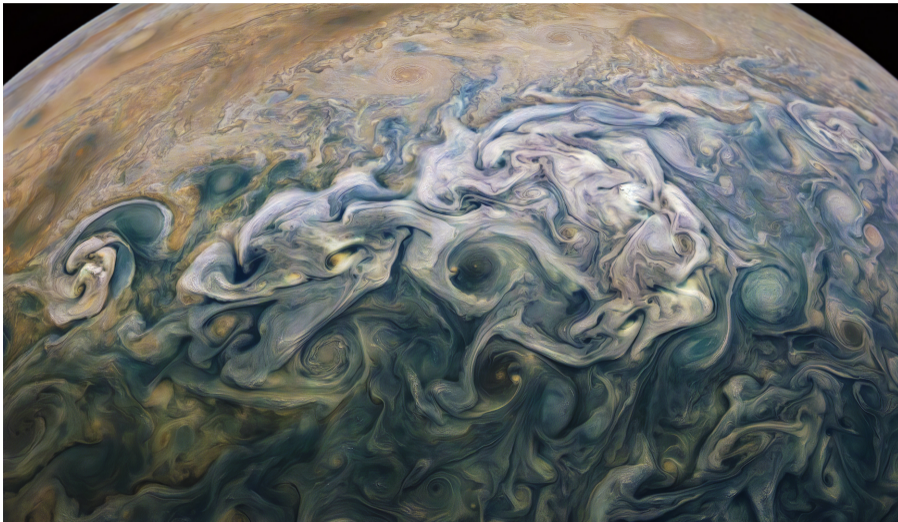


Data-based approach for time-correlated closures of turbulence models

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Alexei Mailybaev - IMPA

September 25th, 2023

Turbulence



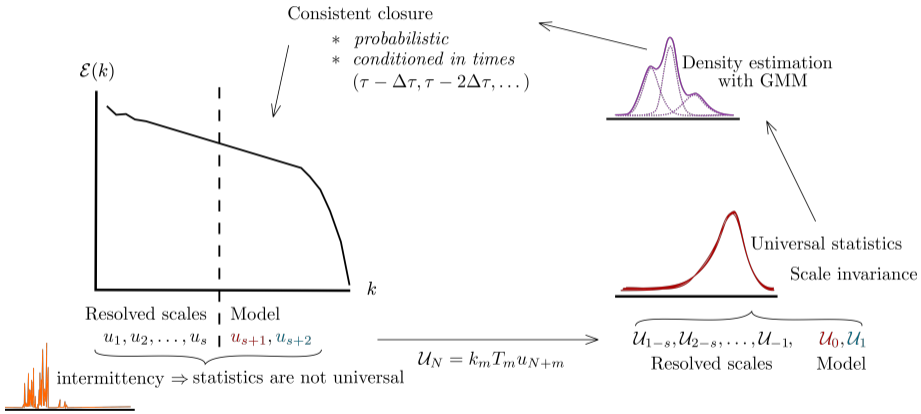
$$Re = \frac{UL}{\nu}, \quad \eta \sim \left(\frac{\nu^3}{\epsilon}\right)^{1/4}, \quad \epsilon \sim \frac{U^3}{L}$$

For a grid with spacing smaller than the Kolmogorov length scale:

$$N = \left(\frac{L}{\eta}\right)^3 \sim Re^{9/4} \tag{1}$$

- Cup of coffee: $Re = 10^4$, grid must have 10^9 points (8GB per array)
- Moving car: $Re = 10^9$, grid must have 10^{16} points (80000000GB per array)

Road map



N.S.

$$\begin{aligned} \partial_t u_i(\mathbf{n}) = & -i \frac{2\pi n_j}{L} \sum_{\mathbf{n}'} \left(\delta_{il} - \frac{n_i n'_l}{n_j n_j} \right) u_j(\mathbf{n}') u_l(\mathbf{n} - \mathbf{n}') \\ & - \nu k_j k_j u_i(\mathbf{n}) + f_i(\mathbf{n}). \end{aligned} \quad (2)$$

L'vov et al. (1995) and Gledzer, Ohkitani, Yamada (1973,1988)

$$\frac{du_n}{dt} = i \left(a k_{n+1} u_{n+2} u_{n+1}^* + b k_n u_{n+1} u_{n-1}^* + c k_{n-1} u_{n-1} u_{n-2} \right) - \nu k_n^2 u_n + f_n \quad (3)$$

Parameters

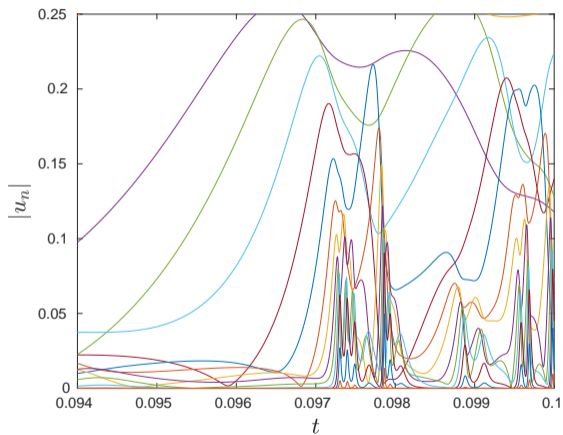
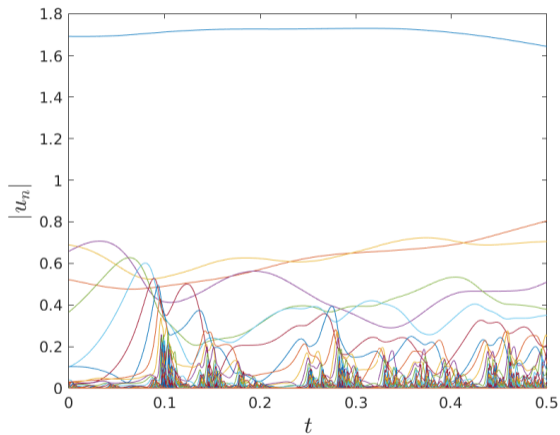
- $a = 1$, $b = -\frac{1}{2}$, $c = \frac{1}{2}$, $\lambda = 2$, $k_0 = 1$ and $k_n = k_0\lambda^n$:
- Inviscid invariants:

