Carnegie Mellon University

The Mallat Scattering Transform for Reduced Order Modelling of Partial Differential Equations

Francis Ogoke, Michael Glinsky*, Amir Barati Farimani

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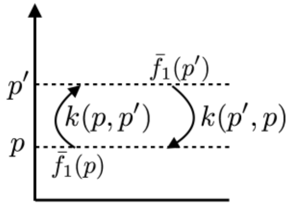
Connection of MST to MLDL, kinetic theory, field theory, and topology

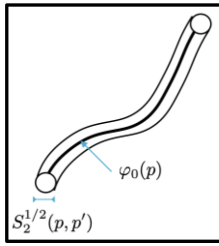
- The Mallat Scattering Transform is a deep Convolutional Network with pre-determined weights
- Manifold safe Wigner-Weyl transform that leads to a Generalized Master Equation through the BBGKY hierarchy
- Gives the S-matrix (generalized Green's function) of field theory in scale basis
- Scale-dependent topological indices, giving the co-homology of the dynamical manifold

$p \equiv \lambda, 1/\text{scale, canonical momentum, or quantum numbers}$



$$\frac{\partial \bar{f}_1^2(p,t)}{\partial t} - \frac{\partial \bar{f}^2_{\text{source}}(p,t)}{\partial t} \sim \int dp' \; \bar{f}_2^2(p',p,t) - \bar{f}_2^2(p,p',t) = \int dp' \; \bar{f}_1^2(p',t)\, k(p',p) - \bar{f}_1^2(p,t)\, k(p,p')$$

classical kinetic

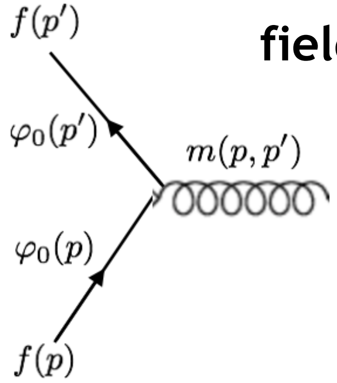


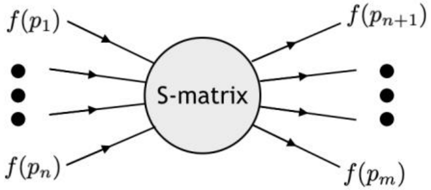
$$S_0[\varphi(p)] = S_0[\varphi_0(p)] - \frac{1}{2}\int dp\, dp' (\varphi(p) - \varphi_0(p))\; S_2^{-1}(p,p')\; (\varphi(p') - \varphi_0(p'))$$

topological

where $k(p,p') \equiv \dfrac{\bar{f}_2^2(p,p',t)}{\bar{f}_1^2(p,t)}$

field theoretical





$$S_1(p) = S_1(|f\rangle) = |f \star \psi_p| \star \phi = \bar{f}_1(p) = \varphi_0(p)$$

state of system

$$S_2(p,p') = S_2(|f\rangle) = ||f \star \psi_p| \star \psi_{p'}| \star \phi = \bar{f}_2(p,p') = 1/m(p,p')$$

deep convolutional network

Feynman diagram

QFT S-matrix

kinetic distribution function

integrated "functional curvature"
that is topological index

transition rates

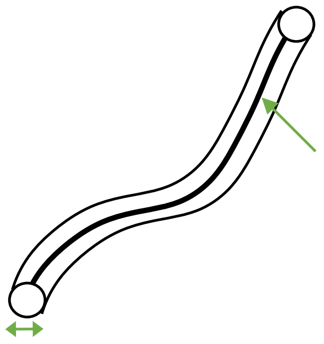
Relationship of MST to algebraic topology: topological invariant (index)

Solving field equations (quantum fluctuations), statistical systems (thermal fluctuations) or data assimilation with uncertainty (data and model fluctuations) can be recast into one of pure geometry, with the complication that the curvature is scale dependent (that is, a non-Riemannian manifold).

