing the model to learn the center well at a early stage of the training.

3. Enforcing physical scaling relations. We know that several quantities (denoted by u) approximately satisfy a scaling relation, i.e., $u(r)$ decays exponentially w.r.t. r, the distance to the blackhole center. To make training easier and more stable, the model is optimized to learn the residual.

$$\log(u(x)) = k|x| + G_\theta(\log(u(x))), \tag{13}$$

where k is estimated through the dataset. We enforce the model output to be smaller than a pre-assgined value C through a regularizer.

5.2 Effective Conservation Law

We apply the angular-integrated conservation law for mass and angular momentum as loss functions. Even without reaching a quasi-steady state, the angular integrated continuity equation and momentum conservation equations should hold. [But for now we abandon the terms associated with the time derivative, by assuming a quasi-steady state (including accretion and feedback) has been reached, then the mass accretion rate and the specific angular momentum transport along the radial direction should be constant.] [This assumption should hold as the domain/level of interest utilized for training has reached a quasi-steady state.]

The integral form of continuity equation

$$\frac{\partial}{\partial t} \int_{r_i}^{r_{i+1}} \langle \rho \rangle_{\theta,\phi} dr + \langle \rho v_r \rangle_{\theta,\phi} |_{r_i}^{r_{i+1}} = 0 \tag{14}$$

and the momentum conservation equation

$$\frac{\partial}{\partial t} \int_{r_i}^{r_{i+1}} \langle \rho v_\phi \rangle_{\theta,\phi} dr + \langle \rho v_r v_\phi - B_r B_\phi \rangle_{\theta,\phi} |_{r_i}^{r_{i+1}} = 0 \tag{15}$$

Removing the time derivative terms, we can use the angular integrated values within each spherical shell to ensure mass and angular momentum conservation:

$$\dot{M} = \langle \rho v_r \rangle_{\theta,\phi} \tag{16}$$
$$\dot{J} = \langle \rho v_r v_\phi - B_r B_\phi \rangle_{\theta,\phi} \tag{17}$$

energy flux and magnetic flux

only train on primative variables (not cons) for GRMHD

time hierarchy

- interpolation: linear/parabolic (or subcycling)
- extrapolation: past time
- interpolation inside FNO $\to$ enforce the semigroup
-

5.3 Single-level

5.4 Two-level

5.5 Nested two-level as multi-level cyclic-zoom

6 Diagnostics

6.1 Hydrodynamics

6.2 MHD

6.3 GRMHD

For consistency, we apply the diagnostics same as the previous GRMHD simulation [11]. The relevant diagnostics include mass flux, magnetic field flux, energy flux, radial momentum flux, and angular momentum flux:

$$\dot{M} \equiv -\int_S \rho u^r \sqrt{-g}\, d\Omega, \tag{18}$$

$$\Phi_{\rm BH} \equiv \sqrt{\pi} \int_S |B^r| \sqrt{-g}\, d\Omega, \tag{19}$$

$$\dot{E} \equiv \int_S T^r{}_t \sqrt{-g}\, d\Omega, \tag{20}$$

$$\dot{p_r} \equiv \int_S T^r{}_r \sqrt{-g}\, d\Omega, \tag{21}$$

$$\dot{L} \equiv \int_S T^r{}_\phi \sqrt{-g}\, d\Omega, \tag{22}$$

where S is the area, $T^r{}_t = (\rho + u + p + b^2) u^r u_t - b^r b_t$, and $T^r{}_\phi = (\rho + u + p + b^2) u^r u_\phi - b^r b_\phi$. Sometimes it is useful to separate the mass flux into inflow and outflow:

$$\dot{M} = \underbrace{-\int_{u^r<0} \rho u^r \sqrt{-g}\, d\Omega}_{\dot{M}_{\rm in}} \underbrace{- \int_{u^r>0} \rho u^r \sqrt{-g}\, d\Omega}_{\dot{M}_{\rm out}}. \tag{23}$$

The dimensionless magnetic flux parameter is defined by

$$\phi_{\rm BH} \equiv \frac{\Phi_{\rm BH}}{\sqrt{\dot{M}}}. \tag{24}$$

The energy flux $\dot{E}$ includes the flux of rest-mass energy, so the "feedback" energy flux is $\dot{M} - \dot{E}$. The efficiency of feedback can thus be defined by

$$\eta \equiv \frac{\dot{M} - \dot{E}}{\dot{M}}. \tag{25}$$

The efficiency is positive (negative) when energy is transported outward (inward). We can further separate the feedback power into the hydrodynamic part and the electromagnetic (EM) part

$$\dot{E}_{\rm hydro} = -\int_S \left[(\rho + u + p) u^r u_t + \rho u^r\right] \sqrt{-g}\, d\Omega, \tag{26}$$

$$\dot{E}_{\rm EM} = -\int_S \left(b^2 u^r u_t - b^r b_t\right) \sqrt{-g}\, d\Omega, \tag{27}$$

7 Problem Setups and Datasets

7.1 Newtonian MHD from large-scale zoom-in

- floor and cap
- output frequency
- downsampled size/resolution

7.2 GRMHD

The initial condition is a cloud of gas with constant mass density $\rho = \rho_0$ and constant angular momentum. We cho

8 Results

9 Discussion and Conclusion

[HYW: Conclusions.] In this work, we present a method combining neural operator and direct numerical simulations for accretion and feedback problem, in both magnetohydrodynamic and general relativistic magnetohydrodynamic simulations.

We demonstrate the validity of the method by training on MHD and GRMHD simulations of magnetized Bondi accretion onto a central black hole.

(1)

(2)

(3)

* begin

* end

This is aimed to motivate the future development of machine-learning-based subgrid models in galactic and cosmological simulations, capturing both the statistically averaged mass and energy feedback information and the variability simultaneously.

[HYW: Future Prospective.] The method presented in this paper is a first step (two-level version) towards a multi-level cyclic-zoom/multi-zone neural operator framework for simulations around a central accretor.

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