

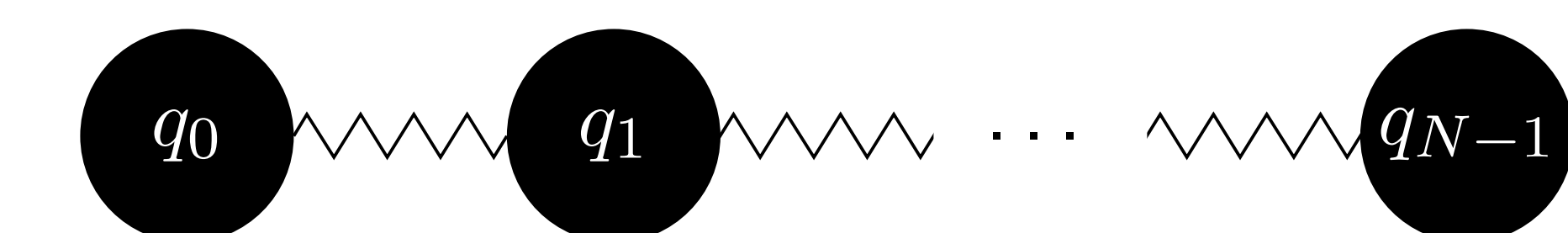
Relaxation in the strongly nonlinear β -FPUT chain for small N

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Introduction

Fermi-Pasta-Ulam-Tsingou (FPUT) systems are one-dimensional chains of N masses and springs with nonlinear interactions.



In this study, nearest neighbors interact with harmonic potentials (weighted by α) and quartic terms (weighted by ξ):

$$V = \sum_{i=1}^{N-1} \left[\frac{\alpha}{2} (q_i - q_{i-1})^2 + \frac{\xi}{2} (q_i - q_{i-1})^4 \right]$$

The complicated dynamics of these systems motivated one of the world's first numerical computer simulations in 1954¹. In strongly nonlinear cases, studies from theoretical perspectives remain a major challenge today. Here, we present one method for overcoming these challenges.

Motivations:

Autocorrelation functions (ACFs) describe how initial conditions continue to influence the system over time. If this influence declines, the system is said to relax. Can we compute these ACFs without simulation? The Recurrence Relations Method (RRM) does this, but can yield non-convergent results. Are there ways around this issue?

Goals:

We aim to apply the RRM to small FPUT chains in the canonical ensemble, try to mitigate the limitations of the method as best we can, and compare results with numerical simulations.

Theory^{2,3}

We perturb the chain with an impulse p_0 to the first particle. How will its momentum $p_0(t)$ evolve over time? First, expand $p_0(t)$ in a Hilbert space, with basis bearing initial conditions and coefficients bearing the weight these conditions carry over time:

$$p_0(t) = \sum_{n=0}^{d-1} a_n(t) f_n$$

Theory^{2,3} (cont.)

A recurrence relation generates the next basis vector from the previous two:

$$f_{n+1} = \hat{L} f_n + \Delta_n f_{n-1}$$

➤ L is the Liouvillian operator:

$$\hat{L} f = \sum_{i=0}^{N-1} \left(\frac{\partial H}{\partial p_i} \frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial f}{\partial p_i} \right)$$

➤ Δ_n is the recurrent:

$$\Delta_n \equiv \frac{|f_n|^2}{|f_{n-1}|^2} \equiv \frac{\int f_n^2 e^{-\beta H} d\mathbf{p} d\mathbf{q}}{\int f_{n-1}^2 e^{-\beta H} d\mathbf{p} d\mathbf{q}}$$