The effective action, entropy, or inverse "Fisher Information" is introduced as

$$S[\varphi(p)] = -\ln Z[J] + \int dp\, J(p)\, \varphi(p)$$

The action in the path integral, $S_0[\varphi(p)]$, can be expanded around the stationary path $\varphi_0(p)$ such that $\left.\frac{\delta S}{\delta \varphi}\right|_{\varphi_0} = 0$



$$S_0[\varphi(p)] = S_0[\varphi_0(p)] - \frac{1}{2}\int dp\, dp' (\varphi(p) - \varphi_0(p))\; S_2^{-1}(p,p')\; (\varphi(p') - \varphi_0(p'))$$

needs to be normalized to $\frac{S_2(p,p')}{\varphi_0(p)}$

where $S_2(p,p') \equiv -\left(\frac{\delta^2 S_0[\varphi_0(p)]}{\delta\varphi(p)\,\delta\varphi(p')}\right)^{-1} = \frac{1}{Z[J]}\left.\frac{\delta^2 Z[J]}{\delta J(p)\,\delta J(p')}\right|_{J=0}$ is the integrated curvature, that is topological index

Relation of MST to Generalized Master Equation: manifold safe Wigner-Weyl transformation

Wigner-Weyl transformation takes operators to/from classical phase space (1927).
The Key is a modified Wigner-Weyl transform that is manifold safe.
Need a local Fourier kernel (Mother Wavelet) with a partition of unity (Father Wavelet).

$$\text{modified Wigner map} = \tilde{W}[\hat{A}] \equiv \int ds\, \psi_p^*(-s) \left\langle q+s \middle| \hat{A} \middle| q-s \right\rangle \psi_p(s) = A(q,p)$$

$$\text{modified Wigner function} = \tilde{W}[\hat{\rho}] = \tilde{W}[\,|f\rangle\langle f|\,] = |f \star \psi_p|^2 = \tilde{W}_f(q,p)$$

Has all of the properties of the conventional Wigner-Weyl transformation, plus has the correct commutator

Now we can identify and calculate,

$$\bar{f}_1(p) \equiv E(\tilde{W}[\hat{f}]) = \sum_i |f \star \psi_p| \star \phi_i = S_1[p]f$$

$$\bar{f}_2(p,p') \equiv E(\tilde{W}[\hat{f}\hat{f}]) = \sum_i ||f \star \psi_p| \star \psi_{p'}| \star \phi_i = S_2[p,p']f$$

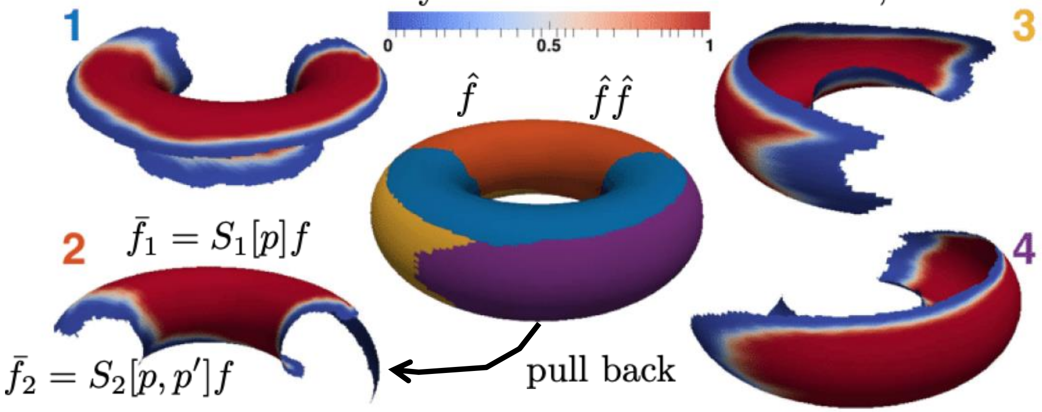
This is the Mayer Cluster expansion on the manifold.

