A latent space solver for PDE generalization

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Introduction

Solutions to Partial Differential Equations (PDEs) depend on PDE conditions such as geometry of computational domain, boundary conditions and source terms. Many existing approaches in machine learning use direct inferencing to predict PDE solutions given a representation of the conditions. The PDE conditions can be sparse and high dimensional and cause generalization problems in ML approaches. Moreover, a direct inferencing approach is not flexible and does not allow solution initialization or correction of solution trajectory. The ML-based hybrid solver presented here uses lower dimensional representations of PDE conditions and combines it with iterative inferencing procedures to improve generalizability.

Latent space solver

Latent space representation of PDE solutions and PDE conditions

Fig. 1 shows the neural network architectures used to determine the compressed latent space vectors of the various PDE conditions, such as geometry of computational domain, BCs and source term distributions, and PDE solutions (u_1 and u_2). The PDE conditions, as well as the PDE solutions are compressed into their lower dimensional latent vectors, η_g, η_h, η_b, η, using CNN encoder-decoder type networks.

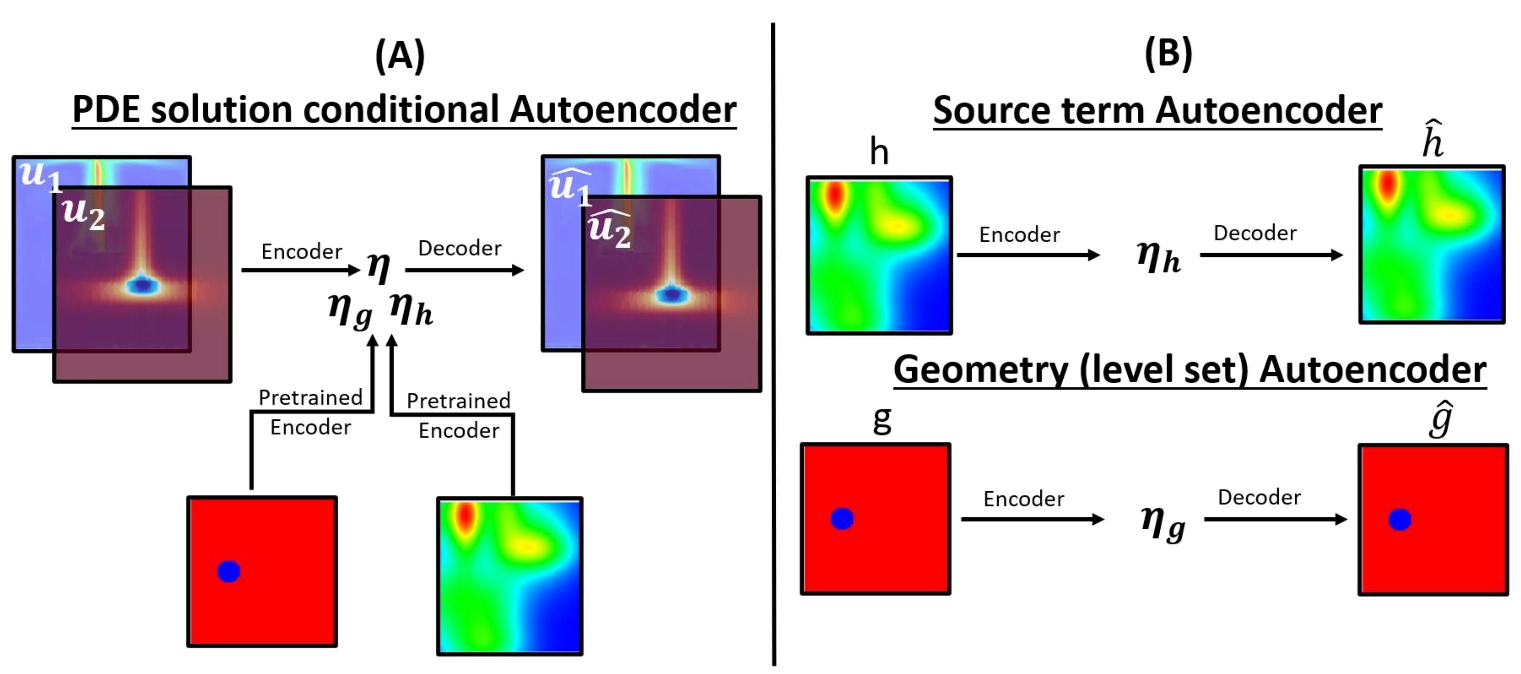

Fig. 1: Autoencoders for PDE solutions and PDE conditions

Iterative inferencing strategy

Fig. 2 shows the hybrid latent space solver methodology proposed in this work for using the Autoencoder networks to infer at unknown and unseen conditions. Given a coarse solution, the latent vectors (η) are obtained using the encoder network. Similarly, latent vectors are also obtained for the PDE conditions (η_g, η_h). The latent space solver uses the trained encoder-decoder networks to iteratively to update the PDE solution latent vector and at convergence, decodes the converged PDE solutions

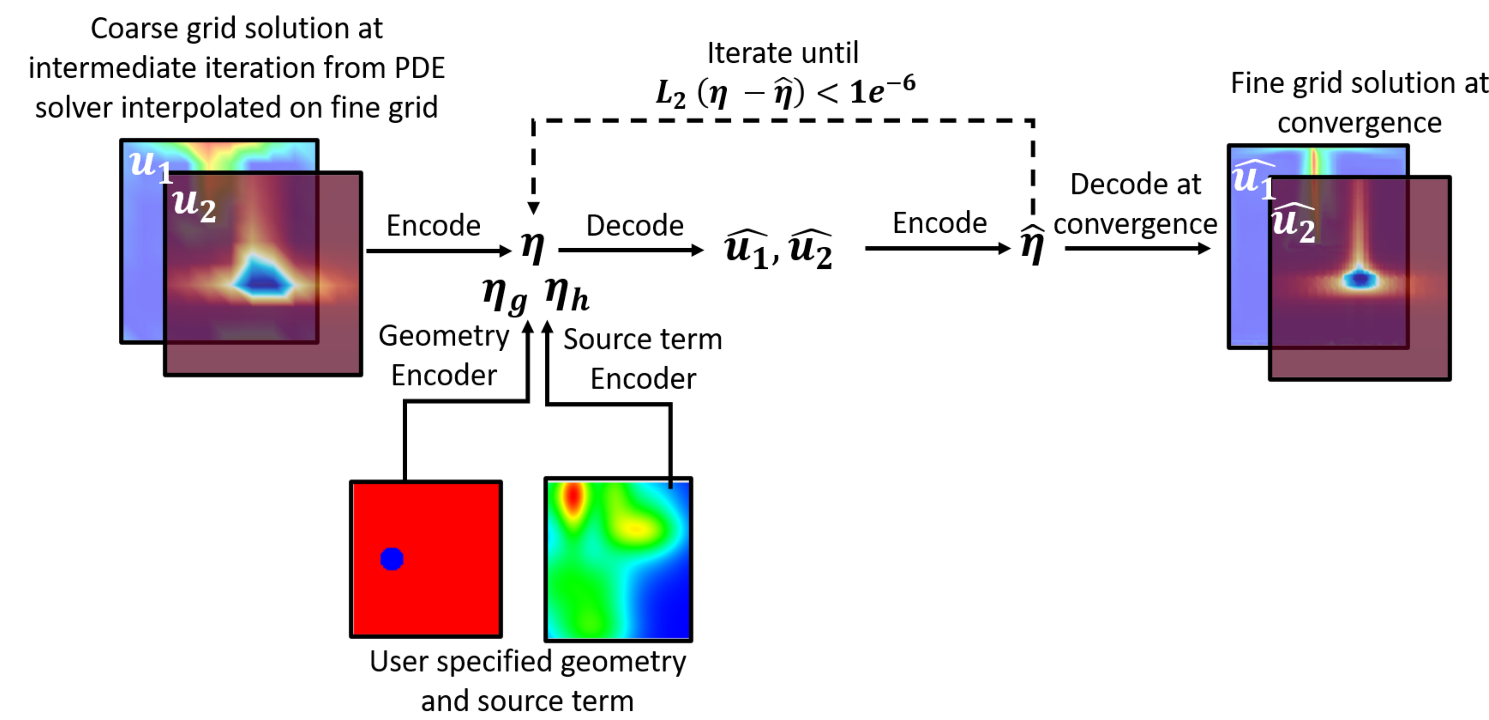

Fig. 2: Latent space solver: iterative inferencing strategy

Advantages

- The iterative procedure used for inferencing allows PDE solution initialization and alteration of solution trajectory during iterations using existing PDE solvers
- The PDE solution is conditioned by dense, lower dimensional representations of PDE conditions, thus enhancing the generalizability.

