Physics for Deep Learning and Deep Learning for Physics

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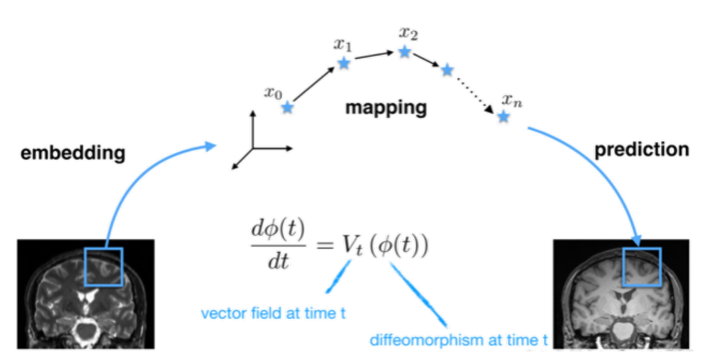
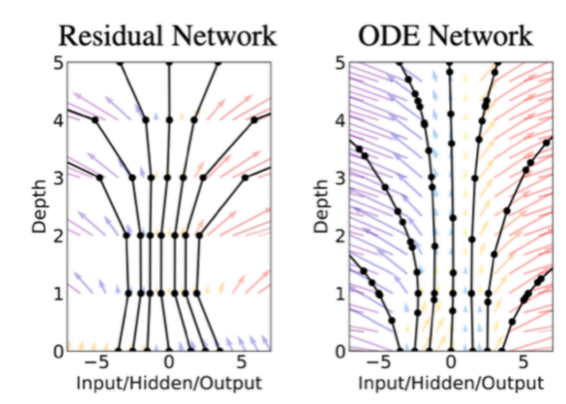
Observations

- Deep neural networks are extremely popular but require well-defined mathematical frameworks
- Some neural behave like dynamical systems, here an example of a Res-Net similar to an ODE in the limit



