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NeuraSim Error Analysis

Antonio Giménez Nadal

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Obtaining the Results

NeuraSim Error Analysis

- The figures presented in this report can be generated using the data from Pando at:

*/scratch/daep/partage/NeuraSim_SharedCases/2021_08_17_VKrot_XX_A_XX_dx_0.3_RE_100_CFL
_0.2_REFERENCE_case_736/*

- And executing there the following script:

NeuraSim Error Analysis

```
from analysis.post_proc import *

in_dir = ['./results_cg/', './results_lt_grad_2_4/', './results_no_lt/', './results_nolt_3/', './results_nolt_grad_2_4/']

meta_analysis(in_dir, [forces_time], config_dir=['./'], y_lim=[-5, 3], meta_within_case=True)
meta_analysis(in_dir, [forces_time], config_dir=['./'], y_lim=[-5, 3], meta_within_alpha=True)

meta_analysis(in_dir, [forces_phase_diagram], in_ref='./reference/', config_dir=['./'], meta_within_case=True)
meta_analysis(['./results_cg/', './results_lt_grad_2_4/', './results_nolt_grad_2_4/'], [forces_phase_diagram], in_ref='./reference/', config_dir=['./'], meta=True)
meta_analysis(in_dir, [forces_phase_diagram], in_ref='./reference/', config_dir=['./'], precision=True) #Forcoefcient examples

meta_analysis(in_dir, [evaluate_precision], in_ref='./reference/', config_dir=['./'], meta=True)
meta_analysis(in_dir, [evaluate_precision], in_ref='./results_cg/', config_dir=['./'], meta=True)

meta_analysis(in_dir, [evaluate_performance], in_ref='./results_cg/', config_dir=['./'])

meta_analysis(in_dir, [divergence_time], config_dir=['./'], meta_within_case=True)
meta_analysis(in_dir, [divergence_timestep], config_dir=['./'])
```

Configuration of simulation

NeuraSim Error Analysis

- config_simulation.yaml

```
save_field_x_ite: 20
#####
# DISCRETIZATION #
#####
Nx: 736
Ny: 736
Nt: 10000
CFL: 0.2

#####
# SOLVER IA #
#####
ite_transition: 0
network_params:
    new_train: 'new'

#####
# NORMALIZATION #
#####
normalization:
    normalize: True
    scale_factor: 10.0

#####
# GEOMETRY #
#####
Lx: 224
Ly: 224
BC_domain_x: OPEN
BC_domain_y: STICKY
D: 15
xD: 75

#####
# PHYSICAL FORCES #
#####
Reynolds: 100.0
```