Mother wavelet $\psi_p \sim$ convolution filter

Father wavelet $\phi \sim$ pooling

$|\cdot| \sim$ activation function

Partition of Unity on the manifold of a torus, T^2



The MST is a transformation into the **sparse** Koopman basis

Using the BBGKY hierarchy, and the ideas of Bogoliubov,

$$\boxed{\frac{\partial W(p,t)}{\partial t} = \int dp'\ W(p',t)\,k(p',p) - W(p,t)\,k(p,p')}$$

$$W(p,t) \equiv \mu(p)\ \bar{f}_1^2(p,t)$$

$$\mu(p) \equiv \text{ measure or density of states}$$

$$\int dp\ \frac{\partial W(p,t)}{\partial t} = 0$$

$$\text{detailed balance } => \ W_{th}(p)\,k(p,p') = W_{th}(p')\,k(p',p)$$

$$W_{th}(p) \equiv \mu(p)e^{-E(p)/k_BT} \text{ or } \mu(p)e^{(i/\hbar)E(p)} \text{ or } \mu(p)e^{-E(p)/\sigma^2}$$

$$k(p,p') \equiv \begin{cases} \frac{\bar{f}_2^2(p,p')}{\bar{f}_1^2(p)} & \text{for } p' < p \\ -\sum_{p''\neq p} k(p,p'') & \text{for } p' = p \\ \frac{\mu(p')}{\mu(p)} e^{\Delta E/k_BT}\frac{\bar{f}_2^2(p',p)}{\bar{f}_1^2(p')} & \text{for } p' > p \end{cases}$$

$$\boxed{\frac{\partial W_p(t)}{\partial t} = K_{pp'}\,W_{p'}(t)}$$

$$\text{where } K = \begin{array}{c c} & p' \rightarrow \\ p \downarrow & \begin{pmatrix} \ddots & \cdots & k(p',p) \\ \vdots & -\sum_{p\neq p'} k(p',p) & \vdots \\ k(p',p) & \cdots & \ddots \end{pmatrix} \end{array} = \begin{pmatrix} \ddots & \cdots & \frac{\bar{f}_2^2(p',p)}{\bar{f}_1^2(p')} \\ \vdots & -\sum_{p\neq p'} k(p',p) & \vdots \\ \frac{\mu(p)}{\mu(p')} e^{\Delta E/k_BT}\frac{\bar{f}_2^2(p,p')}{\bar{f}_1^2(p)} & \cdots & \ddots \end{pmatrix}$$

$$\text{and } \Delta E \equiv E(p') - E(p)$$

Dynamics converge exponentially to the attractive manifold

$$K_{pp'} = f(\mu_p, (\bar{f}_2/\bar{f}_1)_{pp'}, (\bar{f}_2/\bar{f}_1)_{p'p}) \;\text{ or }\; f(\mu_p, (\bar{f}_2/\bar{f}_1)_{pp'}, E_p/k_B T) \quad \text{for } p' > p$$

μ_p from Dirac normalization

$(\bar{f}_2/\bar{f}_1)_{pp'}$ from MST, or $(\bar{f}_2/\bar{f}_1)_{pp'}$ and E_p from Lagrangian

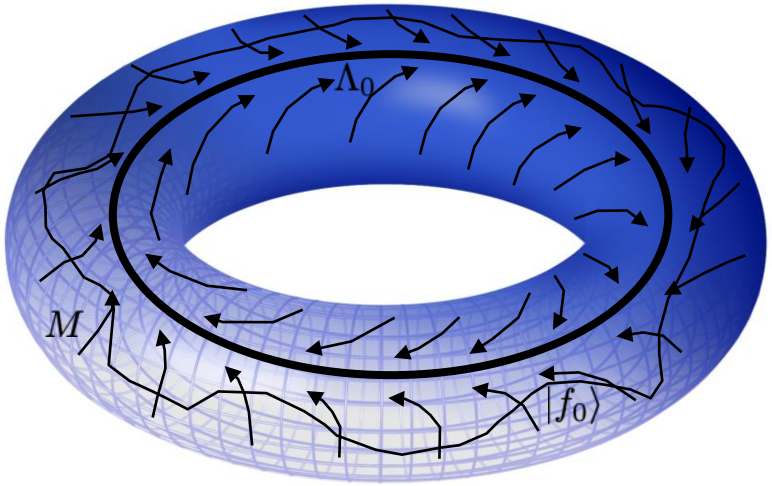
$k_B T$ from data, largest of quantum, thermal or measurement fluctuations

decompose $K = U\,\Sigma\,U^T$ where $\Sigma = \mathrm{diag}(\sigma_p)$ and rotate $\widetilde{W}_p(t) = U^T\,W_p(t)$

$$\frac{\partial \widetilde{W}_p(t)}{\partial t} = \Sigma\,\widetilde{W}_p(t) \text{ with solution } \boxed{\widetilde{W}_p(t) = e^{\sigma_p t}, \text{ where } \sigma_p \leq 0}$$