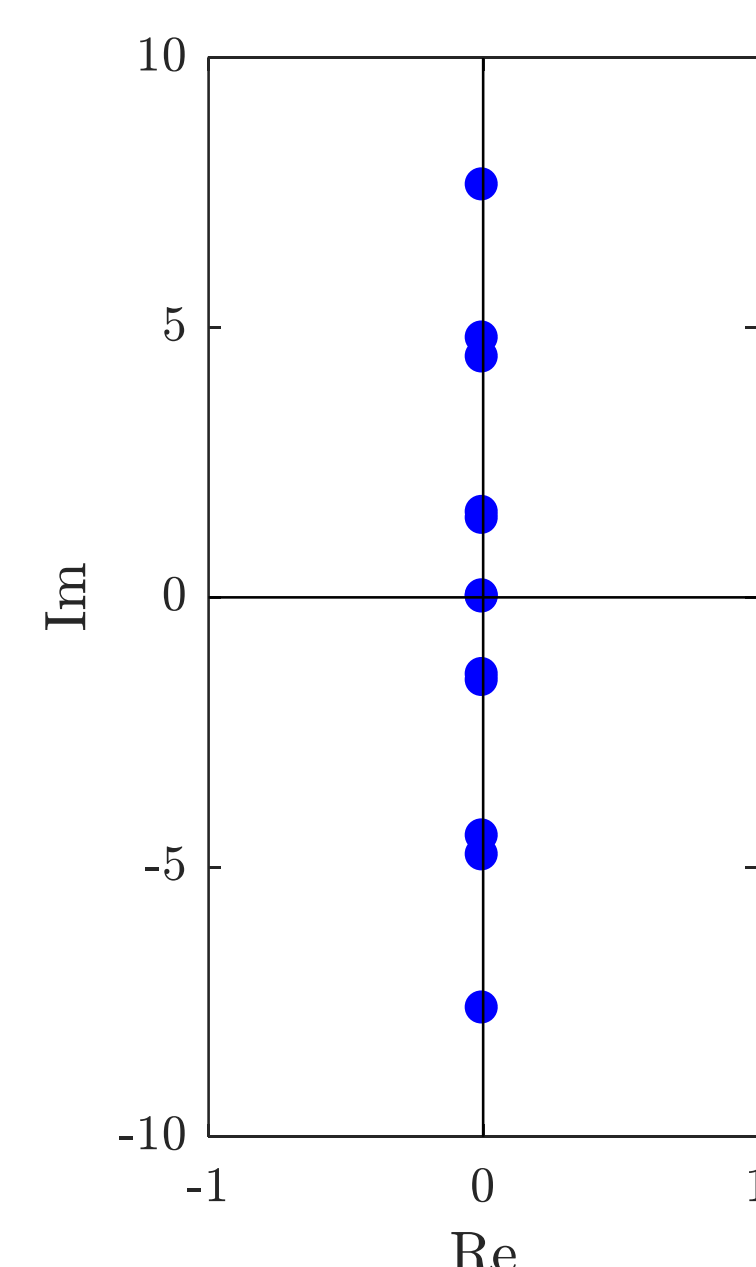
If we set the first basis vector $f_0 = p_0$, then the first coefficient $a_0(t)$ becomes the ACF for $p_0(t)$. The Laplace transform of the ACF, $a_0(z)$, is a continued fraction:

$$a_0(z) = \frac{1}{z + \frac{\Delta_1}{z + \frac{\Delta_2}{z + \dots}}}$$

The ACF itself is then the inverse Laplace transform of the continued fraction:

$$a_0(t) = \frac{1}{2\pi i} \lim_{t \rightarrow \infty} \int_{\gamma-it}^{\gamma+it} a_0(z) e^{zt} dz$$

This is a complex contour integral. By the residue theorem, the result depends on the singularities (or poles) of $a_0(z)$ in the complex plane. These poles turn out to be located symmetrically on the imaginary axis at $\pm i\omega_k$, as shown.



Poles in $a_0(z)$.