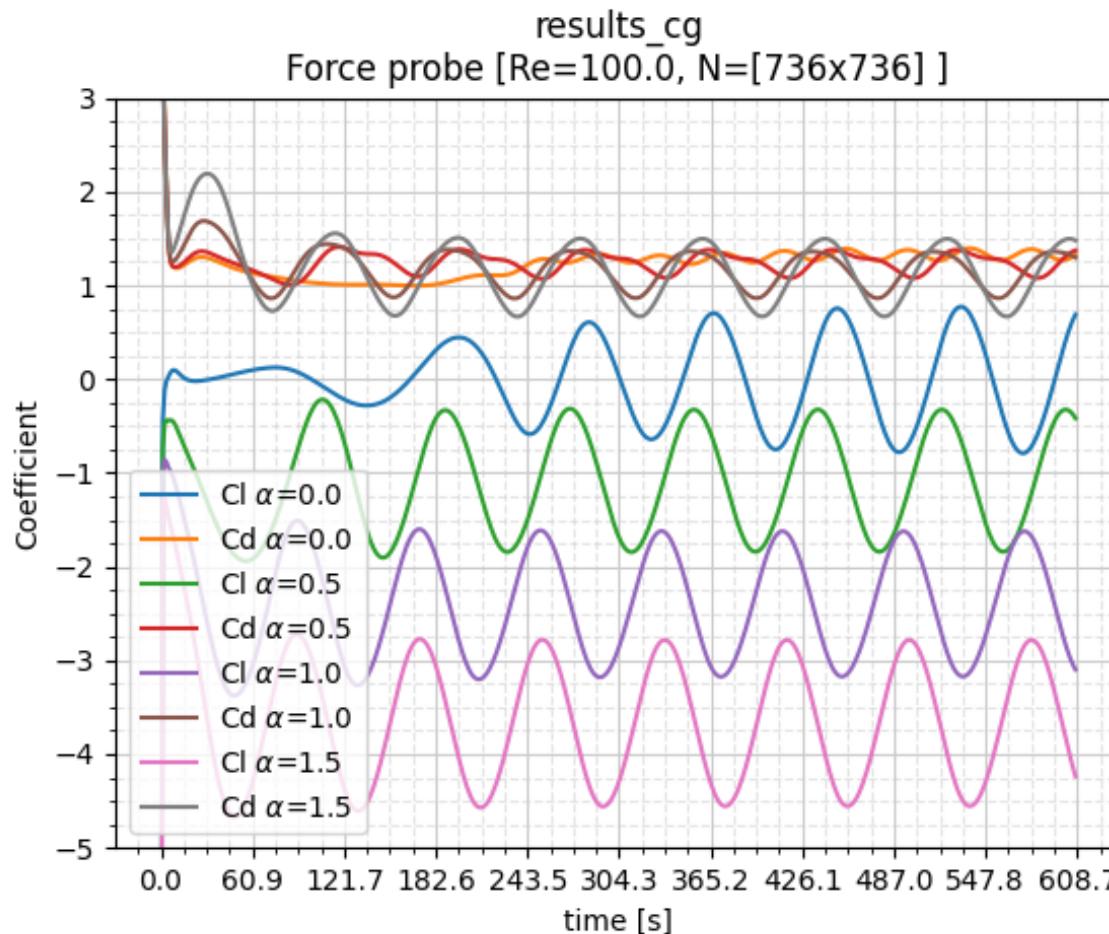
Results

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- Types of UNETS:
- no_lt: trained without long term only with the dataset [no_lt, nolt_3]
- no_lt_grad: trained with long term included but without having it differentiated [nolt_grad_2_4]
- lt_grad: trained with long term and also differentiated [lt_grad_2_4]

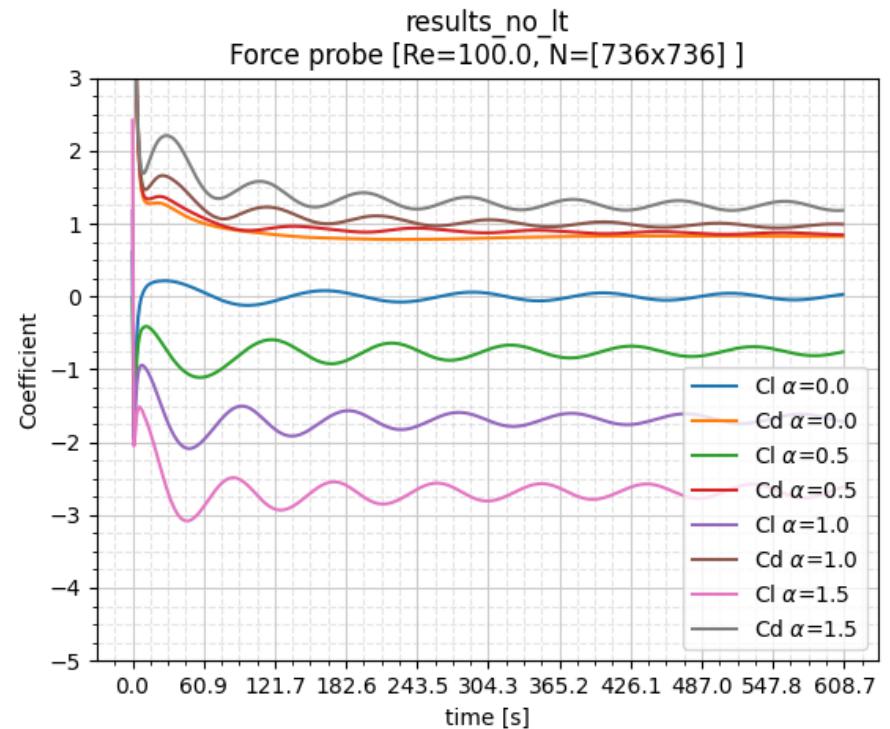
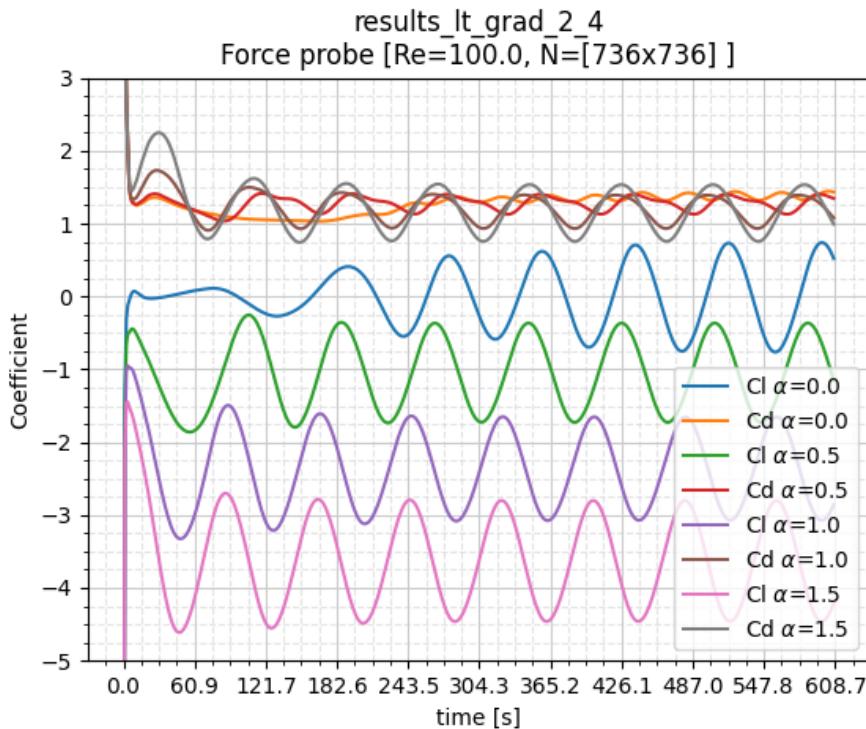
NeuraSim Error Analysis