$W_p(t)$ converges exponentially onto null space of K, Λ_0, with $\sigma_p = 0$ (that is, emergent behavior)

the emergent behavior is the projection of the initial state onto the null space manifold, $\Lambda_0 \subset M$



finite difference of the Generalized Master Equation stable if $\Delta t \ll 1/|\sigma_p|_{\max}$

Λ_0 is the dynamical attractive manifold, and is **sparse**

Renormalization group provides theoretical guarantee of sparsity

The dimension of the subspace is given by $\mathrm{PDF} \sim k^{\beta_i(k)}$, where $N_i = N_{\text{coupling constants}} + N_{\text{fields}}$ is the Kodaira dimension of the dynamical manifold, or the dimension of the dynamical attractive manifold. The dynamics converge to a subspace that is the solution of the Renormalization Group Equations

Applied to ϕ^4 field theory, the RGEs are given by

$$\frac{\mathrm{d}(\log c_i)}{\mathrm{d}(\log k)} = f(\log k)$$

$$\log(\mathrm{PDF}) = \sum_k \beta_i(k) \log(k)$$

With the solution:

$$\phi(k) \sim k^{\beta_\phi(k)}$$

$$\gamma(k) \sim k^{\beta_\gamma(k)}$$

$$m(k) \sim k^{\beta_m(k)}$$

$[\beta_\phi(k), \beta_\gamma(k), \beta_m(k)]$ act as the unit vectors of the subspace, $\hat{\beta}_i$ in $\log k$, which defines the Reduced Order Model, or latent space

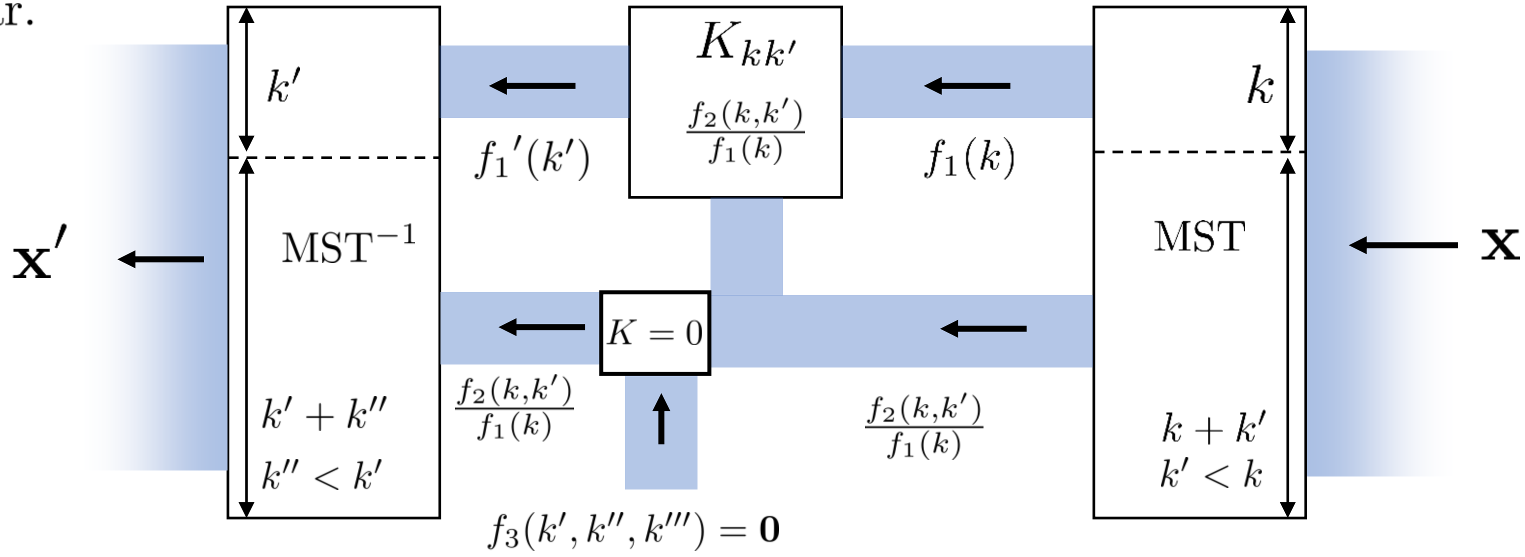
The MST can be incorporated into a traditional autoencoder propagation model (PropNet)

