

Contents

Dedication	iii
Abstract	iv
Kurzfassung	v
1 Introduction	1
1.1 Computational Sciences	1
1.2 Scientific Machine Learning	3
1.3 Turbulence and fusion	4
1.3.1 Pathway to fusion energy and the role of turbulence in it	5
1.3.2 Modeling turbulence in fusion devices	6
1.3.3 Derivation	7
1.3.4 2D Hasegawa-Wakatani to 2D Navier-Stokes	11
1.4 Large Eddy Simulation	12
1.4.1 Neural Networks in LES	12
1.5 Building Scientific Machine Learning Simulation Benchmarks	13
1.5.1 Structure of this dissertation	14
2 The Hasegawa-Wakatani model of drift-wave turbulence	15
2.1 Practical Introduction	15
2.2 Modified Hasegawa-Wakatani	16
2.3 Phases of the HW Model	17
2.3.1 Initialization	17
2.3.2 Linear Phase	18
2.3.3 Turbulent Phase	18
2.4 Discretization of the HW model	19
2.4.1 Complexity	19
2.4.2 Adiabatic Coefficient c_1	20
2.4.3 Drive strength κ	21
2.4.4 Viscosity coefficient ν and order N	21
2.4.5 Box size	22
2.4.6 Boundary conditions	22
2.4.7 Spatial resolution	22
2.5 Numerical Methods	23

3	Quantitative analysis of the Hasegawa-Wakatani model	30
3.1	Scalar properties	31
3.1.1	Turbulent Particle Flux: Γ_n	31
3.1.2	Primary counteracting sink: Γ_c	32
3.1.3	Remaining Sinks	32
3.1.4	Energy and Enstrophy	33
3.2	Temporal Properties	33
3.3	Spectral Properties	33
3.3.1	Spectral description $\Gamma_n(k_y)$	34
3.4	Data Generation	35
3.4.1	Hyperparameter Spaces	35
3.5	Empirical model for Γ_n	42
4	Applying machine learning to physical simulations	44
4.1	Contextualization	44
4.2	Theory	44
4.3	Accelerating LES with the help of NNs	46
4.4	Implementation	47
4.4.1	ResNet	47
4.4.2	UNet	49
4.4.3	Loss Calculation	49
4.4.4	Temporal unrolling	50
4.4.5	Early stopping	51
4.4.6	Data Selection	51
4.4.7	Data pre-processing	52
4.4.8	Normalizations	52
5	A data-driven model for Hasegawa-Wakatani	54
5.1	The potential-based surrogate correction (PSC)	54
5.2	Flow of information through the hybrid network	55
5.3	Explored parameter space	57
5.3.1	Step type	57
5.3.2	Step size	57
5.3.3	Learning rate and optimizer	57
5.3.4	Batch sizes	58
5.3.5	Different unrolling for loss and validation	58
5.3.6	Include diffusion	58
5.3.7	Adjusted standard deviation	58
5.4	Limitations	59
5.4.1	Reducing Physical Resolution	59
5.4.2	An empirical look at the effects of lossy compression in HW2D	61

6	Evaluating the Results	67
6.1	The drawbacks of physical space evaluations	67
6.1.1	Autocorrelations	68
6.1.2	Autocorrelations in lowerscale space	71
6.2	On challenges and achievements of long-term stability	74
6.2.1	Reaching stable and visually identical results	74
6.2.2	Comparing physical space losses	76
6.3	Timetraces	77
6.4	Averages	79
6.4.1	Evaluating average values	79
6.5	Spectral Comparisons	82
6.5.1	Physical Spectra	82
6.5.2	Spectral Turbulent Particle Flux $\Gamma_n(k_y)$	86
6.5.3	Spectral Phase Shift	88
6.6	Comparison of statistical distributions	90
6.6.1	Methodology	90
6.6.2	Distributions: Γ_n	92
6.6.3	Distributions: Γ_c	94
6.6.4	Distributions: $\partial_t E$	95
6.6.5	Distributions: $\partial_t U$	97
6.6.6	Final words on the almost ideal simulator	98
6.7	Evaluation of the model	99
7	Conclusion	101
7.1	Summary	101
7.2	Outlook	104
	List of Figures	107
	List of Tables	111
	Bibliography	112