- Let's view first the forces evolution over time for the different solvers



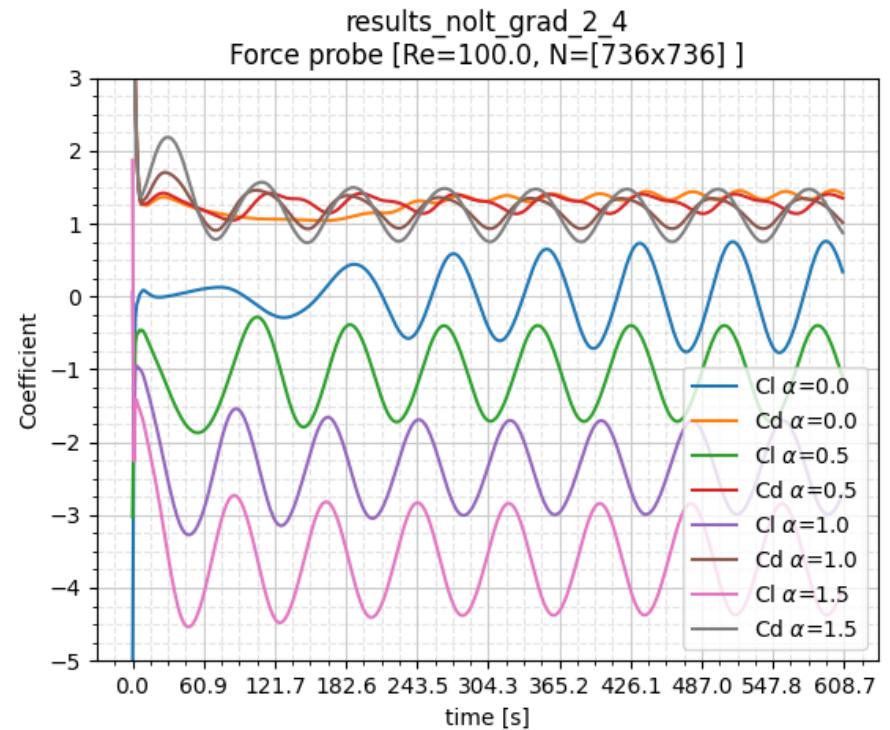
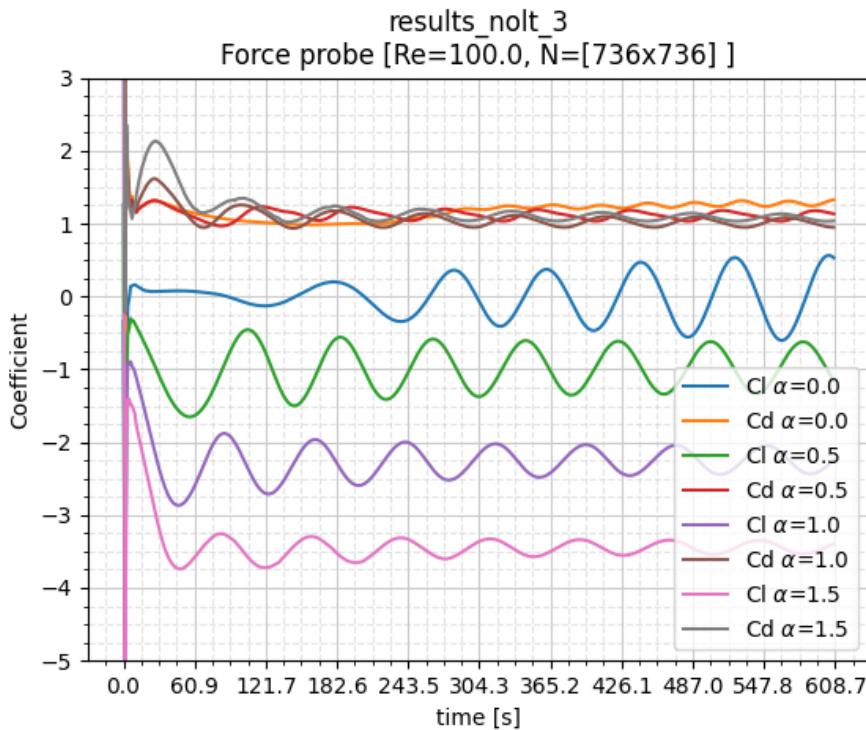
NeuraSim Error Analysis