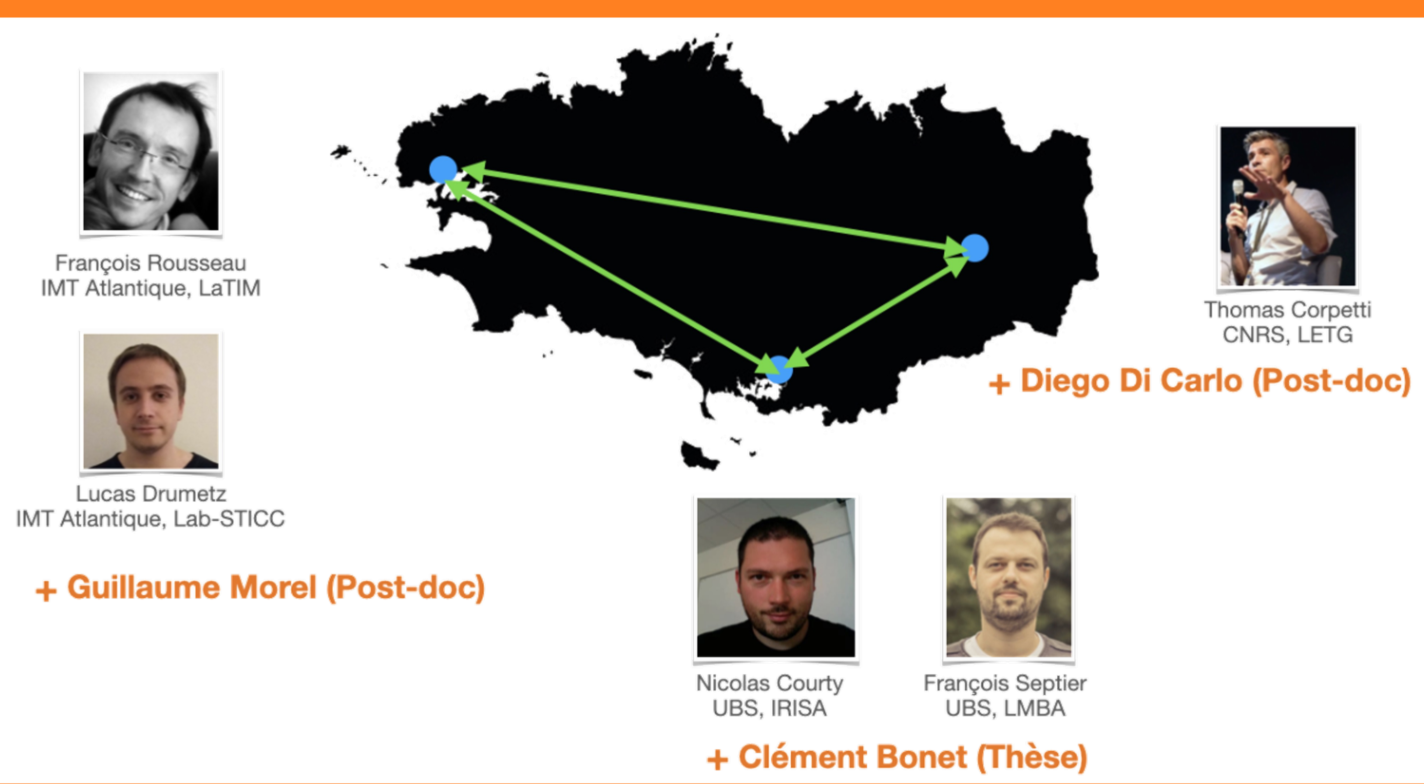


A residual network defines a discrete sequence of finite transformations, whose combination is a way of building diffeomorphisms. A ODE network defines a vector field, which continuously transforms the state.

Goals of the project

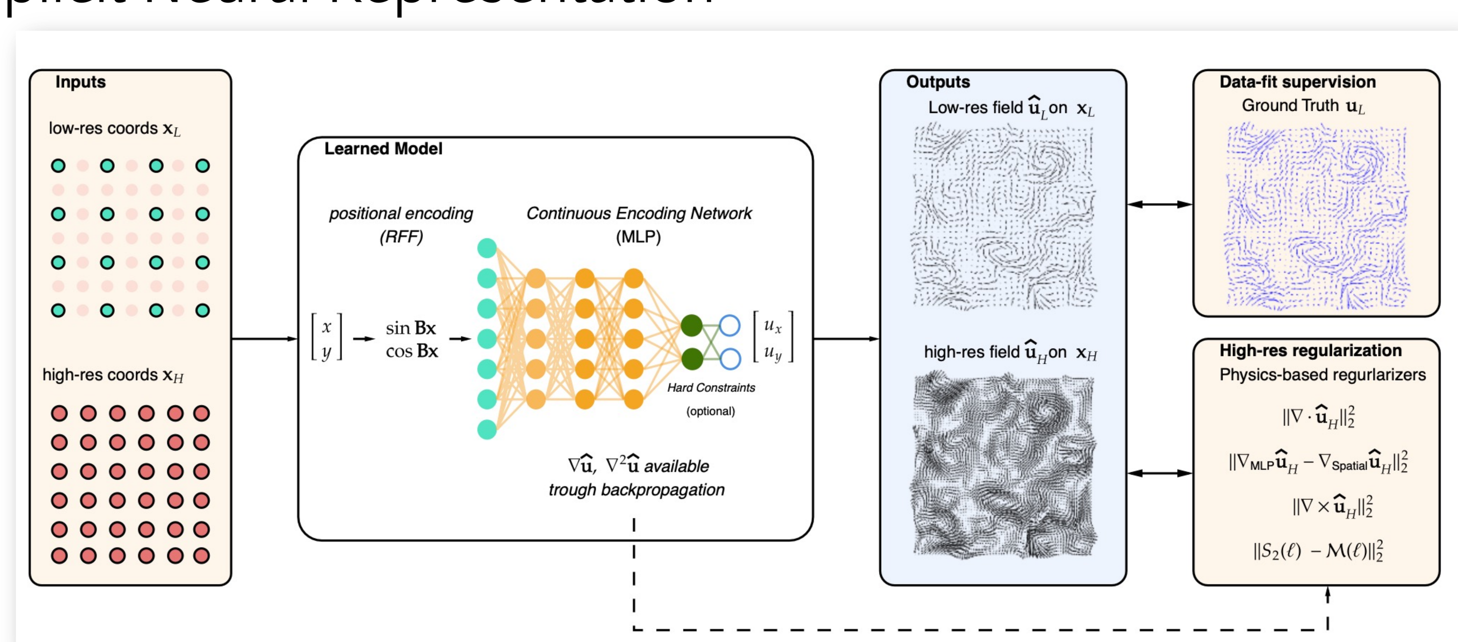
- How can a learning system be expressed as a dynamical system?
- How can learning-based methods help in simulating complex dynamic systems?
- How to handle the probabilistic nature of data ?