The transition kernel, or the generator of infinitesimal time translations on the dynamical variable $u(x,t)$ can be taken as

$$K[u(x,t);t] = \frac{-i}{\hbar}\hat{H}(t), \text{ where } u(x,\Delta t) = u(x,0) + \Delta t\ K[u(x,0);t]$$

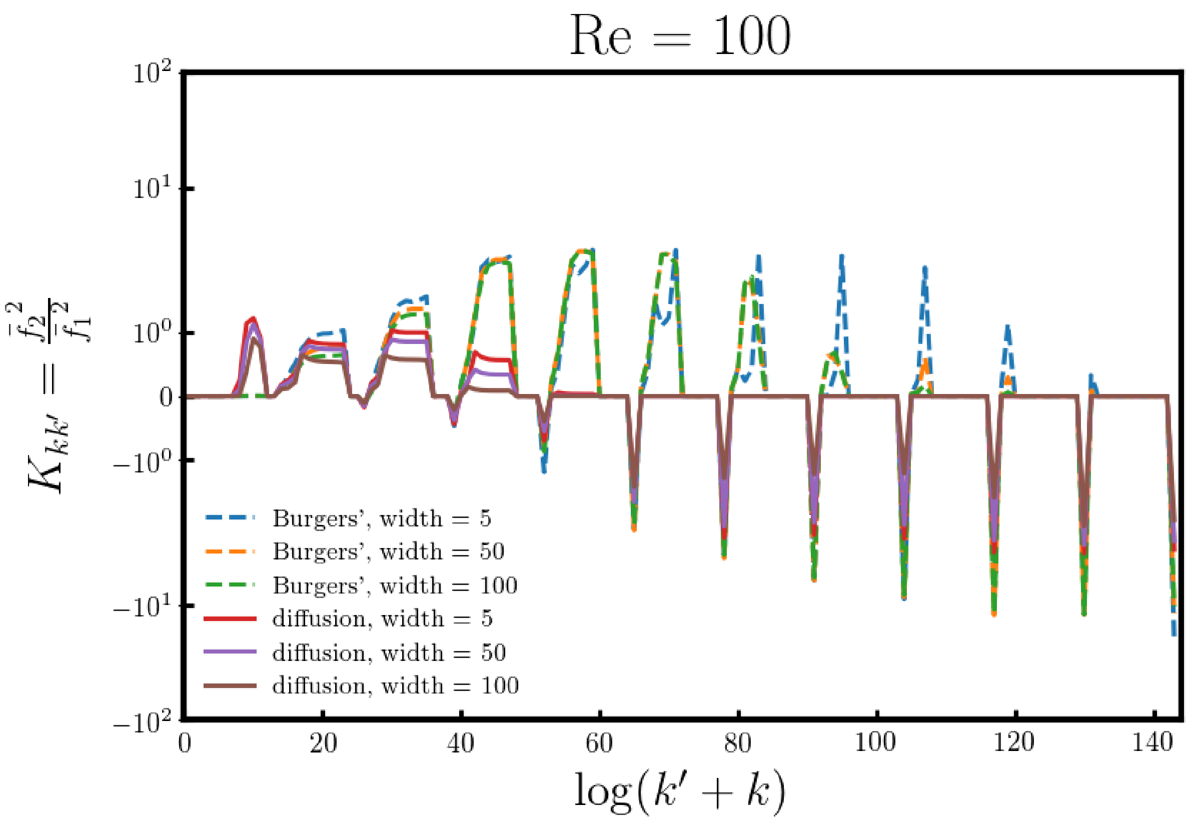
$$\boxed{K[u(x,t);t] \text{ has the form: } K[u(x)] = h^{-1}[\tilde{u}(k')]\ K_{kk'}\ h[u(x)]}$$