- Let's view first the forces evolution over time for the different solvers



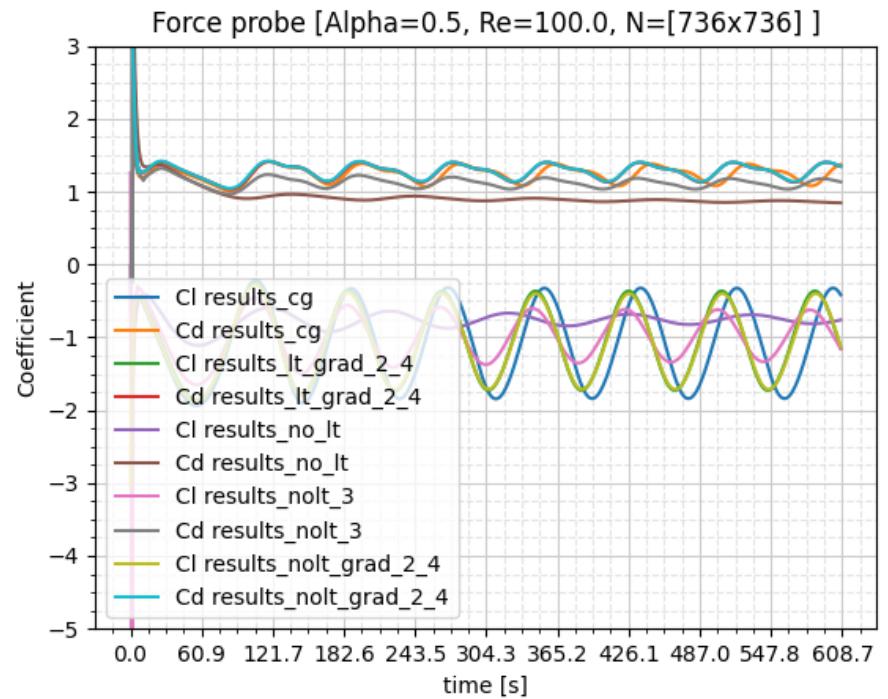
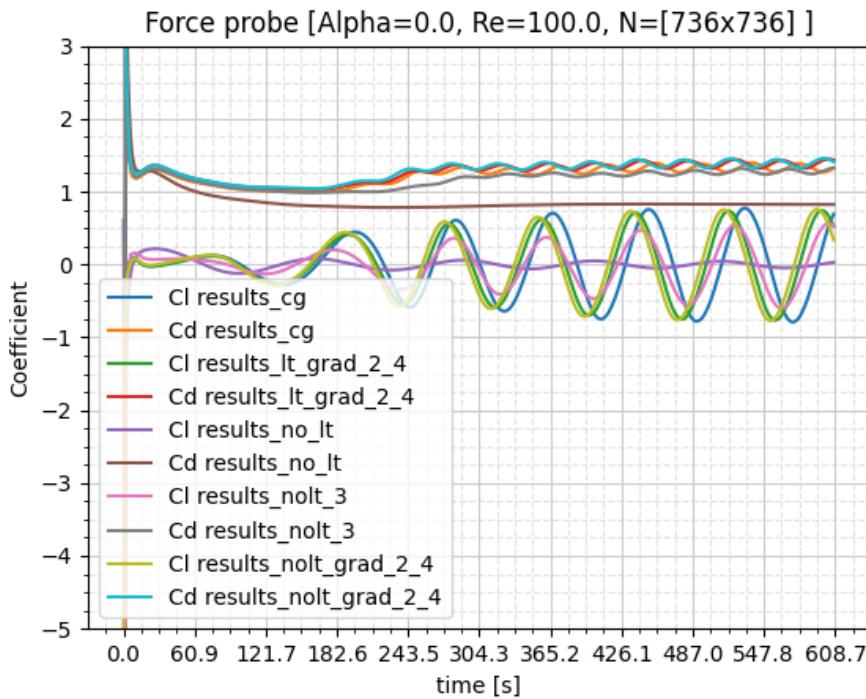
NeuraSim Error Analysis