$$E = \sum |u_n|^2 \quad (4)$$

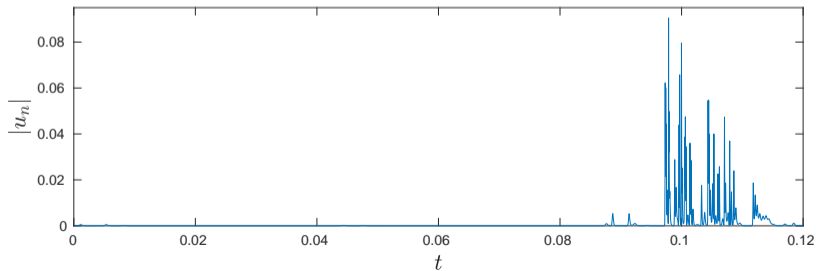
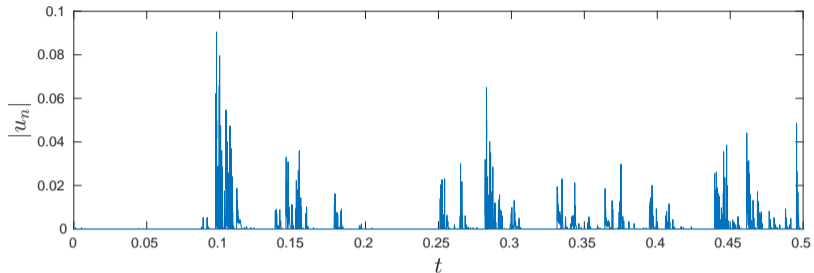
$$H = \sum (-1)^n k_n |u_n|^2 \quad (5)$$

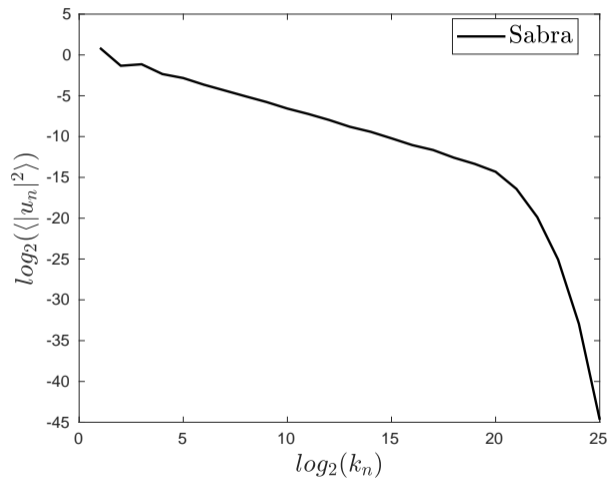
Numerics

- $n = 30$
- $u_{-1} = u_0 = u_{n+1} = u_{n+2} = 0$ (for now)
- $\nu = 10^{-8}$, $f_1 = 1 + i$, $u_n(0) = k^{-1/3} e^{iq_n}$ for $n = 1, 2$

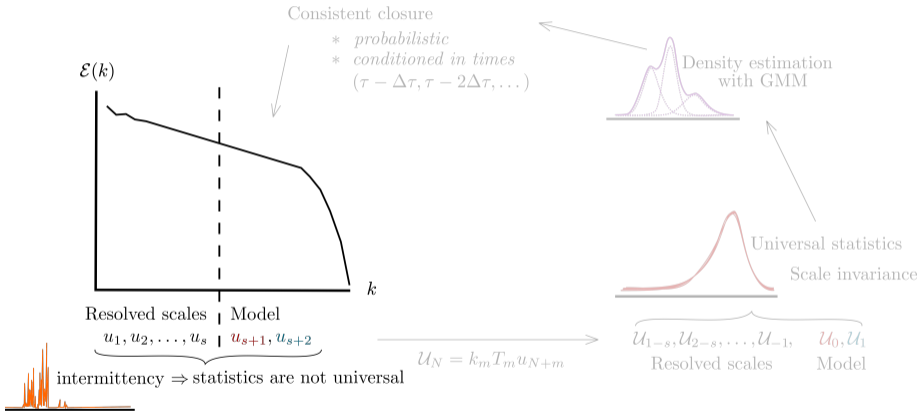


Intermittency





Road map



$$z_n = w_n e^{i\Delta_n}, \quad (6)$$

$$w_n = \left| \frac{u_n}{u_{n-1}} \right|, \quad (7)$$

$$\Delta_n = \arg(u_n) - \arg(u_{n-1}) - \arg(u_{n-2}), \quad (8)$$

PHYSICAL REVIEW E **95**, 043108 (2017)

Optimal subgrid scheme for shell models of turbulence

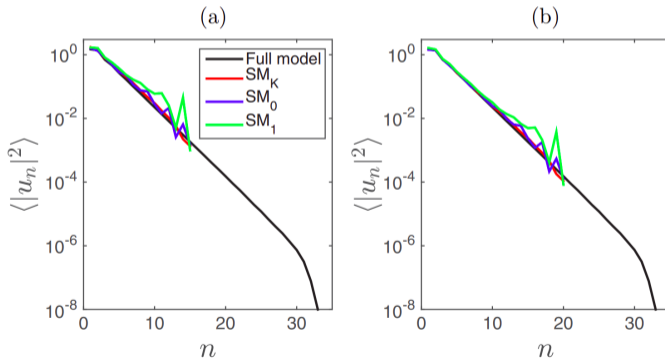
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[Kolmogorov, 1962]

[Benzi, 1993]

Choose a reference shell m [Mailybaev, 2021]

$$T_m(t) = \left(k_0^2 U^2 + \sum_{n < m} k_n^2 |u_n|^2 \right)^{-1/2} \quad (9)$$

