Numerical analysis for scientific machine learning

Jiaxi Zhao

17th Apr, 2024

Scientific machine learning is applied to a broad range of computational problems, including

1. Steady-state simulations & inverse problems
2. Unsteady (transient) simulations
3. Eigenvalue problems

Many classical physical processes belong to the first two categories well the third class contains mostly quantum problems.

Steady-state simulations & inverse problems

Most of the steady-state simulations and inverse problems can be formulated as

$$\mathcal{L}(\mathbf{u}, \mathbf{y}) = 0, \quad \mathbf{y} = \phi_\theta(\mathbf{u}).$$

One example of special interests is the **Reynolds-averaged Navier-Stokes equation**:

$$\left(\langle \mathbf{U} \rangle \cdot \nabla\right) \langle \mathbf{U} \rangle + \frac{\partial \langle \mathbf{u} u_j \rangle}{\partial x_j} = -\frac{1}{\rho} \nabla p + \nu \Delta \langle \mathbf{U} \rangle ,$$
$$\nabla \cdot \langle \mathbf{U} \rangle = 0.$$

Great flexibility to choose the scheme for solving these problems: pseudo transient, Newton method, iterative methods, etc.

Unsteady (transient) simulations

Two leading applications are **Large eddy simulation** and **Molecular dynamics**.

$$\partial_t \mathbf{u} = \mathcal{L}(\mathbf{u}, \mathbf{y}, t), \quad \mathbf{y} = \phi_\theta(\mathbf{u}, t).$$

Temporal and spatial discretization

Stability and convergence analysis

Eigenvalue problem

Density functional theory

$$E = E_{\mathrm{Kin}}[\{\psi_i^\sigma\}] + E_{\mathrm{Har}}[\rho] + E_{\mathrm{Ext}}[\rho] + E_{\mathrm{XC}}[\rho]$$

Quantum many-body problem (Quantum Monte Carlo)

$$\min_\theta \frac{\left\langle \psi_\theta(\mathbf{r}_1, \cdots, \mathbf{r}_n) | \widehat{H} | \psi_\theta(\mathbf{r}_1, \cdots, \mathbf{r}_n) \right\rangle}{\langle \psi_\theta(\mathbf{r}_1, \cdots, \mathbf{r}_n) | \psi_\theta(\mathbf{r}_1, \cdots, \mathbf{r}_n) \rangle}$$

There are tons of works focusing on learning the exchange-correlation functional $E_{\mathrm{XC}}[\cdot]$ and plugging into the SCF loops to improve the accuracy, which can be formalized into the following eigenvalue problem:

$$\min_{\|\mathbf{v}\|=1} \mathbf{v}^T (H_0 + \phi_\theta) \mathbf{v}.$$

Key features

There are several key features in the numerical analysis of SciML:

1. Low-dimensional structures induced by the data, as for real applications the data is always sparse but structured. The data-driven surrogate can only be trusted in a low-dimensional space.

2. Statistical properties of the data-driven surrogate, such as the bias and asymptotic normality. These could be integrated with the numerical analysis to obtain a precise analysis of simulation dynamics.