Equivariance and generalization in neural networks

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Based on: S. Bulusu, M. Favoni, A. Ipp, D. I. Müller, D. Schuh, *Preprint* (2021) [2103.14686]

Code: gitlab.com/openpixi/scalar-ml

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Doktoratskolleg Particles and Interactions

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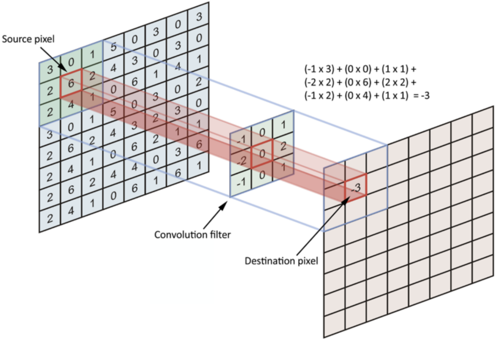
- Convolutional neural networks (CNNs) incorporate translational symmetry under certain circumstances
- Investigate generalization capabilities in terms of different lattice sizes and different physical parameters

CNNs



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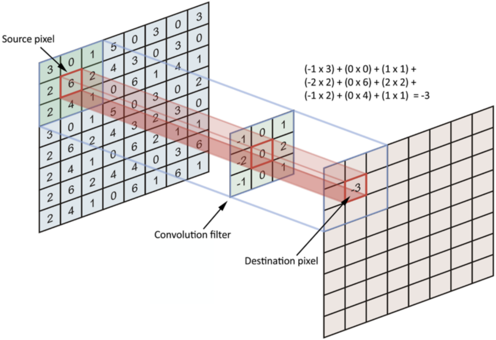
CNNs



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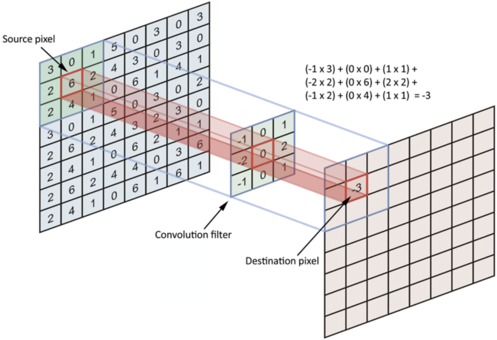
- Equivariance vs invariance

CNNs



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- Equivariance before a global pooling layer is a sufficient condition for output invariance

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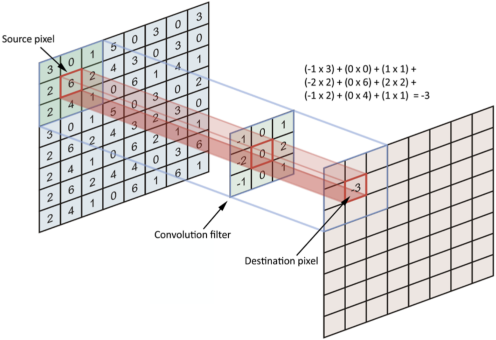

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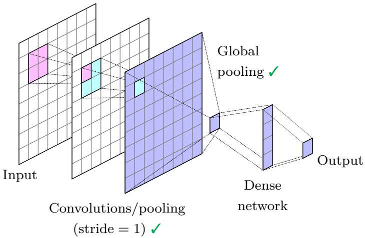
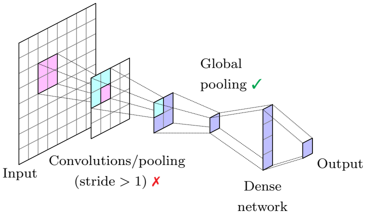
- Equivariance vs invariance
- Equivariance before a global pooling layer is a sufficient condition for output invariance
- Does translational symmetry make a significant difference?