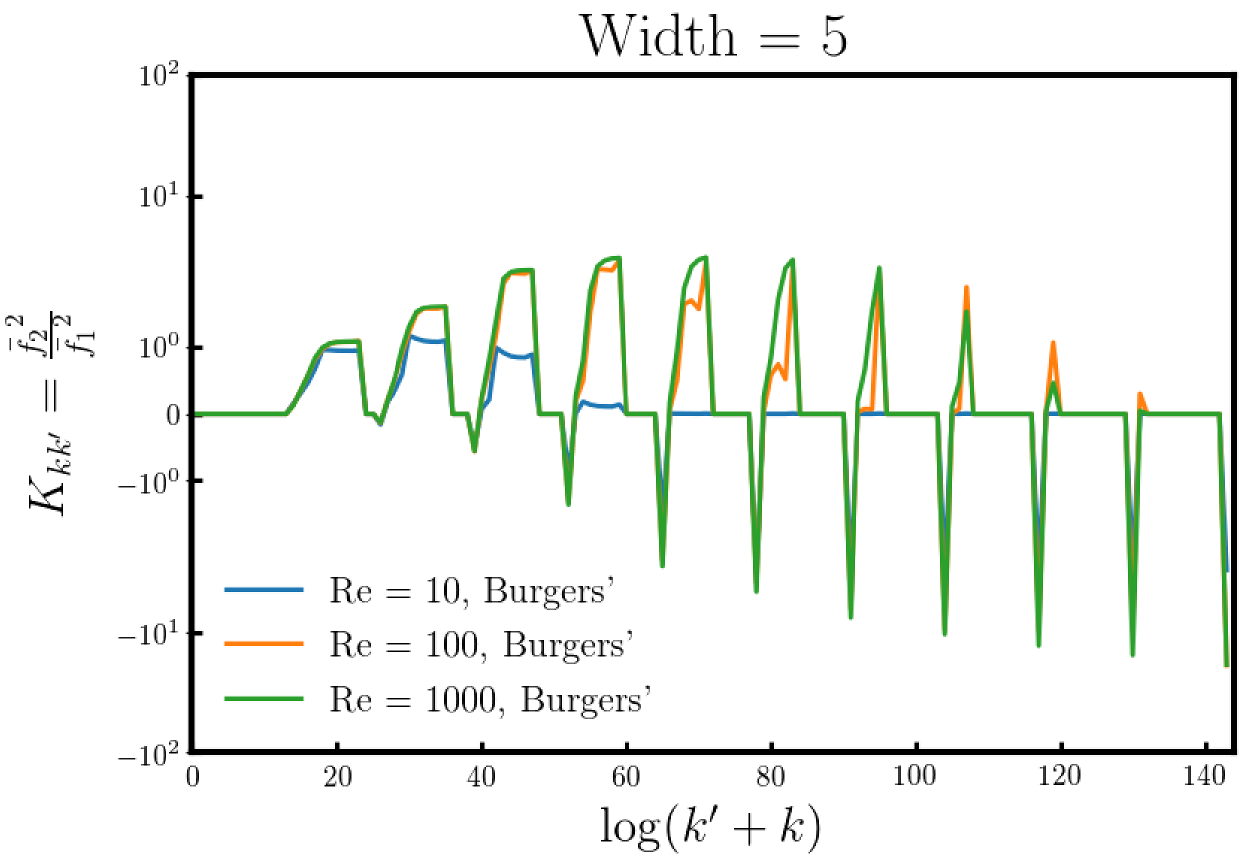
Taking $h[u(x)] : u(x) \to \tilde{u}(k)$ as the MST, it acts as a Convolutional Network **encoder**, a functional transformation into the Koopman basis where $K_{kk'}$ is linear.