Consortium



Simulating complex dynamic systems

- PINNUS: PINNs for Unsupervised Super-resolution
- Train a PINN on low resolution images of turbulence
- Use regularizers to perform super resolution and denoising on sparse data
- Sub-grid model (Kolmogorov theory) at higher scales
- Regularization of vorticity for spatial gradient consistency
- Implicit Neural Representation



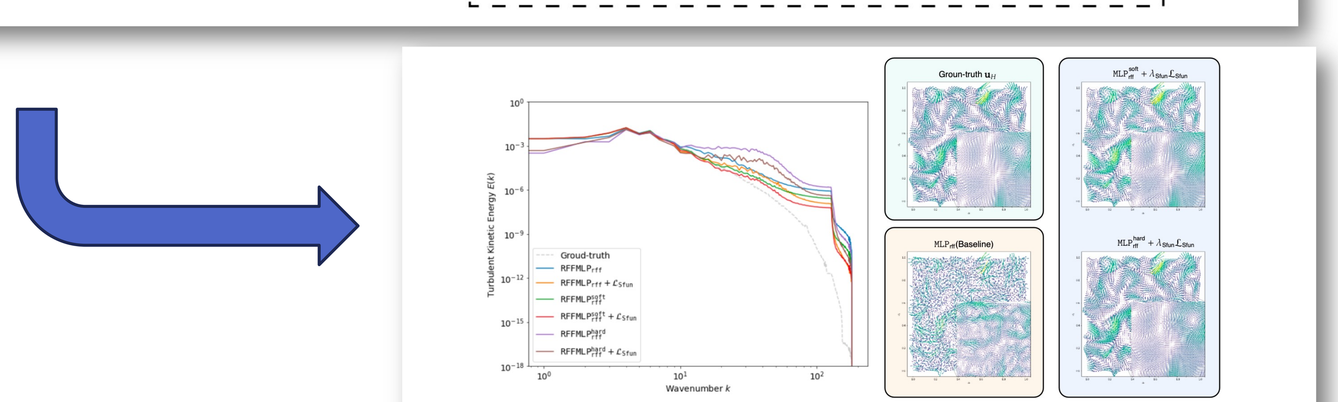
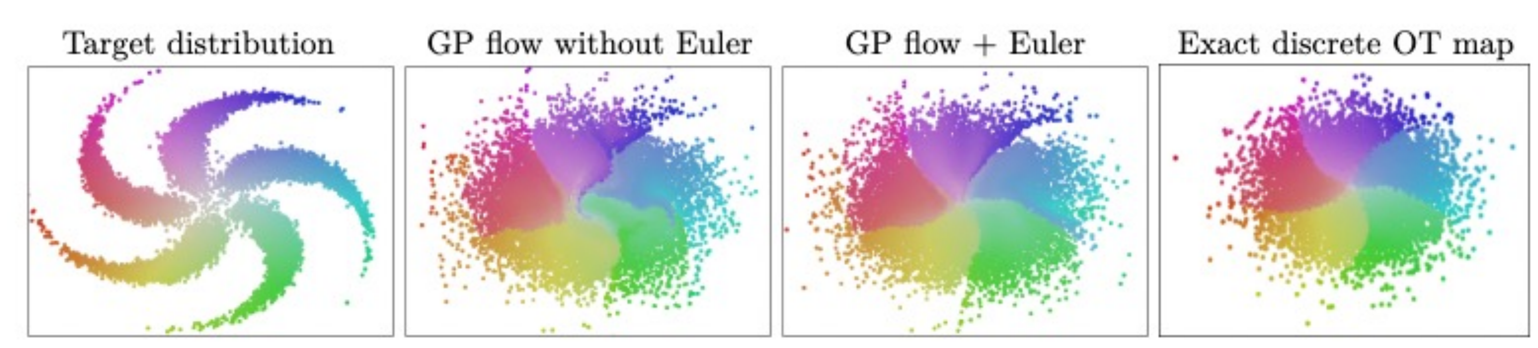