- Let's view first the forces evolution over time for the different solvers



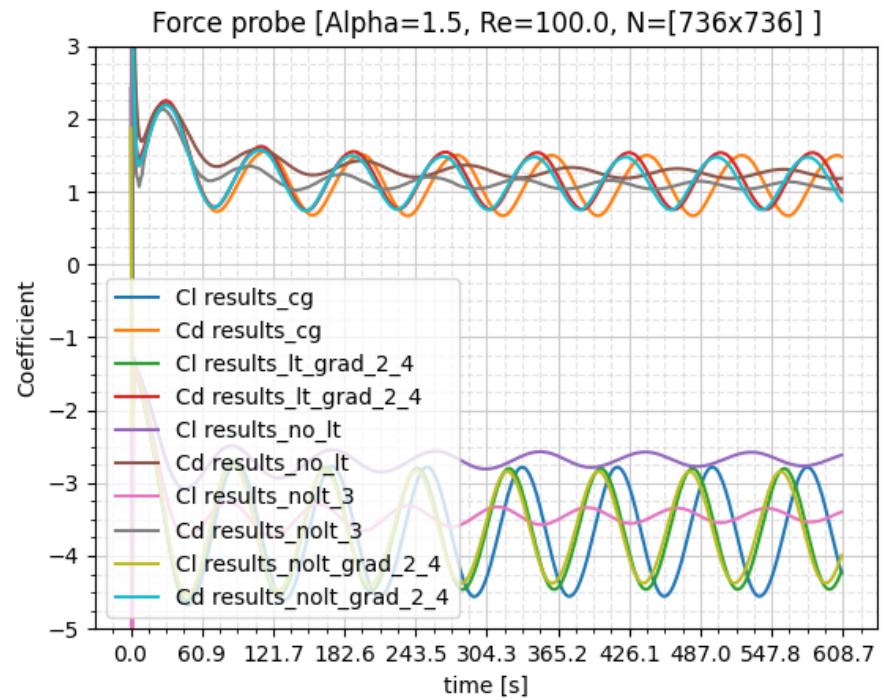
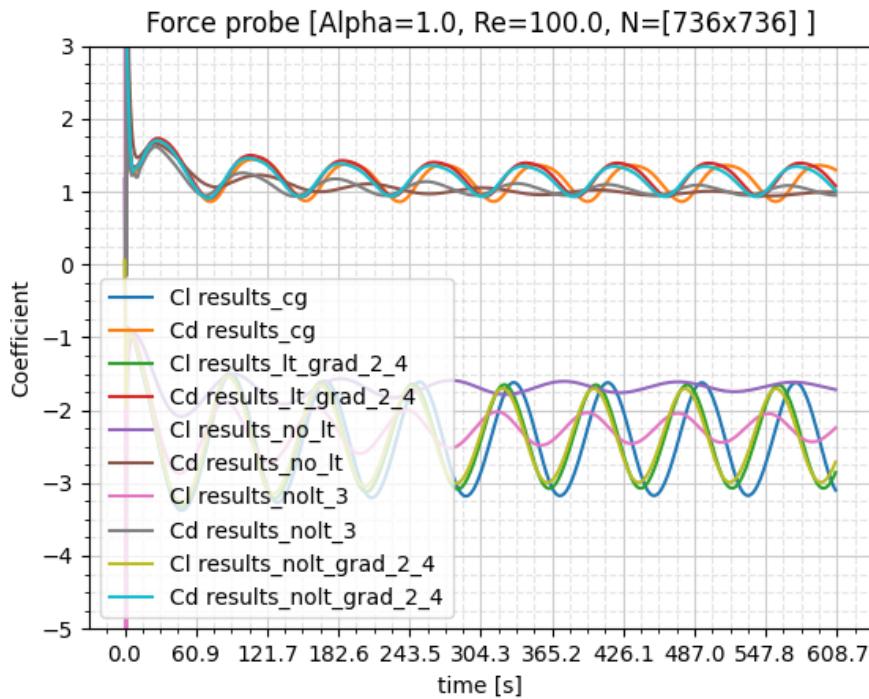
NeuraSim Error Analysis