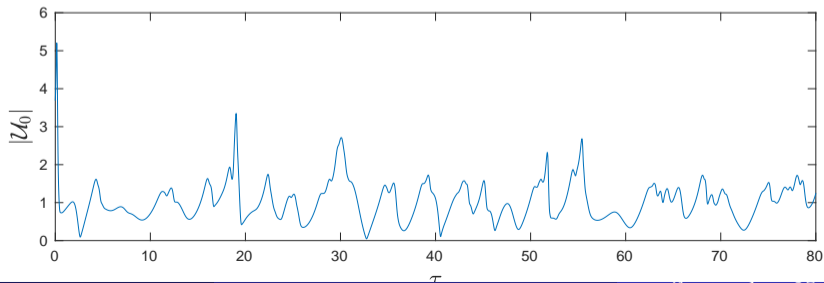
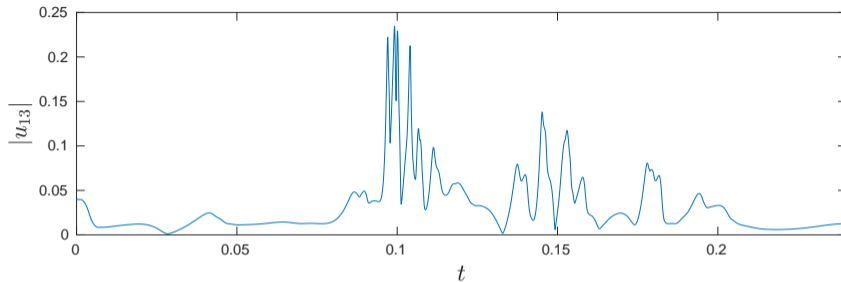
Define the change of variables

$$\tau = \int_0^t \frac{dt'}{T_m(t')} \quad (10)$$

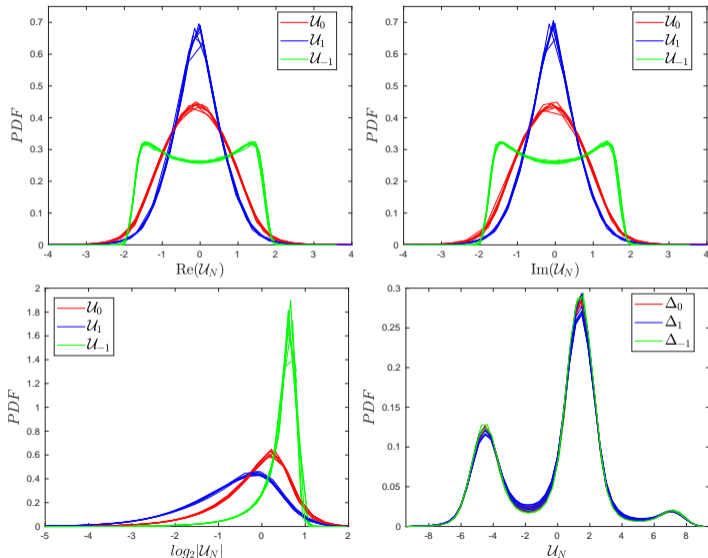
$$\mathcal{U}_N = k_m T_m(t) u_{N+m}(t) \quad (11)$$

- Shrinks long periods of time where nothing happens
- Stretches short periods of time where a lot happens
- Gives a new sense of symmetry

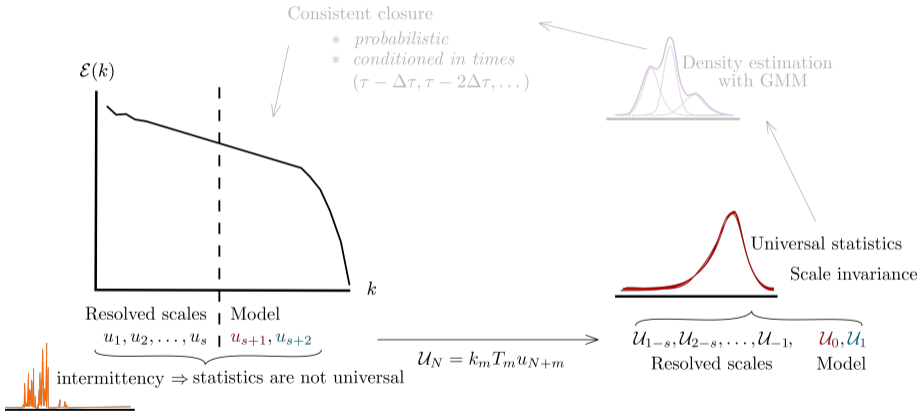
Rescaled Model



Hidden Symmetry



Road map



$$\begin{aligned} \frac{d\mathcal{U}_N}{d\tau} = & i(k_{N+1}\mathcal{U}_{N+2}\mathcal{U}_{N+1}^* - \frac{1}{2}k_N\mathcal{U}_{N+1}\mathcal{U}_{N-1}^* + \frac{1}{2}k_{N-1}\mathcal{U}_{N-1}\mathcal{U}_{N-2}) \\ & + (\xi + \xi_f)\mathcal{U}_N + \nu k_m^2 T_m \left(-k_N^2 + \sum_{J<0} k_J^4 |\mathcal{U}_J|^2 \right) \mathcal{U}_N + T_m^2 k_m f_{N+m} \end{aligned} \quad (12)$$

where

$$\xi = \sum_{N<0} k_N^3 \operatorname{Im} \left(2\mathcal{U}_N^* \mathcal{U}_{N+1}^* \mathcal{U}_{N+2} - \frac{1}{2} \mathcal{U}_{N-1}^* \mathcal{U}_N^* \mathcal{U}_{N+1} - \frac{1}{4} \mathcal{U}_{N-1}^* \mathcal{U}_N \mathcal{U}_{N-2}^* \right) \quad (13)$$

$$\xi_f = -T_m^2 \sum_{N<0} k_{N+m} k_N \operatorname{Re} \left(\mathcal{U}_N^* f_{N+m} \right) \quad (14)$$

$$T_m = \frac{1}{k_0 U} \left(1 - \sum_{N<0} k_N^2 |\mathcal{U}_N|^2 \right)^{1/2} \quad (15)$$