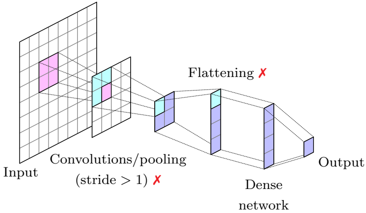
Architecture types



Equivariant architecture (EQ)



Strided architecture (ST)



Flattening architecture (FL)

Physical system

- Complex scalar field in 1+1D with nonzero chemical potential

$$S = \int \mathrm{d}x_0 \mathrm{d}x_1 \left(|D_0 \phi|^2 - |\partial_1 \phi|^2 - m^2 |\phi|^2 - \lambda |\phi|^4 \right), \quad D_0 = \partial_0 - i\mu \tag{1}$$

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- Discretized action

$$S_{lat} = \sum_x \left(\eta|\phi_x|^2 + \lambda|\phi_x|^4 - \sum_{\nu=1}^{2} \left(e^{\mu\,\delta_{\nu,2}} \phi_x^* \phi_{x+\hat{\nu}} + e^{-\mu\,\delta_{\nu,2}} \phi_x^* \phi_{x-\hat{\nu}} \right) \right), \quad \eta = 2D + m^2 \tag{2}$$

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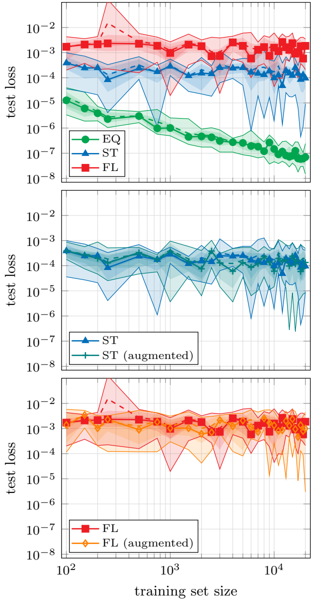
- Sign problem solved by a dual formulation: $\phi_x \to \{k_{x,\nu}, l_{x,\nu}\}$ integer fields, Gattringer, Kloiber, arxiv:1206.2954
- Regression task: predicting observables

$$n = \frac{1}{N} \sum_x k_{x,2}, \qquad |\phi|^2 = \frac{1}{N} \sum_x \frac{W(f_x + 2)}{W(f_x)} \tag{3}$$

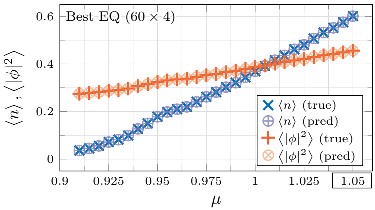
$$f_x = \sum_\nu [|k_{x,\nu}| + |k_{x-\hat{\nu},\nu}| + 2(l_{x,\nu} + l_{x-\hat{\nu},\nu})], \quad W(f_x) = \int_0^\infty \mathrm{d}x\, x^{f_x+1} \mathrm{e}^{-\eta x^2 - \lambda x^4} \tag{4}$$

Architecture comparison



- Systematic architecture search with optuna, Akiba et al., arxiv:1907.10902
- 10 instances of the winning architectures are retrained from scratch for various training set size
- EQ beats ST and FL for any number of training samples
- EQ improves with more samples, while the other two do not
- Data augmentation does not help the two non-equivariant architectures

Silver blaze phase transition



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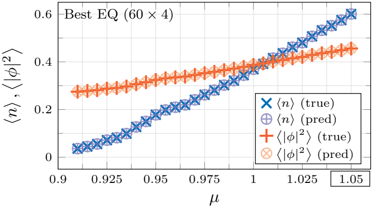
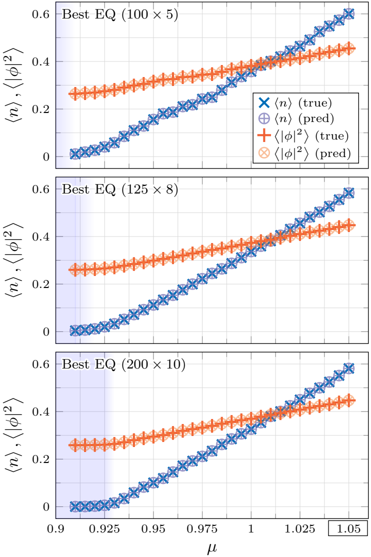
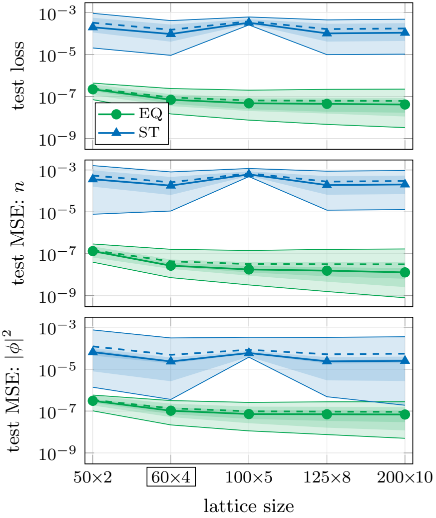