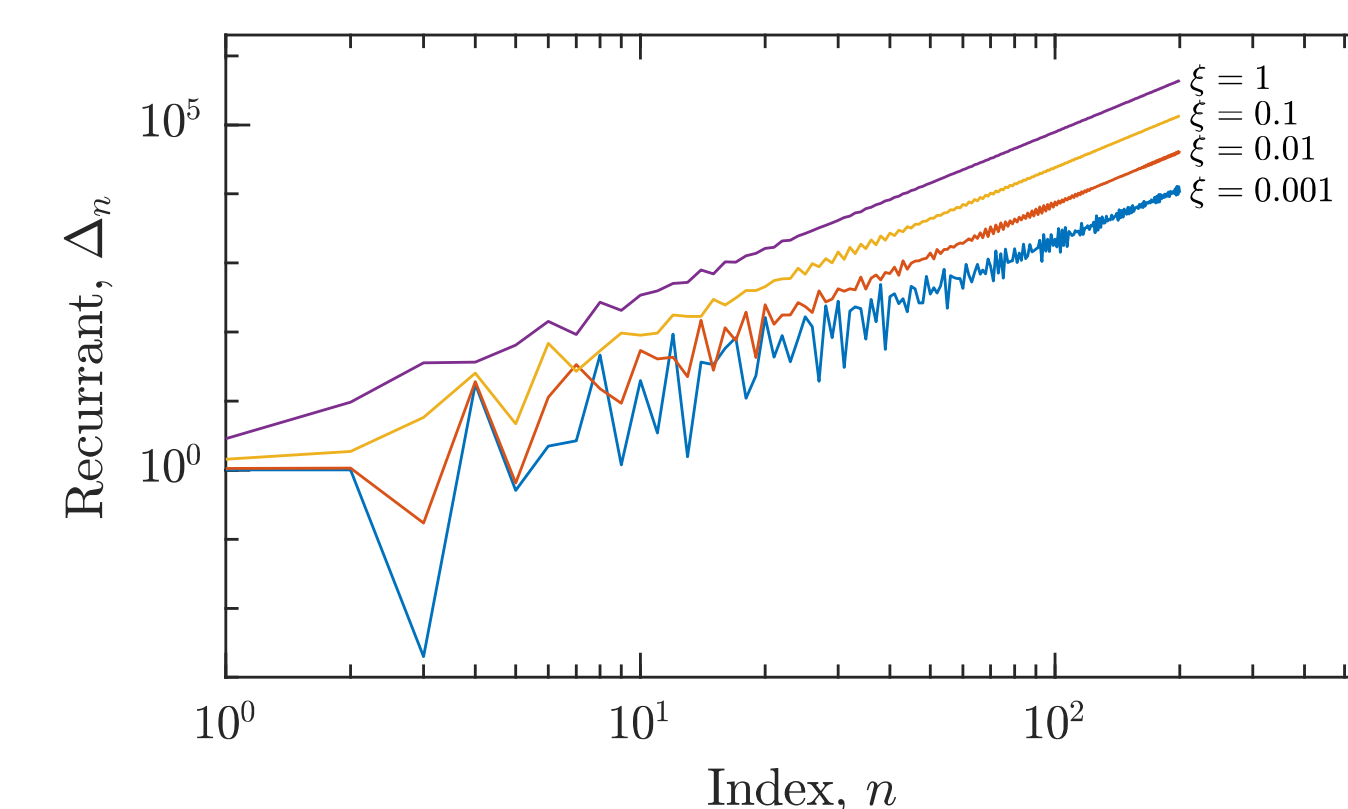
Because of this, summing the residues yields a real cosine series for the ACF:

$$a_0(t) = \sum_k A_k \cos(\omega_k t)$$

The ACF's frequencies ω_k are given by the locations of the continued fraction's poles.