- Or equivalently the same results but separated by alphas:



NeuraSim Error Analysis

- Or equivalently the same results but separated by alphas:

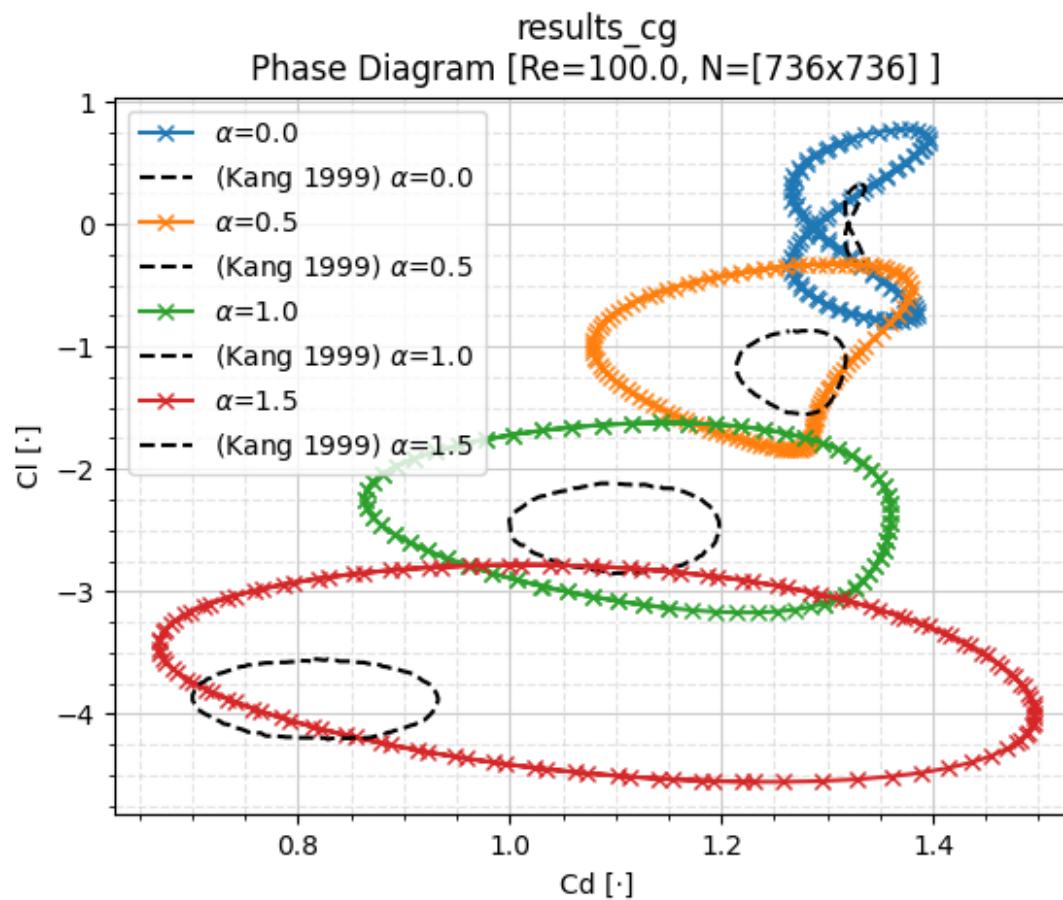


NeuraSim Error Analysis

- It appears that for all the alphas, the neural nets without long term have a significantly higher difference in amplitude compared with the rest of networks and the CG. And from what we know as ground true, a higher error. Checking in this way what was expected.
- Regarding the rest of the networks. Compared with the CG. It appears there is a phase difference. Being the CG more advance in time. While the rest of the networks, share an almost equal phase.