Experiments

Case setup and training

The hybrid solver is demonstrated for a 3-D, steady-state electronic cooling case with natural convection shown in Fig. 4. There are 5 solution variables, 3 components of velocity, pressure and temperature. The chip is electronically heated using a power source with random spatial distributions (example in Fig. 4). The chip heating results in two-way coupling of physics.

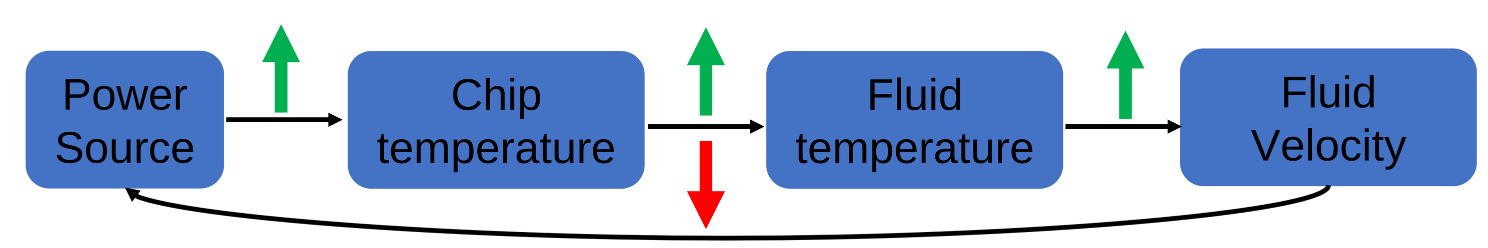

Fig. 3: Two-way physics coupling

The training data for the autoencoders consists of PDE solutions from 200 spatial distributions of power source but generalizes to a wider range of power source distributions (examples in Fig. 5-8).