Figure: (left) Turbulent Energy Spectra against resolution scale for different models (ground-truth spectra in gray dashed line). (right) Ground-truth and reconstructed vector fields with proposed models.

Geodesic Gaussian Preserving Flows

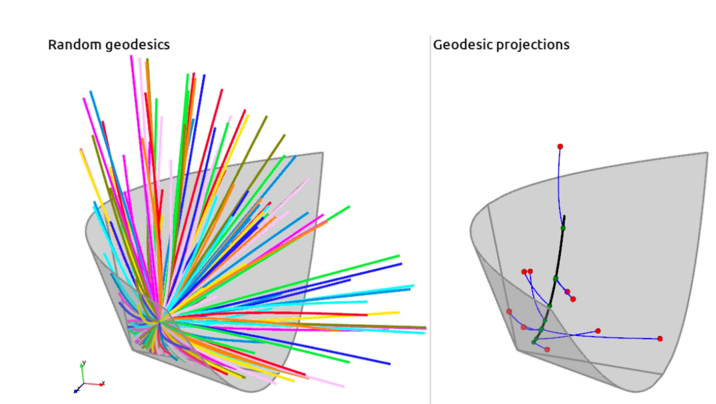
- Goal : turning Normalizing Flows into Monge Maps with Geodesic Gaussian Preserving Flows
- Brenier's polar factorization to transform any trained Normalizing Flow into a more Optimal Transport efficient version without changing the final density
- Construction of high dimensional divergence free functions
- The path leading to the estimated Monge map is constrained to lie on a geodesic in the space of volume-preserving diffeomorphisms thanks to Euler's equation



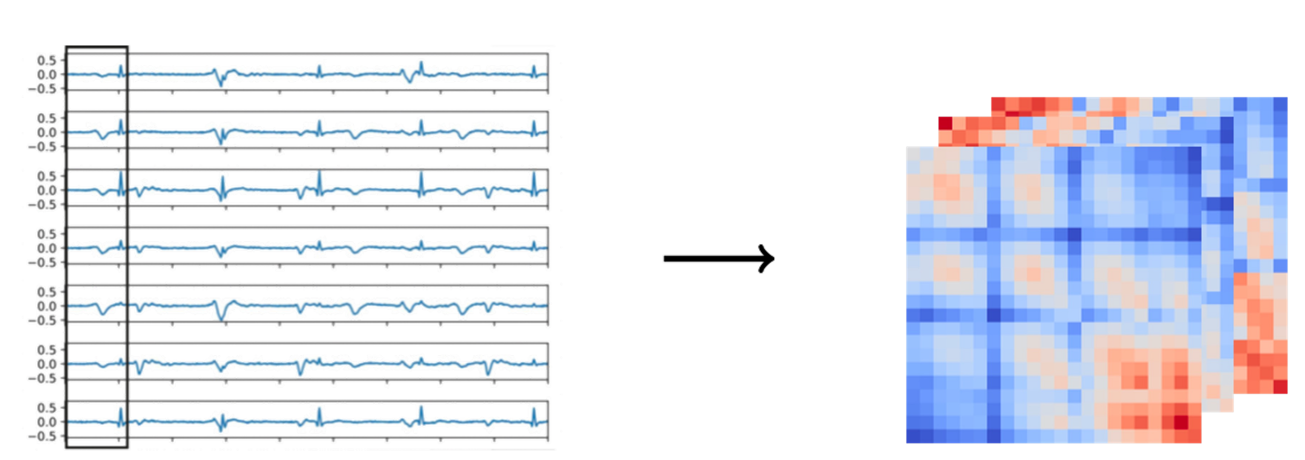
Comparison of GP flow with and without Euler for the Pinwheel test case. Euler regularization leads to a better convergence result