Training on both phases is not necessary as long as the expression of the observables is independent of the transition

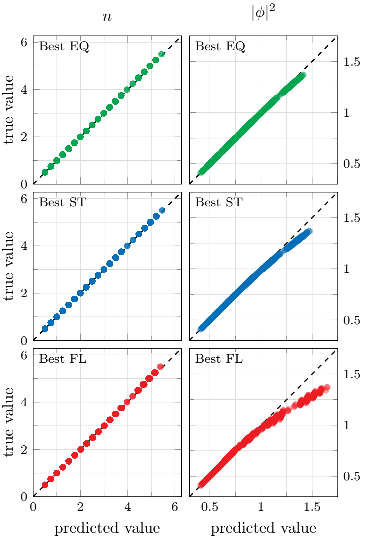


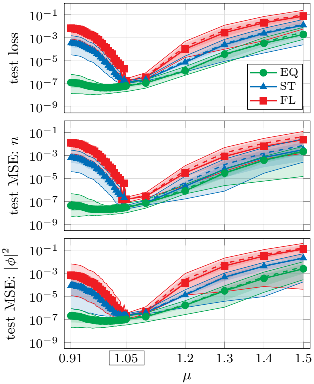
Generalization to other lattice sizes and physical parameters



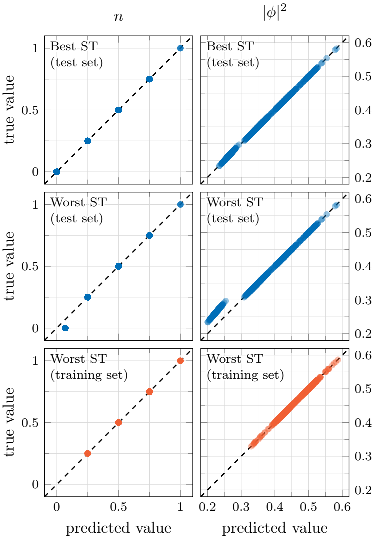
- FL cannot be tested on different lattice sizes
- Training only on 60×4
- Kink in ST at 100×5 due to $s = 2$ in spatial pooling layer
- EQ clearly outperforms ST
- Problem already tackled in literature with an FL trained on both phases on 200×10 reaching test loss of 10^{-6}

Extrapolation to larger chemical potentials





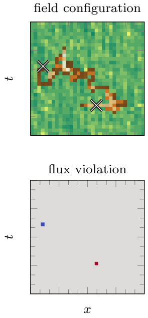
Why do ST and FL fail?



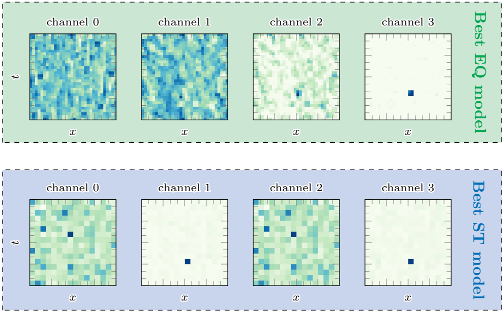
- Worst performing ST instance predicts correctly when tested on $\mu = 1.05$
- Mispredicts values not present in the training set
- Best ST generalizes well
- No EQ instance features a behavior like worst ST

Detecting flux violations

The field k obeys the conservation law $\sum_\nu \left(k_{x,\nu} - k_{x-\hat{\nu},\nu}\right) = 0$. We artificially created flux violations to be detected by the models.