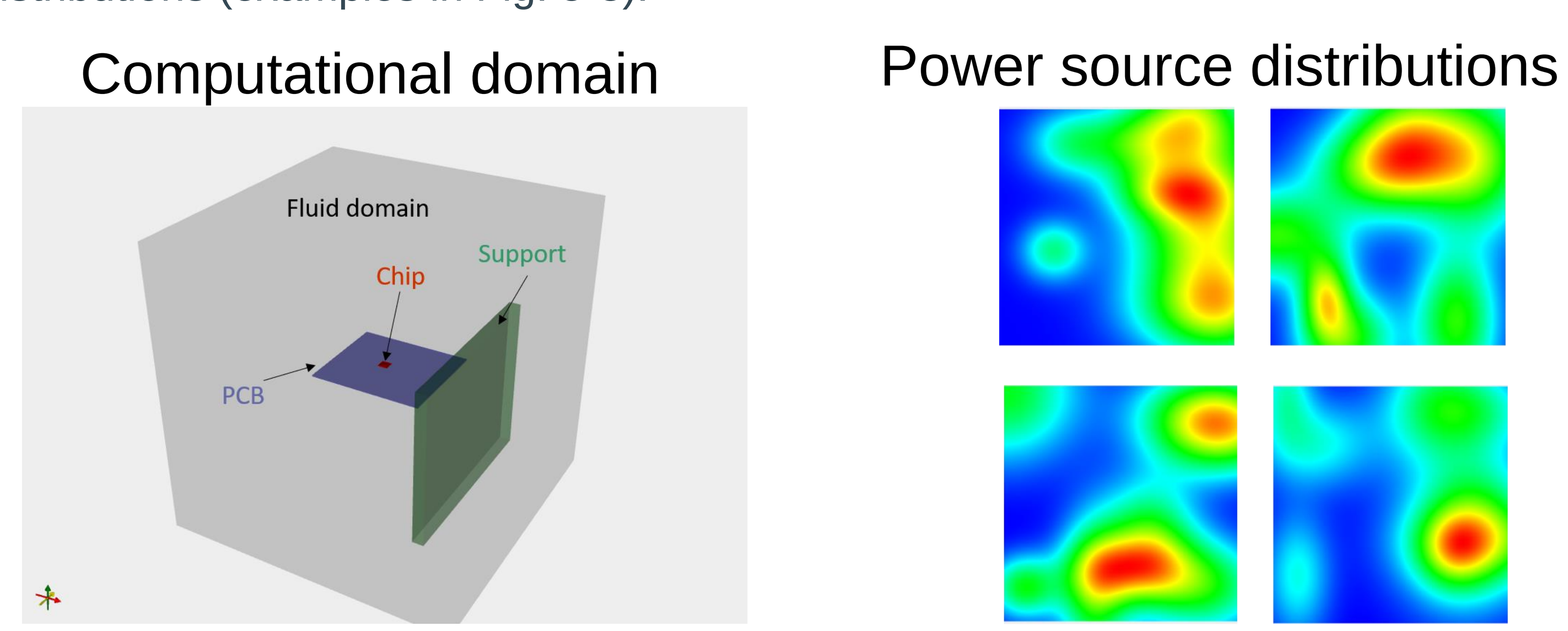

Fig. 4: Computational domain and power source distribution example

Unseen power source distribution: case 1

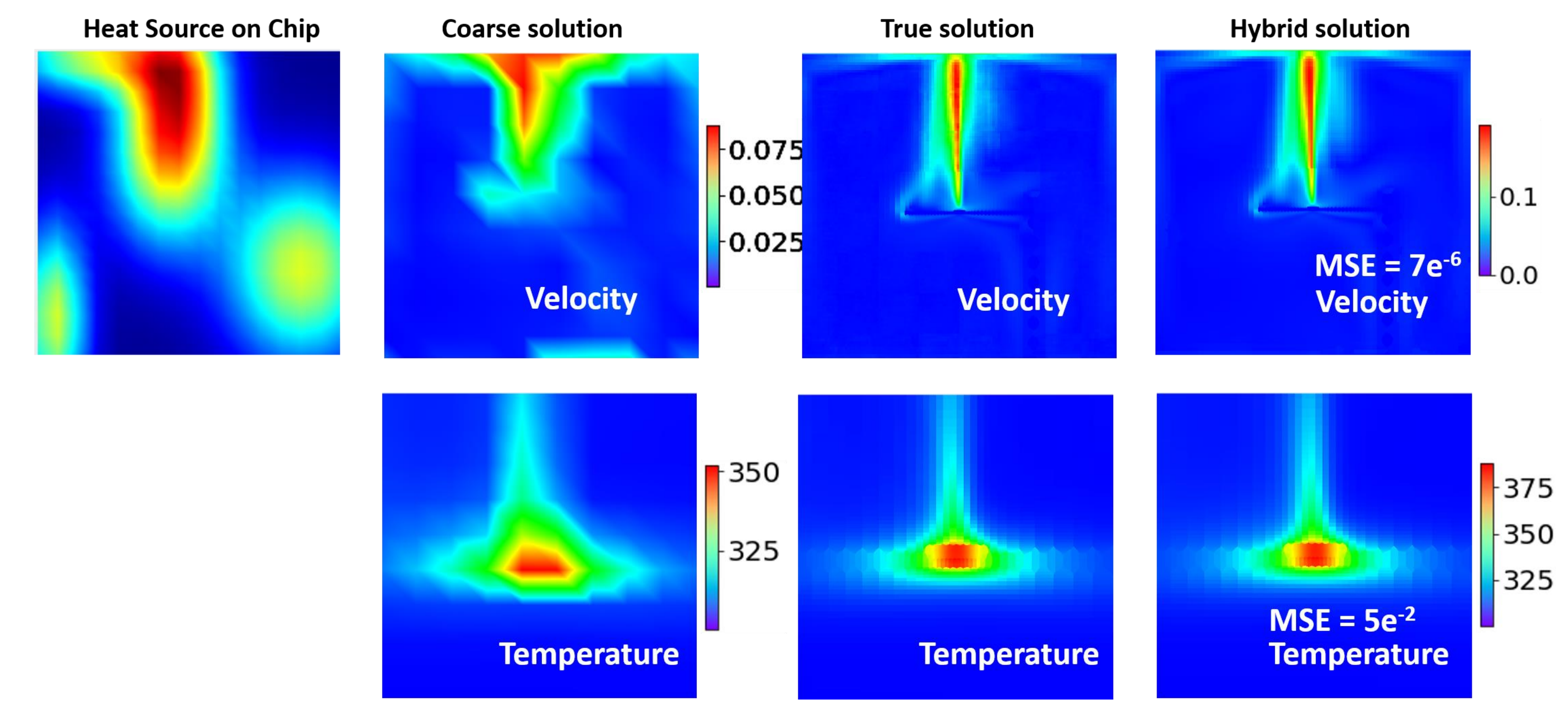