Results

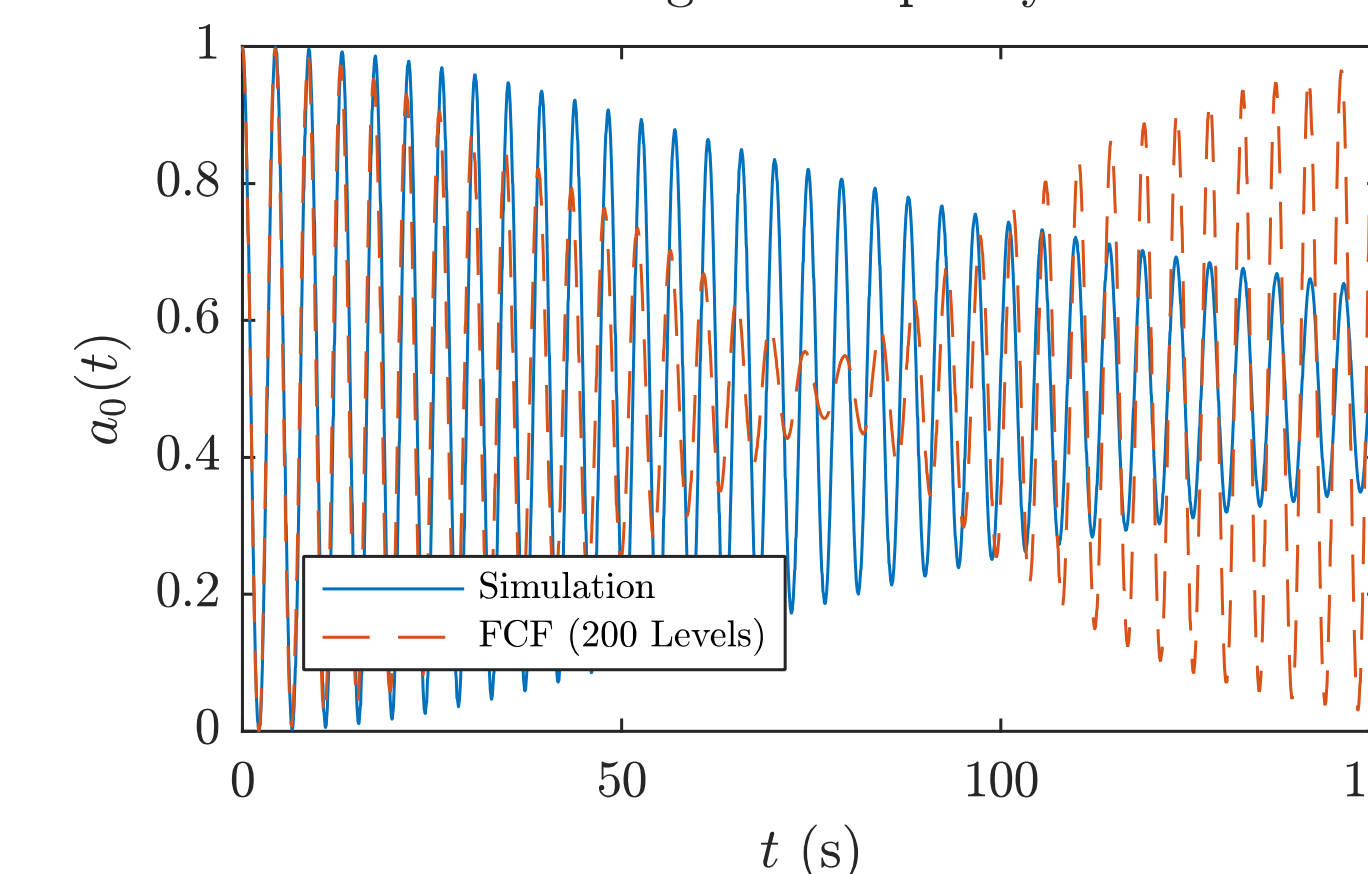
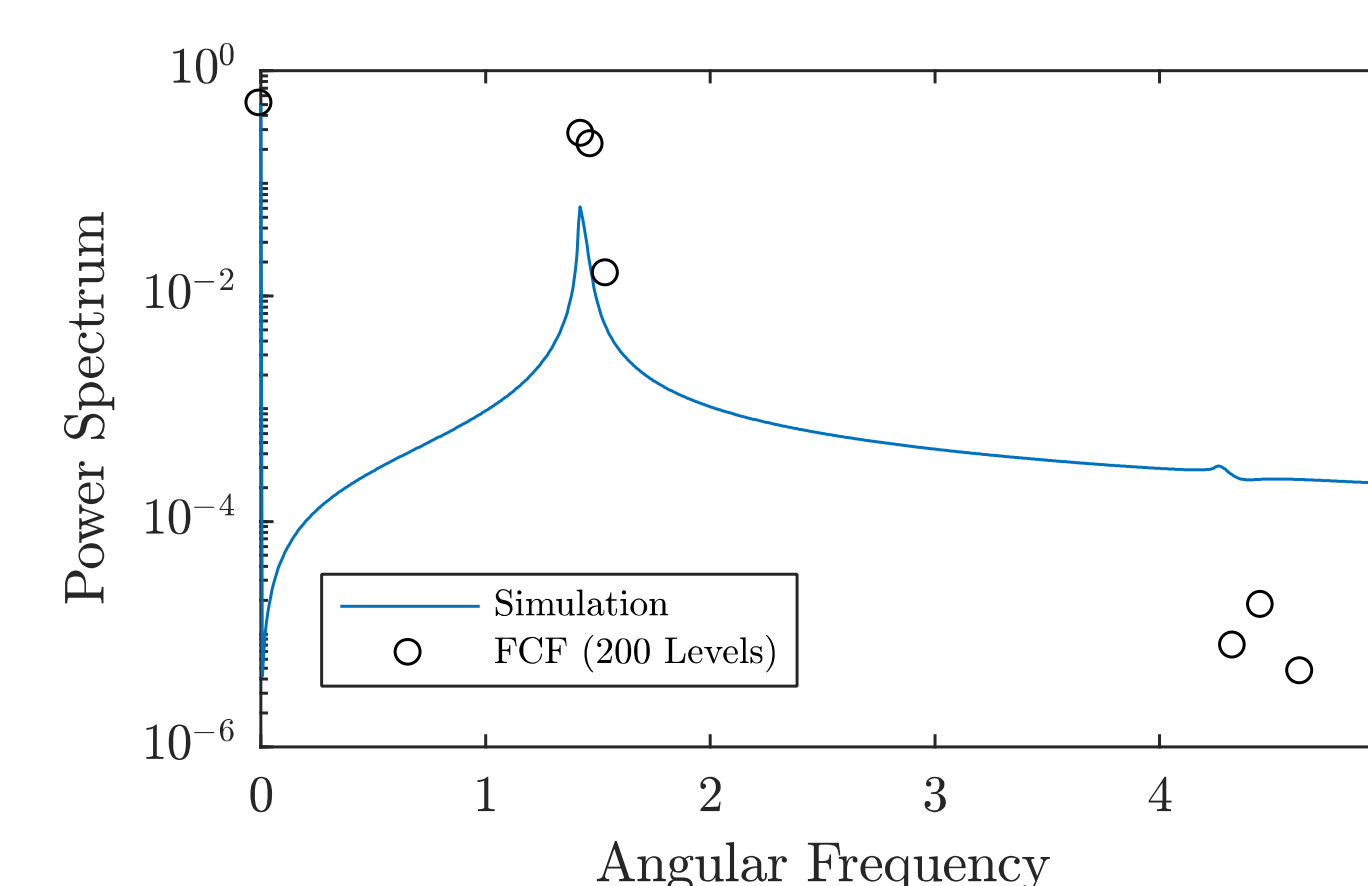
Using Maple, we have currently obtained 200 recurrants for $N = 2$ (shown below).