(a) Example field configuration

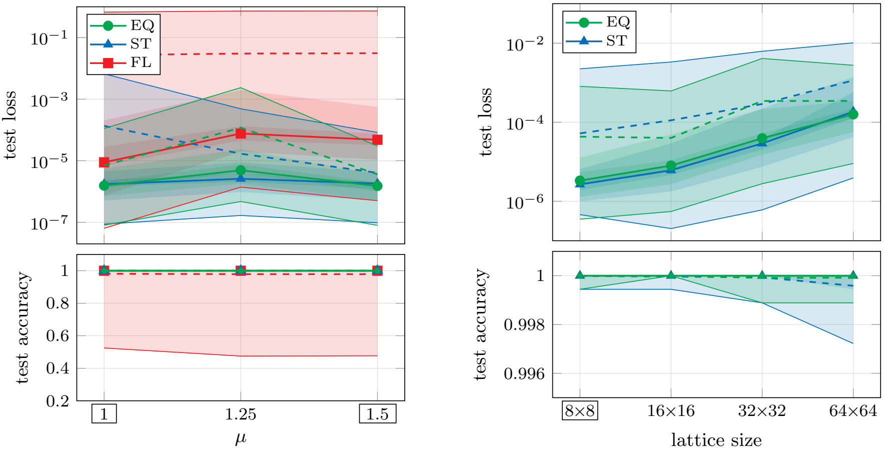


(b) Feature maps of convolutional network in best EQ and ST models

- 2x2 convolutions are necessary for this task
- Similar approach with optuna

Results

Training at $(\eta, \mu) = (4.25, 1)$ and $(4.01, 1.5)$ on 8x8 lattice with $N_{train} = 4000$; testing at $\eta \in \{4.01, 4.04, 4.25\}$, $\mu \in \{1, 1.25, 1.5\}$ on 4 lattice sizes



Counting flux violations

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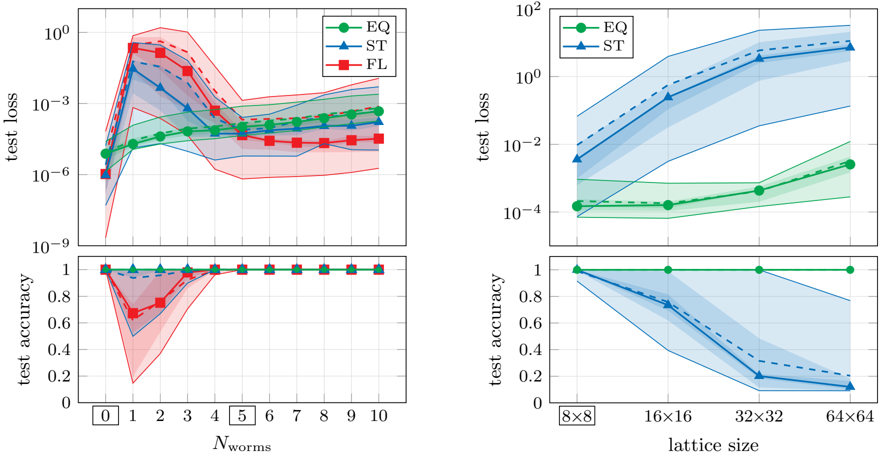

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- In all tasks EQ proved to be a highly reliable choice
- Optuna favoured architectures with $< 10^5$ parameters
- Remarkable generalization capabilities of EQ

Backup slides

First task optuna winners

EQ	ST	FL
Conv(1 $\times$ 1, 4, 64) LeakyReLU Conv(1 $\times$ 1, 64, 48) LeakyReLU Conv(1 $\times$ 1, 48, 80) LeakyReLU Conv(2 $\times$ 2, 80, 80) LeakyReLU GlobalAvgPool Linear(80, 2)	Conv(1 $\times$ 1, 4, 80) LeakyReLU Conv(1 $\times$ 1, 80, 80) LeakyReLU Conv(1 $\times$ 1, 80, 48) LeakyReLU AvgPool(2 $\times$ 2, 2) Conv(2 $\times$ 2, 48, 80) LeakyReLU GlobalAvgPool Linear(80, 2)	Conv(1 $\times$ 1, 4, 64) LeakyReLU Conv(2 $\times$ 2, 64, 80) LeakyReLU AvgPool(2 $\times$ 2, 2) Conv(1 $\times$ 1, 80, 48) LeakyReLU Conv(2 $\times$ 2, 48, 64) LeakyReLU AvgPool(2 $\times$ 2, 2) Conv(1 $\times$ 1, 64, 24) Flatten Linear(360, 24) LeakyReLU Linear(24, 2)
33202	26370	47394

Second task optuna winners

EQ	ST	FL
Conv(2 × 2, 4, 32) LeakyReLU Conv(1 × 1, 32, 32) LeakyReLU GlobalMaxPool Linear(32, 32) LeakyReLU Linear*(32, 1) Sigmoid	Conv*(2 × 2, 4, 16) LeakyReLU MaxPool(2 × 2, 2) Conv(1 × 1, 16, 16) LeakyReLU Conv(1 × 1, 16, 8) LeakyReLU GlobalMaxPool Linear*(8, 32) Linear(32, 1) Sigmoid	Conv*(3 × 3, 4, 8) LeakyReLU MaxPool(2 × 2, 2) Conv(2 × 2, 8, 32) LeakyReLU AvgPool(2 × 2, 2) Conv(2 × 2, 32, 32) LeakyReLU Flatten Linear*(128, 1) Sigmoid
2657	953	5600