Closure for Reduced Models

- Choose a shell s in the inertial range

$$\frac{du_n}{dt} = i(a k_{n+1} u_{n+2} u_{n+1}^* + b k_n u_{n+1} u_{n-1}^* + c k_{n-1} u_{n-1} u_{n-2}) - \nu k_n^2 u_n + f_n \quad (16)$$

for $n = 1, \dots, s$

- Choose $m = s + 1$

$$\begin{aligned} \frac{d\mathcal{U}_N}{d\tau} = & i(k_{N+1} \mathcal{U}_{N+2} \mathcal{U}_{N+1}^* - \frac{1}{2} k_N \mathcal{U}_{N+1} \mathcal{U}_{N-1}^* + \frac{1}{2} k_{N-1} \mathcal{U}_{N-1} \mathcal{U}_{N-2}) \\ & + (\xi + \xi_f) \mathcal{U}_N + \nu k_m^2 T_m \left(-k_N^2 + \sum_{J < 0} k_J^4 |\mathcal{U}_J|^2 \right) \mathcal{U}_N + T_m^2 k_m f_{N+m} \end{aligned} \quad (17)$$

For $N = 1 - s, \dots, -1$.

We need expressions for u_{s+1} and u_{s+2} .

- or -

We need expressions for \mathcal{U}_0 and \mathcal{U}_1 .

[Biferale, Mailybaev, Parisi, 2017]

$$\frac{|u_{s+2}|}{|u_{s+1}|} = \frac{|u_{s+1}|}{|u_s|} = \lambda^{-1/3}, \quad (18)$$

$$\Delta_{s+1} = \Delta_{s+2} = \frac{\pi}{2}. \quad (19)$$

Choosing the the shell velocities' phases θ_n as to satisfy $\theta_n = \theta_{n-1} + \theta_{n-2}$,

$$u_{s+1} = |u_s| \lambda^{-1/3} e^{i(\frac{\pi}{2} + \theta_s + \theta_{s-1})}, \quad (20)$$

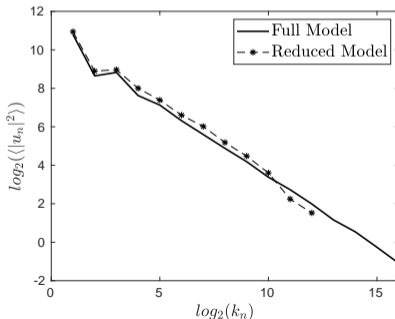
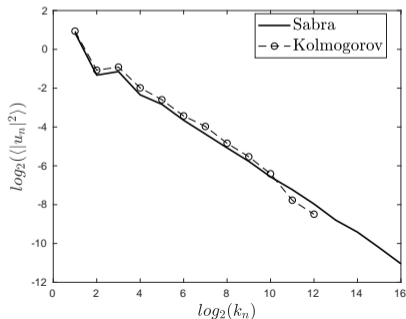
$$u_{s+2} = |u_{s+1}| \lambda^{-1/3} e^{i(\frac{\pi}{2} + \theta_{s+1} + \theta_s)}. \quad (21)$$

Kolmogorov's Closure

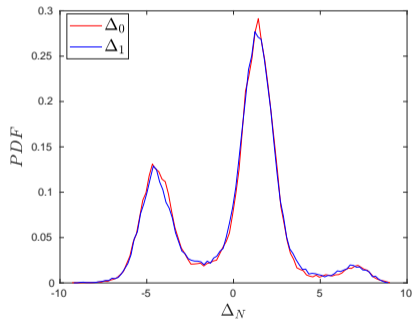
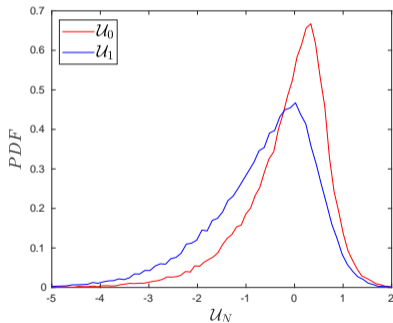
$$\mathcal{U}_0 = |\mathcal{U}_{-1}| \lambda^{-1/3} e^{i(\frac{\pi}{2} + \alpha_{-1} + \alpha_{-2})}, \quad (22)$$

$$\mathcal{U}_1 = |\mathcal{U}_0| \lambda^{-1/3} e^{i(\frac{\pi}{2} + \alpha_0 + \alpha_{-1})} \quad (23)$$

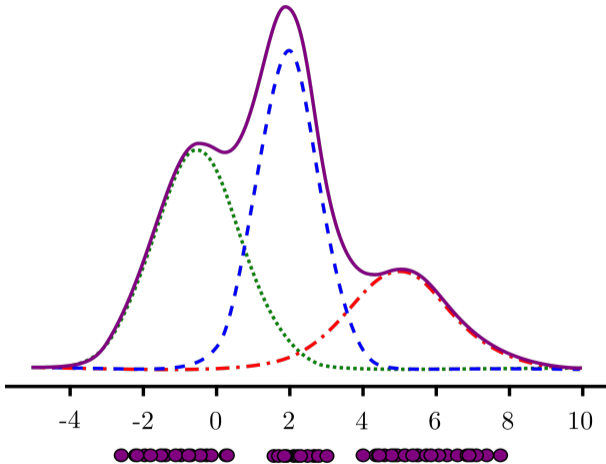
$$\alpha_N = \arg(\mathcal{U}_N) = \theta_{N+m}$$



How do we go about making this *probabilistic*?