Fig. 5: Contour Plot comparisons of ML-Solver vs Ansys Fluent for case 1 along plane YZ

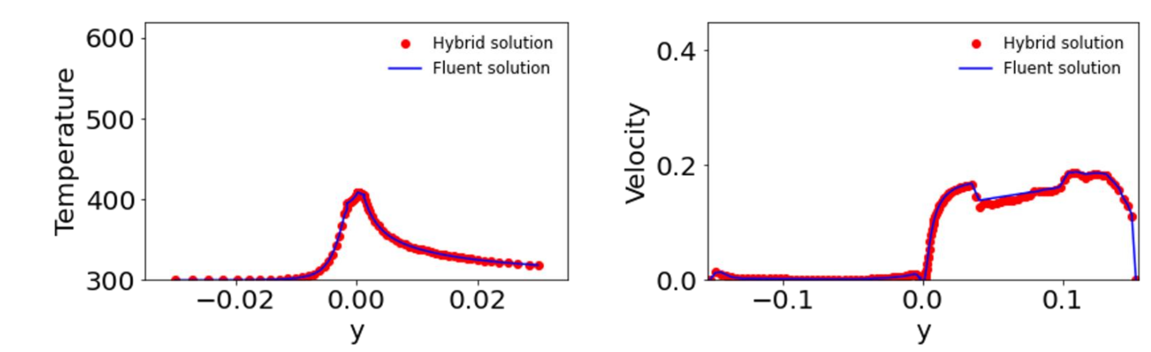

Fig. 6: Line Plot comparisons of ML-Solver vs Ansys Fluent for case 2 along line Y