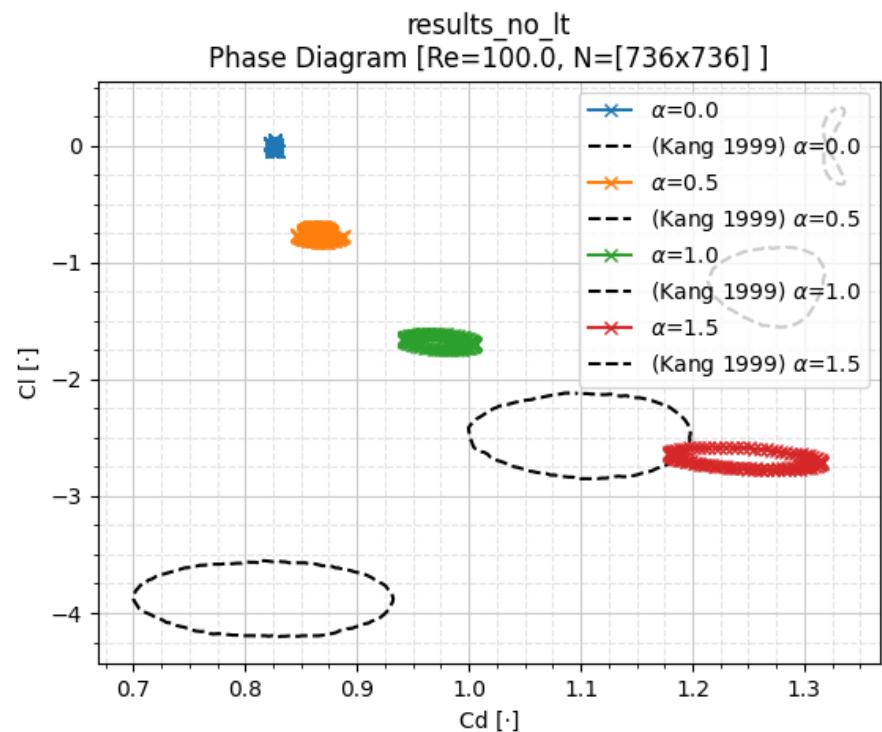
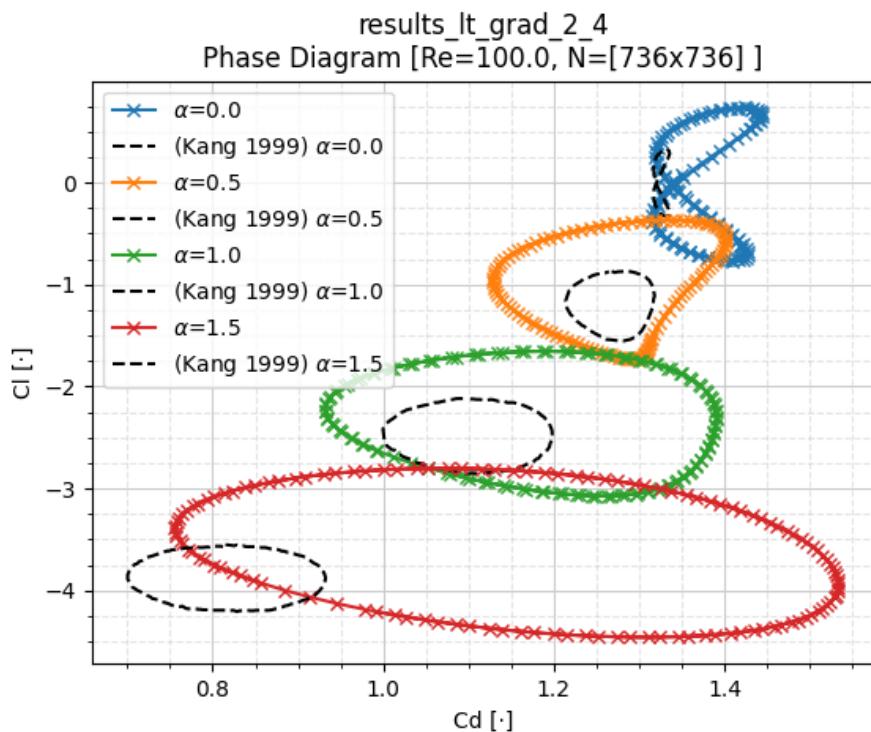
NeuraSim Error Analysis