Gaussian Mixture Models



Say we have N data samples from a distribution we don't know.

$$p(\mathbf{x}) = \sum_{k=1}^K \pi_k \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \quad (24)$$

$$\mathcal{N}(\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2} |\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right) \quad (25)$$

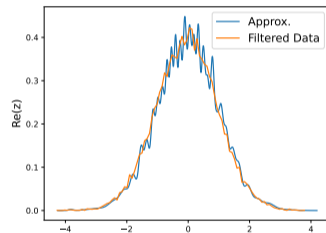
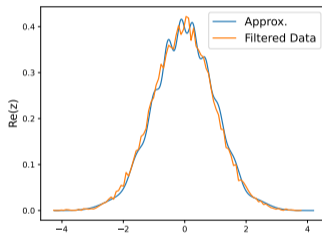
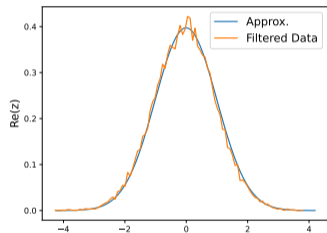
$$\sum_{k=1}^K \pi_k = 1. \quad (26)$$

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^k \pi_j \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \quad (27)$$

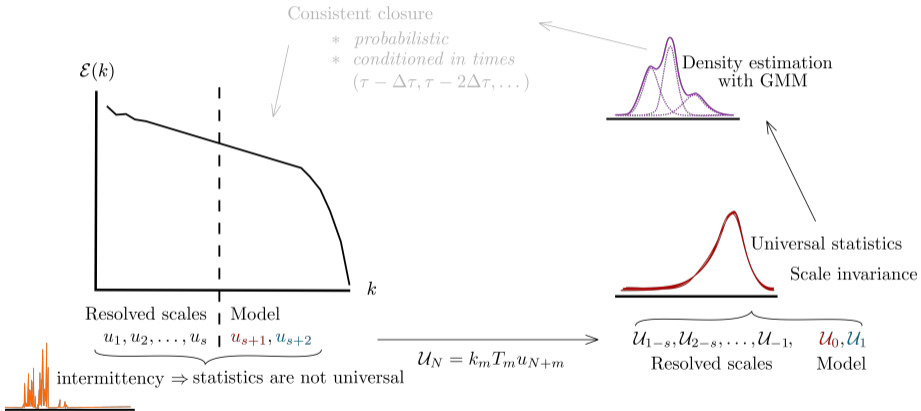
$$Q(\boldsymbol{\theta}^*, \boldsymbol{\theta}) = \sum_{n=1}^N \sum_{k=1}^K \gamma(z_{nk}) (\ln \pi_k^* + \ln \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k^*, \boldsymbol{\Sigma}_k^*)) + \lambda \left(\sum_{k=1}^K \pi_k^* - 1 \right) \quad (28)$$

$$\hat{\boldsymbol{\theta}} = \arg \max_{\boldsymbol{\theta}^*} Q(\boldsymbol{\theta}^*, \boldsymbol{\theta}) \quad (29)$$

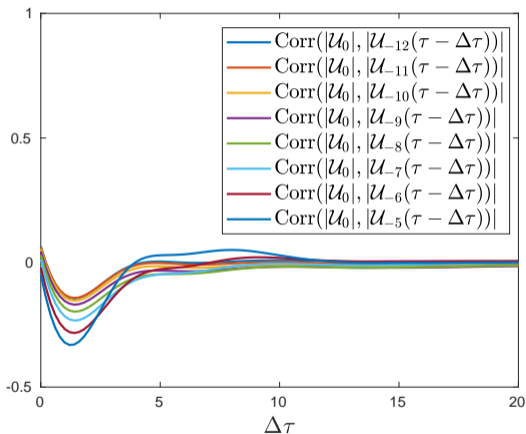
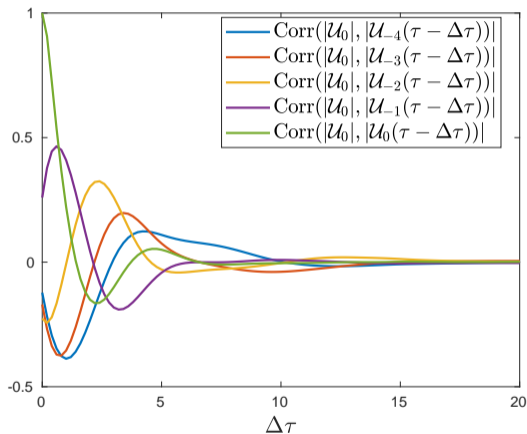
Convergence



Road map



Time Correlation



Only **modules**:

$$\mathcal{U}_0 = 2^{z_0} e^{i(\frac{\pi}{2} + \alpha_{-1} + \alpha_{-2})}, \quad (30)$$

$$\mathcal{U}_1 = 2^{z_1} e^{i(\frac{\pi}{2} + \alpha_0 + \alpha_{-1})}, \quad (31)$$

$$\mathbf{z} = (z_0, z_1) \sim g(\mathbf{z}). \quad (32)$$

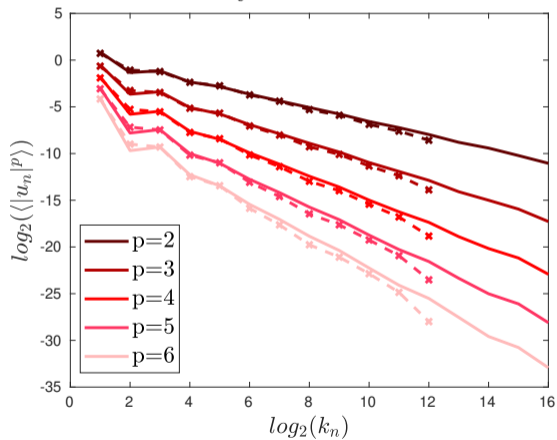
Modules and **phases**:

$$\mathcal{U}_0 = 2^{z_0} e^{i(z_1 + \alpha_{-1} + \alpha_{-2})}, \quad (33)$$

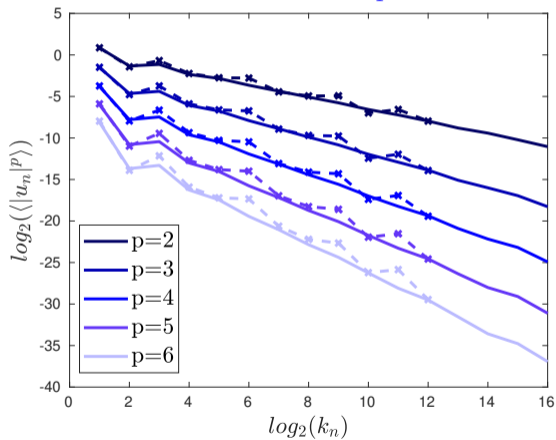
$$\mathcal{U}_1 = 2^{z_2} e^{i(z_3 + \alpha_0 + \alpha_{-1})}, \quad (34)$$

$$\mathbf{z} = (z_0, z_1, z_2, z_3) \sim g(\mathbf{z}). \quad (35)$$

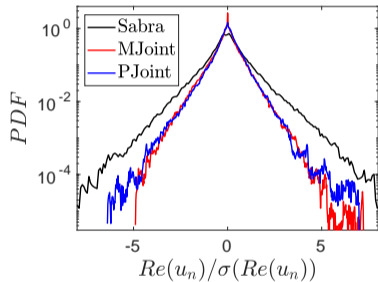
Only modules



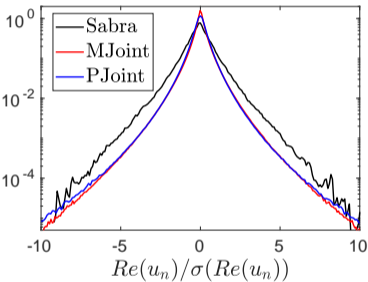
Modules and phases



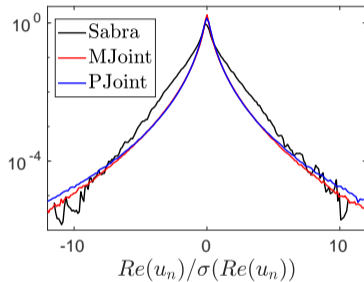
Single-time closures



$n=12$

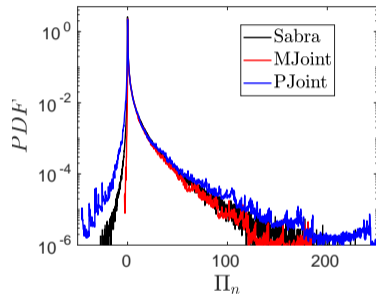


$n=13$

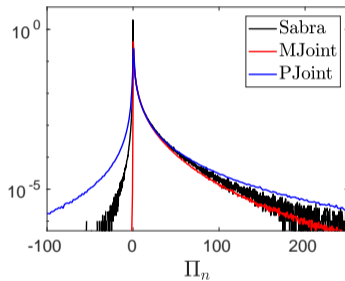


$n=14$

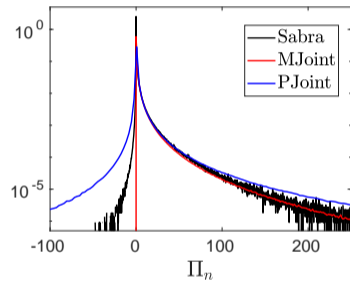
Single-time closures



$n=9$



$n=11$



$n=12$

Conditioning to modules of **three closest** shells:

$$\mathcal{U}_0 = 2^{z_0} e^{i(\frac{\pi}{2} + \alpha_{-1} + \alpha_{-2})}, \quad (36)$$

$$\mathcal{U}_1 = 2^{z_1} e^{i(\frac{\pi}{2} + \alpha_0 + \alpha_{-1})}, \quad (37)$$

$$\mathbf{z} = (z_0, z_1) \sim g(\mathbf{z} | \log_2 |\mathcal{U}_{-3}(\tau - \Delta\tau)|, \log_2 |\mathcal{U}_{-2}(\tau - \Delta\tau)|, \log_2 |\mathcal{U}_{-1}(\tau - \Delta\tau)|), \quad (38)$$

Conditioning to modules and phases of **themselves**:

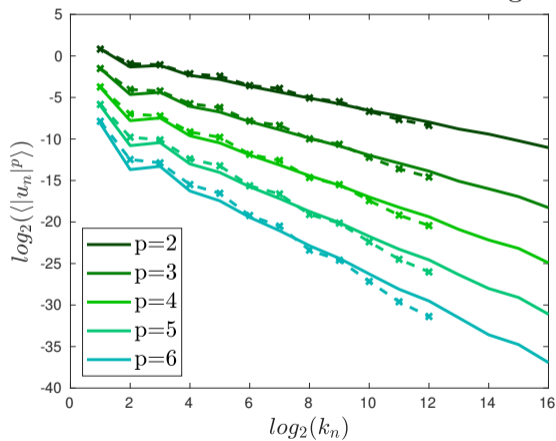
$$\mathcal{U}_0 = 2^{z_0} e^{i(z_1 + \alpha_{-1} + \alpha_{-2})}, \quad (39)$$

$$\mathcal{U}_1 = 2^{z_2} e^{i(z_3 + \alpha_0 + \alpha_{-1})}, \quad (40)$$

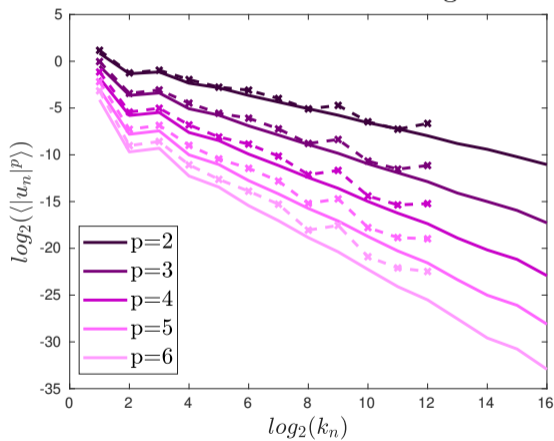
$$\mathbf{z} = (z_0, z_1, z_2, z_3) \sim g(\mathbf{z} | \log_2 |\mathcal{U}_0(\tau - \Delta\tau)|, \Delta_0, \log_2 |\mathcal{U}_1(\tau - \Delta\tau)|, \Delta_1). \quad (41)$$