Sliced-Wasserstein on Manifolds

- Data often lie on manifolds or have an underlying structure which can be captured on manifolds.
- Particular case of Riemannian manifold: Cartan-Hadamard manifolds: Non-positive curvature, complete and connected
- Goal: defining SW discrepancy on Cartan-Hadamard manifolds taking care of geometry of the manifold
- Specification to Hyperbolic Spaces and SPDs with Log-Euclidean metric
- Applications to Machine Learning



M/EEG data:
- Recorded from the brain
- Multivariate time series $X \in \mathbb{R}^{N \times T}$
- Transform X into distribution of SPDs



References

- *Clément Bonet, Titouan Vayer, Nicolas Courty, François Septier, and Lucas Drumetz. Subspace Detours meet Gromov-Wasserstein. Algorithms, 2021.*
- *Clément Bonet, Nicolas Courty, François Septier, and Lucas Drumetz. Efficient Gradient Flows in Sliced-Wasserstein Space. Transactions on Machine Learning Research, 2022.*
- *Clément Bonet, Paul Berg, Nicolas Courty, François Septier, Lucas Drumetz, and Minh-Tan Pham. Spherical Sliced-Wasserstein. International Conference on Learning Representations, 2023.*
- *Clément Bonet, Laetitia Chapel, Lucas Drumetz, and Nicolas Courty. Hyperbolic Sliced-Wasserstein via Geodesic and Horospherical Projections. Annual Workshop on Topology, Algebra, and Geometry in Machine Learning, 2023.*
- *Clément Bonet, Benoît Malézieux, Alain Rakotomamonjy, Lucas Drumetz, Thomas Moreau, Matthieu Kowalski, and Nicolas Courty. Sliced-Wasserstein on Symmetric Positive Definite Matrices for M/EEG Signals. International Conference of Machine Learning, 2023.*
- *Guillaume Mahey, Laetitia Chapel, Gilles Gasso, Clément Bonet, and Nicolas Courty. Fast Optimal Transport through Sliced Wasserstein Generalized Geodesics. Advances in Neural Information Processing Systems, 2023.*
- *Thibault Séjourné, Clément Bonet, Kilian Fatras, Kimia Nadjahi, and Nicolas Courty. Unbalanced Optimal Transport meets Sliced-Wasserstein. Submitted, 2023.*
- *Morel, G., Drumetz, L., Benaïchouche, S., Courty, N., & Rousseau, F. (2022). Turning Normalizing Flows into Monge Maps with Geodesic Gaussian Preserving Flows. arXiv preprint arXiv:2209.10873.*
- *Morel, G., Drumetz, L., Benaïchouche, S., Courty, N., & Rousseau, F. (2022). Turning Normalizing Flows into Monge Maps with Geodesic Gaussian Preserving Flows. Transactions on Machine Learning Research, pp 2835-8856, 2023*
- *Di Carlo, D., Heitz, D., Corpetti, T. & Courty, N. (2022, July). Post processing sparse and instantaneous 2D velocity fields using physics-informed neural networks. In 20th International Symposium on Application of Mlaser and Imaging Techniques to Fluid Mechanics*