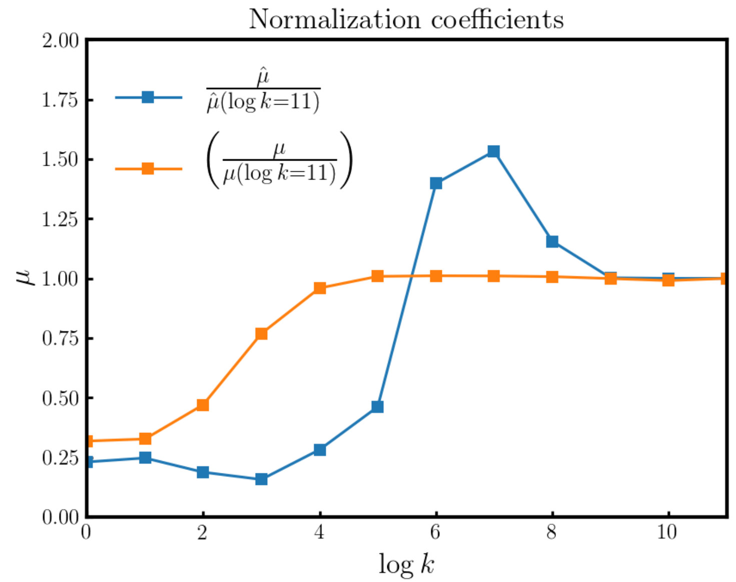
truncate the BBGKY hierarchy, a closure due to statistical realizability

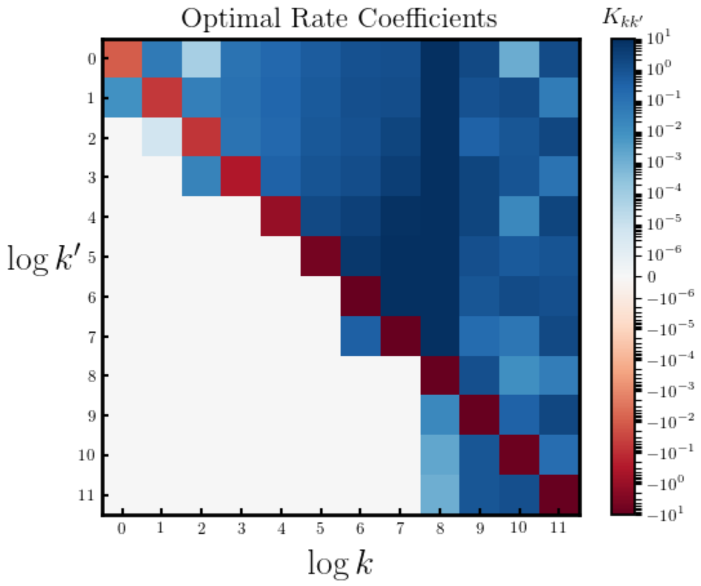
MST rate coefficients are invariant to the initial condition, and extract dynamics of system