Time conditioning, $\Delta\tau = 2.4$

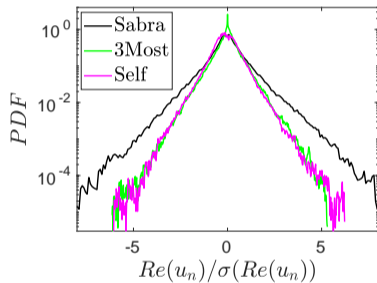
Three-closest conditioning



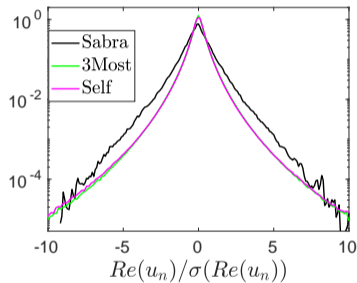
Self conditioning



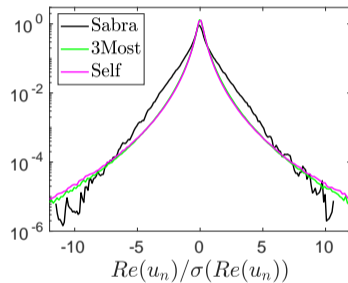
Time conditioning



$n=12$

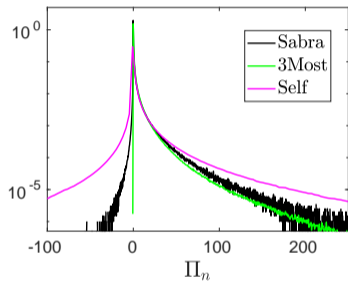


$n=13$

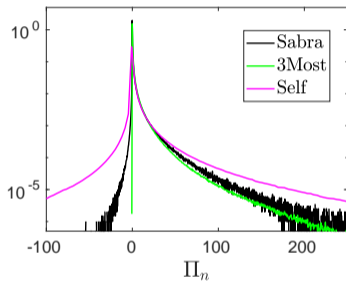


$n=14$

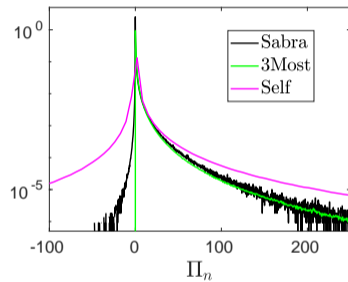
Time conditioning



$n=9$



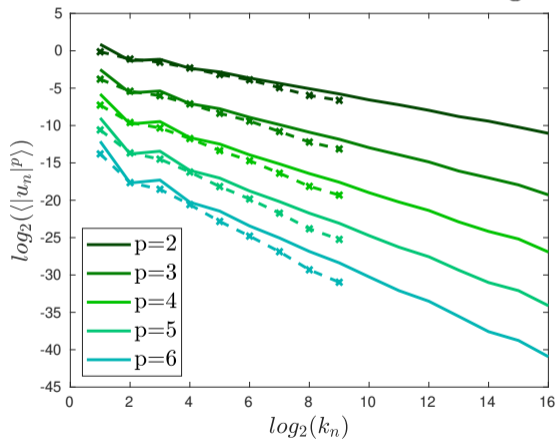
$n=11$



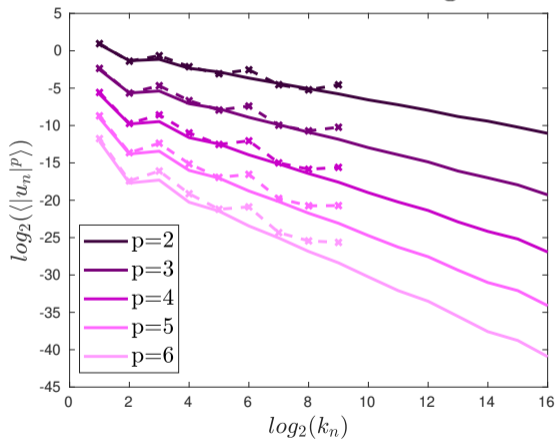
$n=12$

Time conditioning, $\Delta\tau = 2.4$

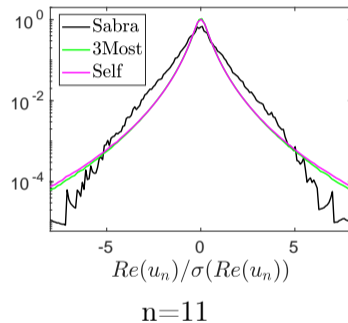
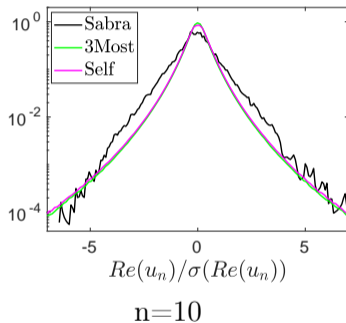
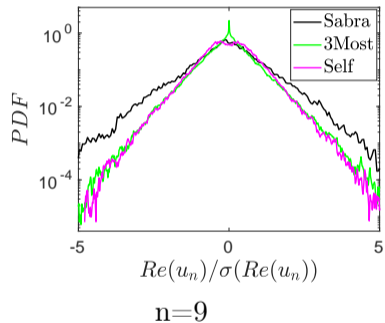
Three-closest conditioning