The star (e.g. Conv*) indicates that the bias in that layer is set to 0

Third task EQ optuna winners

1st EQ	2nd EQ	3rd EQ
Conv(1×1, 4, 32)	Conv(2×2, 4, 8)	Conv(1×1, 4, 4)
LeakyReLU	LeakyReLU	LeakyReLU
Conv(2×2, 32, 8)	Conv(2×2, 8, 8)	Conv(2×2, 4, 8)
LeakyReLU	LeakyReLU	LeakyReLU
Conv(2×2, 8, 16)	Conv(1×1, 8, 4)	Conv(2×2, 8, 4)
LeakyReLU	LeakyReLU	LeakyReLU
Conv(1×1, 16, 8)	Conv(1×1, 4, 8)	Conv(3×3, 4, 1)
LeakyReLU	LeakyReLU	LeakyReLU
GlobalSumPool	GlobalSumPool	GlobalSumPool
Linear(8, 1)	Linear(8, 1)	
1800	456	308

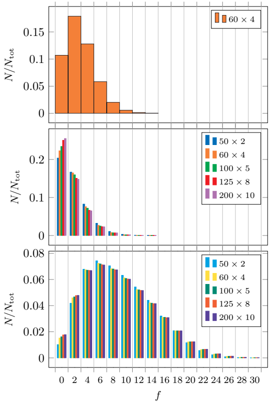
Third task ST optuna winners

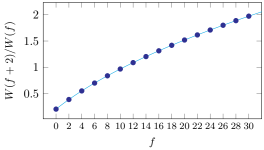
1st ST	2nd ST	3rd ST
Conv(2×2, 4, 16)	Conv(2×2, 4, 4)	Conv(2×2, 4, 4)
LeakyReLU	LeakyReLU	LeakyReLU
Conv(1×1, 16, 32)	MaxPool(2×2, 2)	AvgPool(2×2, 2)
LeakyReLU	Conv(2×2, 4, 4)	Conv(3×3, 4, 16)
Conv(1×1, 32, 32)	LeakyReLU	LeakyReLU
LeakyReLU	GlobalSumPool	GlobalSumPool
AvgPool(2×2, 2)	Linear(4, 1)	Linear(16, 32)
Conv(1×1, 32, 8)		LeakyReLU
LeakyReLU		Linear(32, 1)
GlobalSumPool		
Linear(8, 32)		
LeakyReLU		
Linear(32, 1)		
2336	132	1184

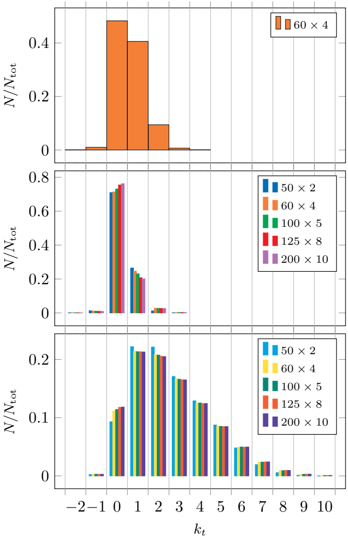
Third task FL optuna winners

1st FL	2nd FL	3rd FL
Conv(2×2, 4, 4)	Conv(2×2, 4, 8)	Conv(2×2, 4, 32)
LeakyReLU	LeakyReLU	LeakyReLU
AvgPool(2×2, 2)	AvgPool(2×2, 2)	AvgPool(2×2, 2)
Conv(3×3, 4, 8)	Conv(3×3, 8, 4)	Conv(3×3, 32, 4)
LeakyReLU	LeakyReLU	LeakyReLU
AvgPool(2×2, 2)	AvgPool(2×2, 2)	AvgPool(2×2, 2)
Flattening	Flattening	Flattening
Linear(8, 4)	Linear(4, 4)	Linear(4, 32)
LeakyReLU	LeakyReLU	LeakyReLU
Linear(4, 32)	Linear(4, 32)	Linear(32, 16)
LeakyReLU	LeakyReLU	LeakyReLU
Linear(32, 1)	Linear(32, 1)	Linear(16, 1)
640	640	2704