Recurrants for $N = 2$ and several ξ .

Recurrants follow a power law trend $\Delta_n \approx an^b$, and best fits show $b \approx 2.5$. However, for growth rates $b > 2$, the continued fraction is **non-convergent**⁴!

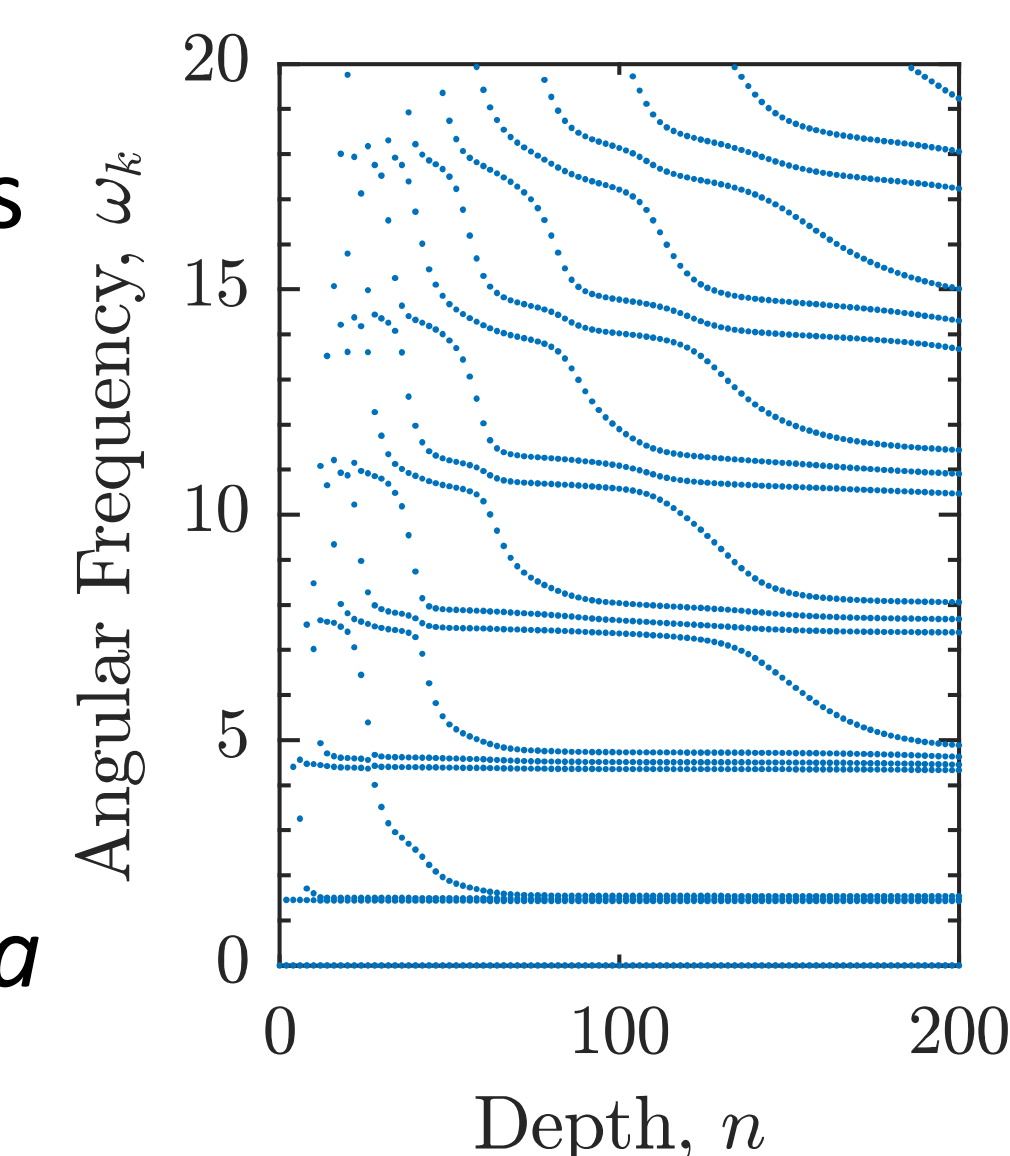
- Truncation to a finite continued fraction (FCF) is not expected to work.
- What if we try truncating anyway, at the best depth we can achieve?



ACF from 200 levels, for $N = 2$ and $\xi = 0.01$.

The frequency agreement is OK, but relaxation (decay envelope) is missing. The **shape** of the frequency spectrum is **not captured** by the discrete poles of the FCF.

- What happens to these frequencies (and imaginary poles) as the fraction gets deeper?