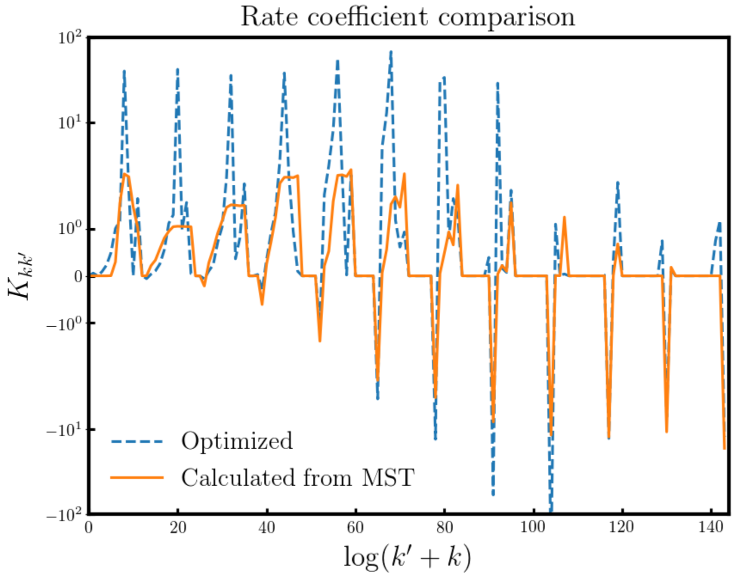


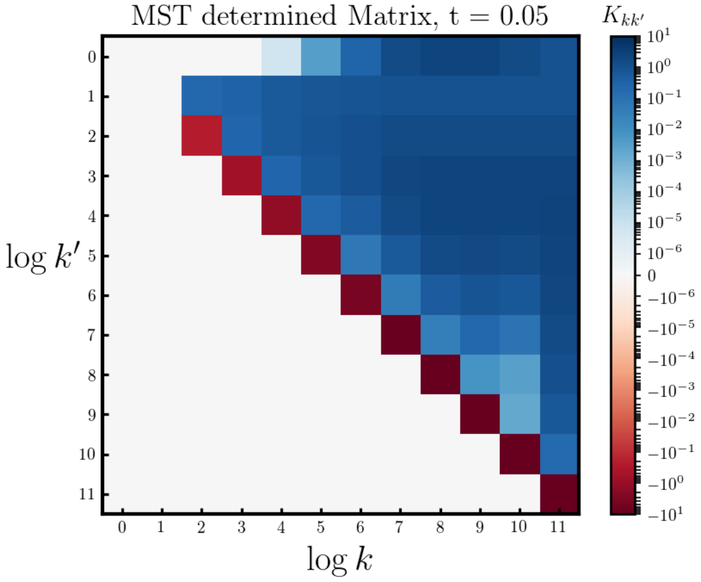


The MST extracts the dynamics of the system with minimal optimization required

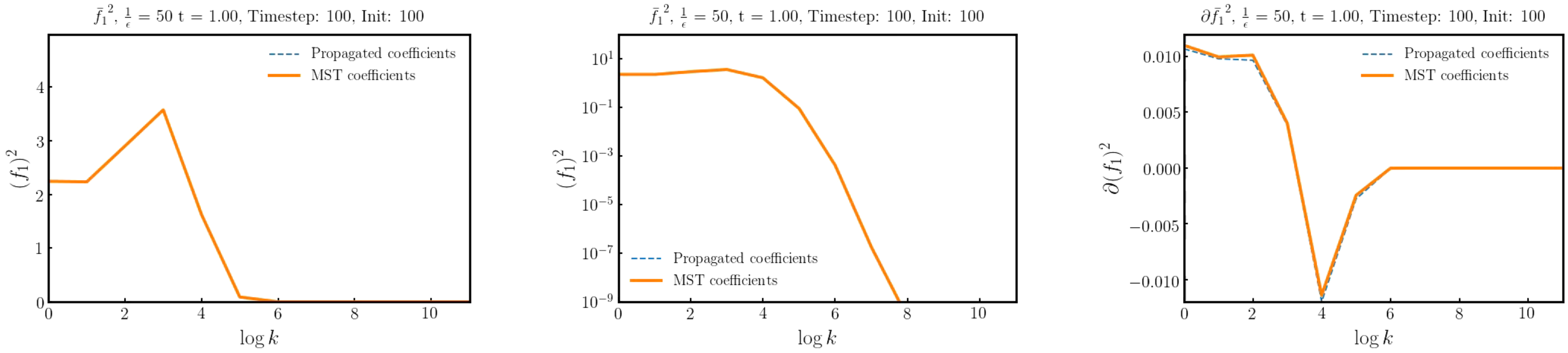








The Generalized Master Equation is able to reproduce the dynamics



In conclusion, the MST:

- Acts as an autoencoder that is principled via physics
- Exposes the dynamics where the representation is optimally sparse with no constraint on the manifold
- Optimally approximates the attractive manifold, that is the latent space or ROM, a very low dimensional linear subspace in this optimal representation.

Future Work

- Deriving the inverse Mallat Scattering Transform, including the field's gauge (that is, phase), to directly reproduce the dynamics
- Fine-tuning optimization to recover coefficients at the small-scale limit
- Extending the MST to two and three dimensional PDEs