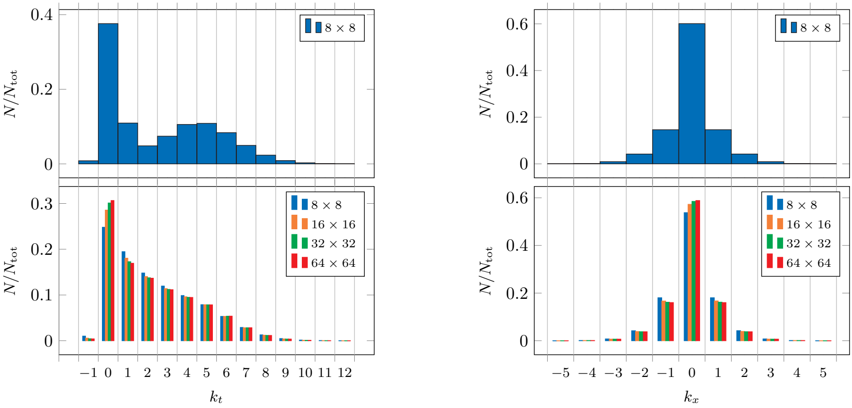
First task data distribution



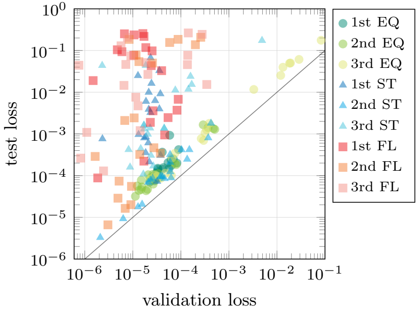


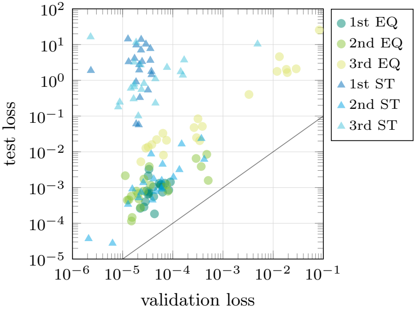


Third task data distribution



Third task: test loss vs validation loss





Test loss vs validation loss table

	validation loss on 8×8		test loss on 8×8		test loss up to 64×64	
	mean	**median**	**mean**	**median**	**mean**	**median**
1st EQ	$\mathbf{4.676 \times 10^{-5}}$	4.137×10^{-5}	$\mathbf{2.108 \times 10^{-4}}$	1.483×10^{-4}	$\mathbf{1.008 \times 10^{-3}}$	8.308×10^{-4}
2nd EQ	1.042×10^{-4}	$\mathbf{2.440 \times 10^{-5}}$	3.525×10^{-4}	$\mathbf{8.783 \times 10^{-5}}$	1.807×10^{-3}	$\mathbf{7.936 \times 10^{-4}}$
3rd EQ	8.992×10^{-3}	3.072×10^{-4}	2.105×10^{-2}	9.163×10^{-4}	1.925	4.031×10^{-2}
1st ST	$\mathbf{2.331 \times 10^{-5}}$	2.173×10^{-5}	9.438×10^{-3}	3.576×10^{-3}	4.446	3.026
2nd ST	8.479×10^{-5}	4.372×10^{-5}	$\mathbf{2.545 \times 10^{-4}}$	$\mathbf{9.340 \times 10^{-5}}$	$\mathbf{3.738 \times 10^{-3}}$	$\mathbf{1.171 \times 10^{-3}}$
3rd ST	2.869×10^{-4}	$\mathbf{2.171 \times 10^{-5}}$	1.676×10^{-2}	1.381×10^{-3}	2.943	9.580×10^{-1}
1st FL	$\mathbf{2.602 \times 10^{-5}}$	1.787×10^{-5}	7.837×10^{-2}	3.817×10^{-2}	-	-
2nd FL	4.004×10^{-5}	1.117×10^{-5}	$\mathbf{5.300 \times 10^{-2}}$	$\mathbf{1.285 \times 10^{-3}}$	-	-
3rd FL	5.805×10^{-5}	$\mathbf{1.031 \times 10^{-5}}$	6.382×10^{-2}	3.556×10^{-2}	-	-