Interview for MatMat group

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Many machine-learning assisted scientific computing methods have an iterative nature, e.g., turbulence modeling, XC functional:

$$\partial_t \mathbf{u} = \mathcal{L}(\mathbf{u}, \mathbf{y}, t), \quad \mathbf{y} = \phi(\mathbf{u}, t), \quad \min_\theta \sum_n \left\| \phi_\theta(\mathbf{u}^{(n)}) - \mathbf{y}^{(n)} \right\|^2,$$

The stability and a-posteriori performance are not satisfactory.

1. Tangent-space regularization method (*published in SISC*)
   - First mathematical formulation and analysis.
   - Non-intrusive and differentiable regularization.
   - Significant improvement over dynamics-agnostic methods.
   - Deployment to practical urban environment simulation (ongoing).
2. Generative subgrid-scale model (*accepted by ICLR 2025 MLMP*)
3. Numerical anlysis of the turbulence modeling (multiscale, data-imbalance, multivaluedness)
4. Distorted plane-wave via normalizing flow (adaptive basis set, smaller cutoff energy, comparable accuracy)
5. Adaptive Gaussian basis set (efficient electron integral, differentiable basis sets)

Mathematics, physics, and programming background

Mathematics & Physics:

1. Mathematics, graduate level course on computational math and analysis: numerical analysis, (numerical) PDE, numerical linear algebra, stochastic analysis, etc.
2. Physics (quantum mechanics, quantum chemistry, solid-state physics, fluid dynamics).

Programming:

1. Core contributor of the *Jrystal* package (pseudopotential, accuracy test modules, exploring the machine-learning XC functionals).
2. Extensive experience with deep-learning framework and models (PyTorch, JAX, generative models, differentiable programming).
3. Familiar with various open-source packages (PySCF, OpenFOAM).

Research vision and contribution to MatMat group

Research vision:

Machine-learning tools can advance scientific computing (differentiable programming, data-centric viewpoint, generative modeling)

Numerical analysis for hybrid algorithms (stability analysis, error estimation, uncertainty quantification)

I aim to contribute to the MatMat group research in the following two aspects:

1. Gradient-accelerated inverse materials design

· Combining stabilization algorithm with inverse design.

· Generative model guided by differentiable DFT calculation.

2. Estimation of simulation errors

· Numerical analysis related to pseudo-potential and XC functional.

· Machine-learning XC functionals and its related problems.