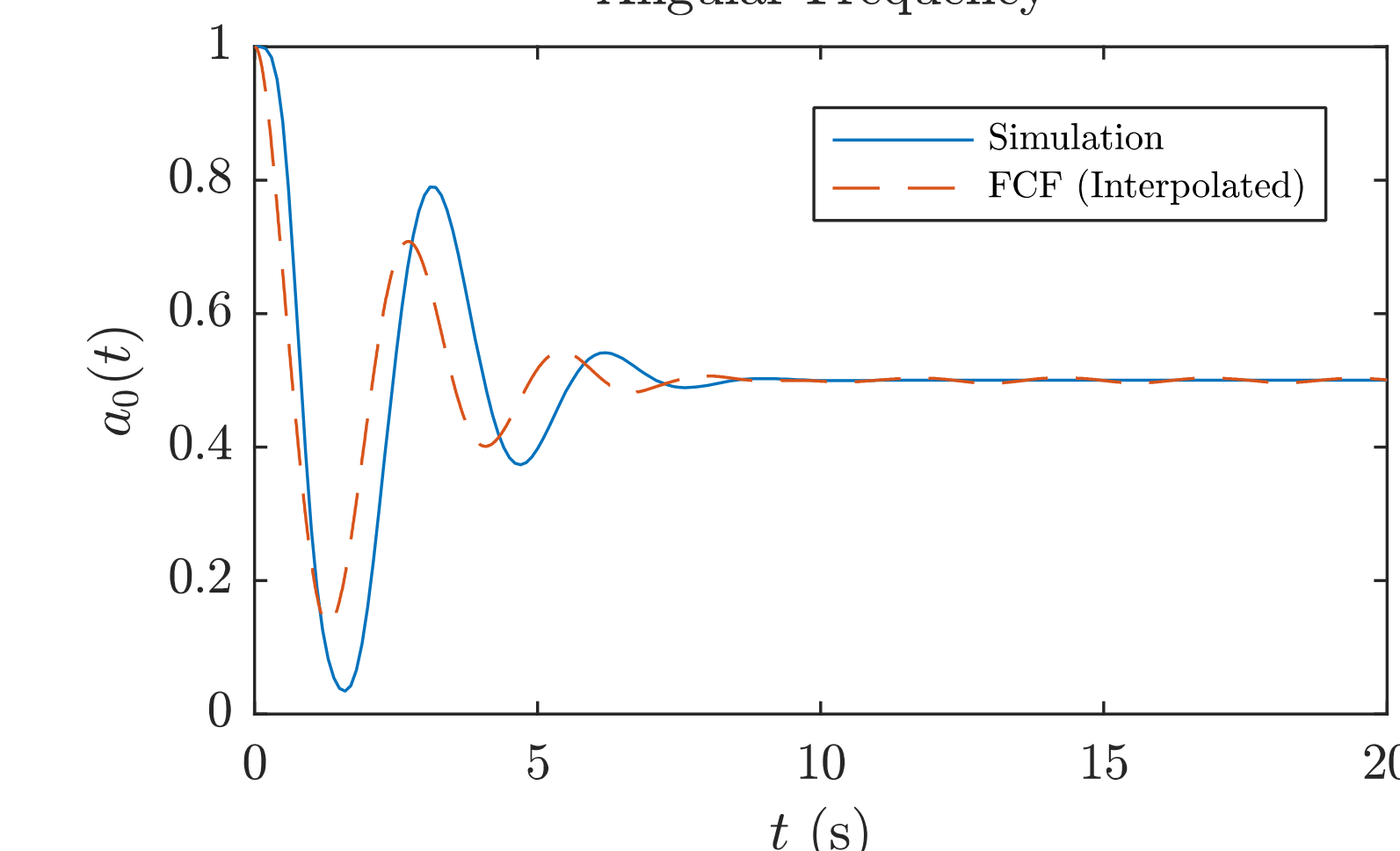
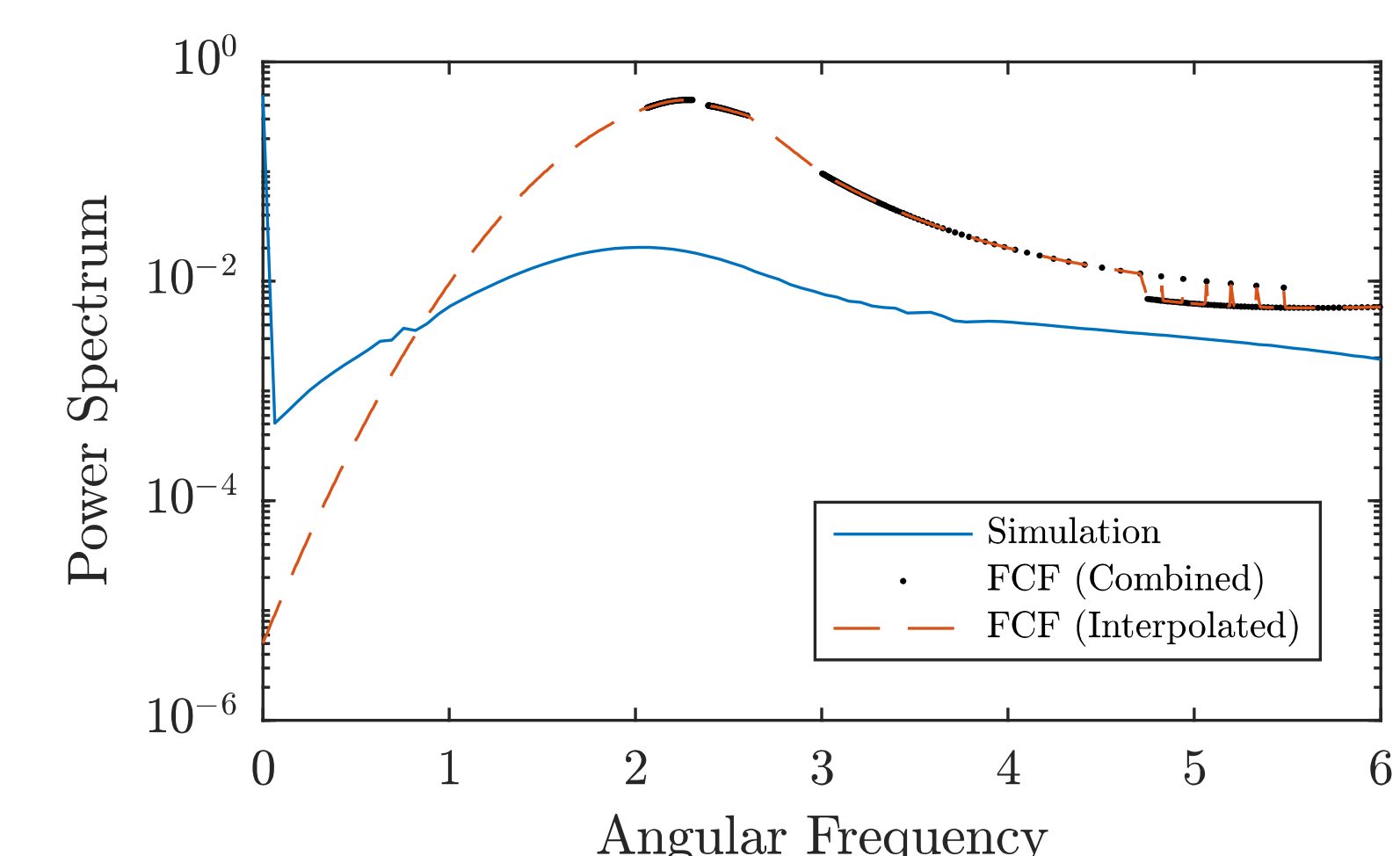


Poles in FCF as a function of depth.

Results (cont.)

Poles appear in **clusters**, consistent across many levels. How can we fill out these clusters with more poles? Our approach:

- Compute poles from **all** available truncation depths individually.
- Combine all sets into one spectrum.
- Interpolate between combined poles.
- Use inverse discrete cosine transform (IDCT) to recover the time domain ACF.



ACF from interpolation, for $N = 2$ and $\xi = 1$.

Conclusion

The Recurrence Relations Method allows us to compute autocorrelation functions in the FPUT chain by casting the Laplace transform of the ACF as a continued fraction. By combining results from many truncation depths, we are able to recover approximate ACFs which compare well with simulation in the strongly nonlinear regime despite the formal non-convergence of the continued fraction. Future work includes extending this approach to other systems and developing more novel fitting techniques in the combined frequency spectra.

References

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- [2] H. Mori, Prog. Theor. Phys. **34** (1965).
- [3] M.H. Lee, Phys. Rev. B **26** (1982).
- [4] S. Sen, Physica A **360** (2006).