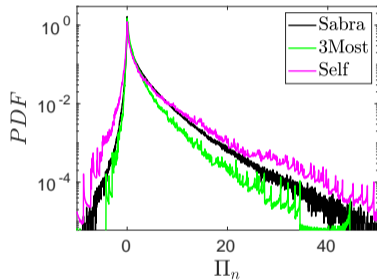
Self conditioning



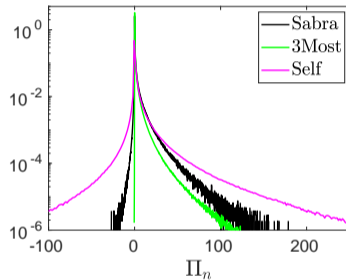
Time conditioning



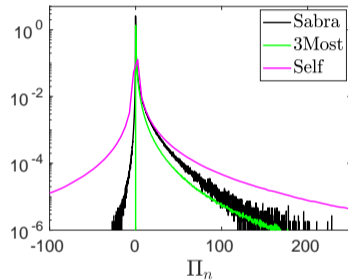
Time conditioning



$n=4$



$n=8$

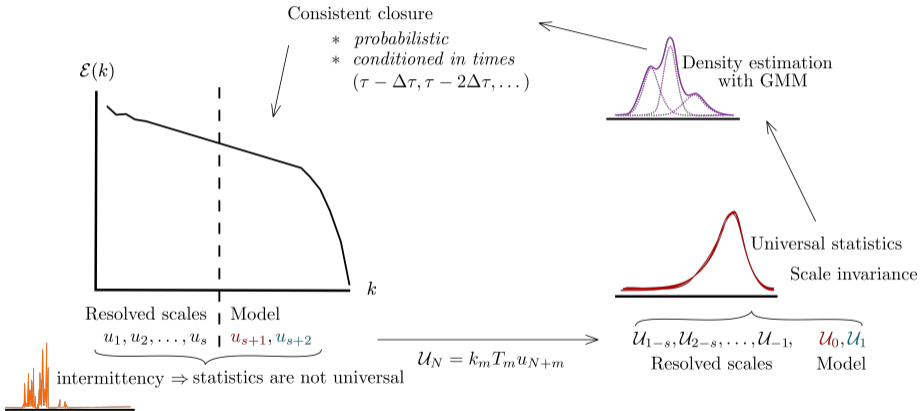


$n=9$

All results

	$ \mathcal{U}_0 $	$ \mathcal{U}_1 $	Δ_0	Δ_1	Conditioning
Half closure	2^{z_0}	$ \mathcal{U}_0 \lambda^{-1/3}$	$\pi/2$	$\pi/2$	\times
Joint	2^{z_0}	2^{z_1}	$\pi/2$	$\pi/2$	\times
Simple cond	2^{z_0}	$ \mathcal{U}_0 \lambda^{-1/3}$	$\pi/2$	$\pi/2$	$ \mathcal{U}_{-1} $ at $\tau - \Delta\tau$
Joint cond	2^{z_0}	2^{z_1}	$\pi/2$	$\pi/2$	$ \mathcal{U}_{-1} $ at $\tau - \Delta\tau$
3-Clos	2^{z_0}	2^{z_1}	$\pi/2$	$\pi/2$	$ \mathcal{U}_{-3} , \mathcal{U}_{-2} , \mathcal{U}_{-1} $ at $\tau - \Delta\tau$
3-Clos 9	2^{z_0}	2^{z_1}	$\pi/2$	$\pi/2$	$ \mathcal{U}_{-3} , \mathcal{U}_{-2} , \mathcal{U}_{-1} $ at $\tau - \Delta\tau$
Long	2^{z_0}	2^{z_1}	$\pi/2$	$\pi/2$	$ \mathcal{U}_{-s} , \dots, \mathcal{U}_{-1} $ at $\tau - \Delta\tau$
Joint phases	2^{z_0}	2^{z_2}	z_1	z_3	\times
Joint cond phases	2^{z_0}	2^{z_2}	z_1	z_3	$ \mathcal{U}_{-1} , \Delta-1$ at $\tau - \Delta\tau$
Self	2^{z_0}	2^{z_2}	z_1	z_3	$ \mathcal{U}_0 , \mathcal{U}_1 , \Delta_0, \Delta_1$ at $\tau - \Delta\tau$
Self 9	2^{z_0}	2^{z_2}	z_1	z_3	$ \mathcal{U}_0 , \mathcal{U}_1 , \Delta_0, \Delta_1$ at $\tau - \Delta\tau$
Global	2^{z_0}	2^{z_2}	z_1	z_3	$ \mathcal{U}_{-2} , \mathcal{U}_{-1} , \Delta_{-2}, \Delta_{-1}$ at τ $ \mathcal{U}_{-2} , \mathcal{U}_{-1} , \mathcal{U}_0 , \mathcal{U}_1 , \Delta_{-2}, \Delta_{-1}, \Delta_0, \Delta_1$ at $\tau - \Delta\tau$
2 Times	2^{z_0}	2^{z_2}	z_1	z_3	$ \mathcal{U}_{-2} , \mathcal{U}_{-1} , \Delta_{-2}, \Delta_{-1}$ at τ $ \mathcal{U}_{-2} , \mathcal{U}_{-1} , \mathcal{U}_0 , \mathcal{U}_1 , \Delta_{-2}, \Delta_{-1}, \Delta_0, \Delta_1$ at $\tau - \Delta\tau$ $ \mathcal{U}_{-2} , \mathcal{U}_{-1} , \mathcal{U}_0 , \mathcal{U}_1 , \Delta_{-2}, \Delta_{-1}, \Delta_0, \Delta_1$ at $\tau - 2\Delta\tau$

Road map



- We have systematically written data-based closures (**probabilistic** and **time-correlated**) for shell models
- Time-correlated closures are working with the present approach
- They may work much better with a better approximation of the densities (other ML tools)
- High-dimensional problems are a significant step in this ladder
- This framework reduced black-box aspects

Thank you!