Unseen power source distribution: case 2

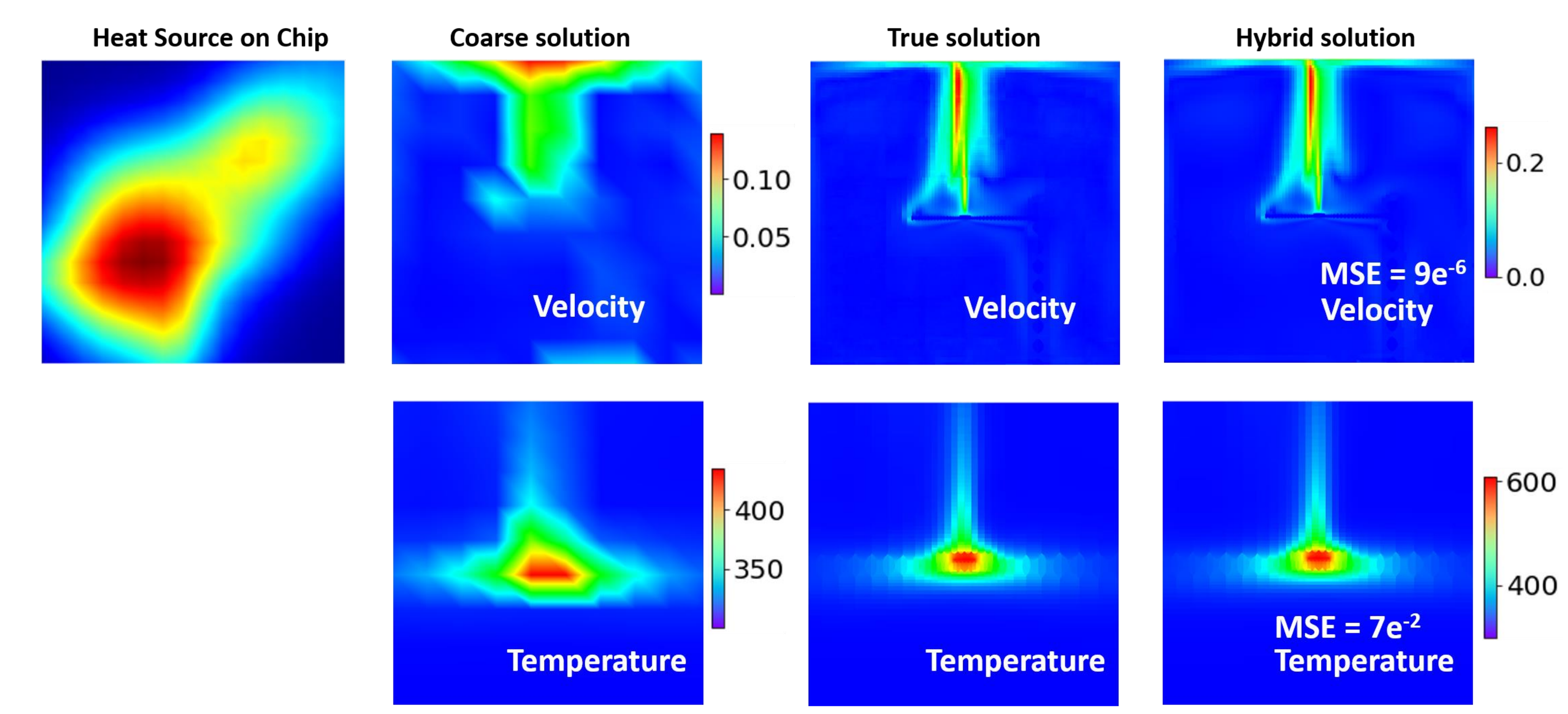

Fig. 7: Contour Plot comparisons of ML-Solver vs Ansys Fluent for case 2 along plane YZ

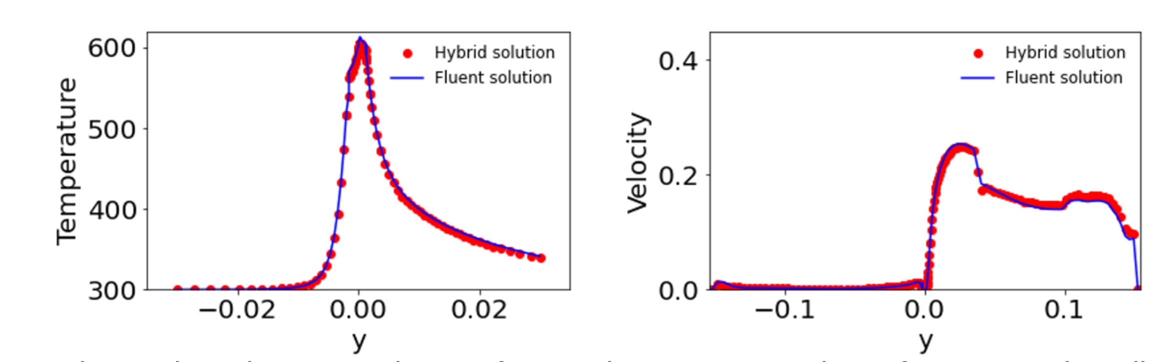

Fig. 8: Line Plot comparisons of ML-Solver vs Ansys Fluent for case 2 along line Y

References

1) Ranade, R., Hill, C., He, H., Maleki, A., & Pathak, J. (2021). A Latent space solver for PDE generalization. arXiv preprint arXiv:2104.02452.

2) Ranade, R., Hill, C., & Pathak, J. (2021). DiscretizationNet: A machine-learning based solver for Navier–Stokes equations using finite volume discretization. Computer Methods in Applied Mechanics and Engineering, 378, 113722.