- Next let's check the phase diagram



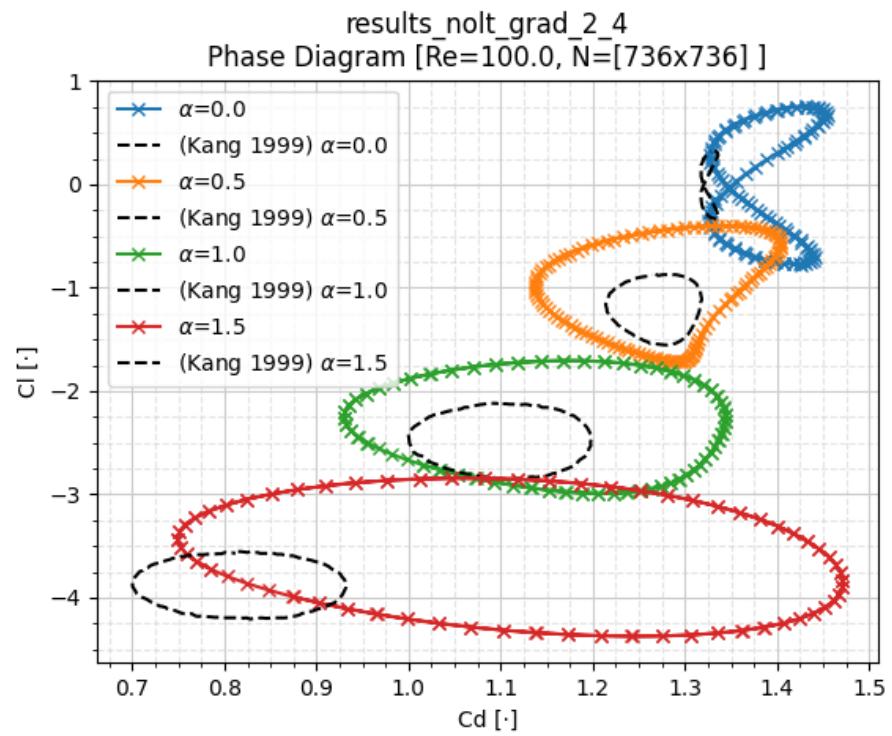
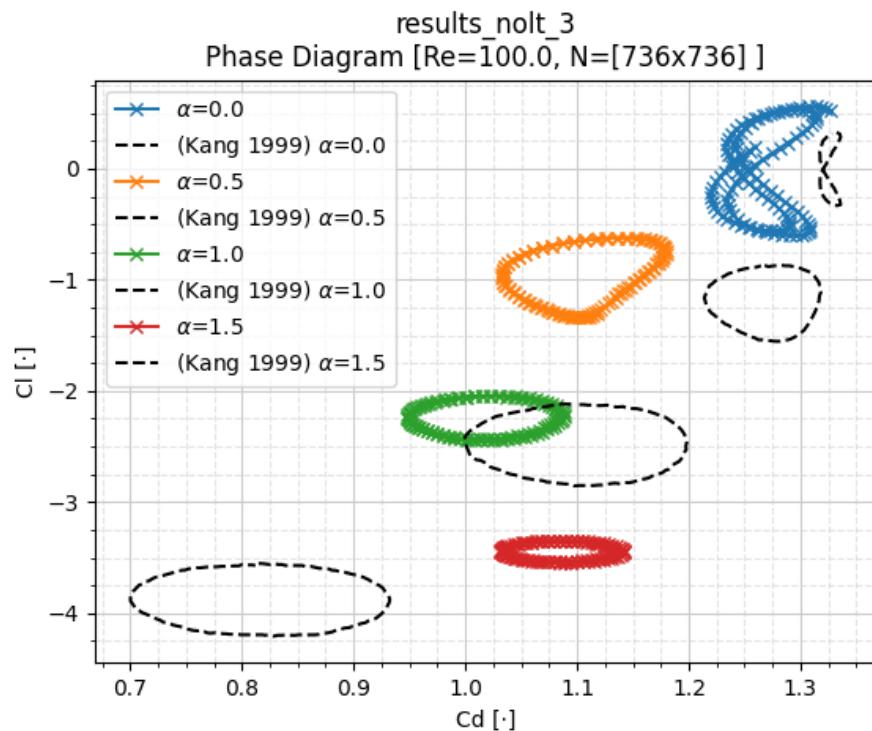
NeuraSim Error Analysis

- Next let's check the phase diagram



NeuraSim Error Analysis

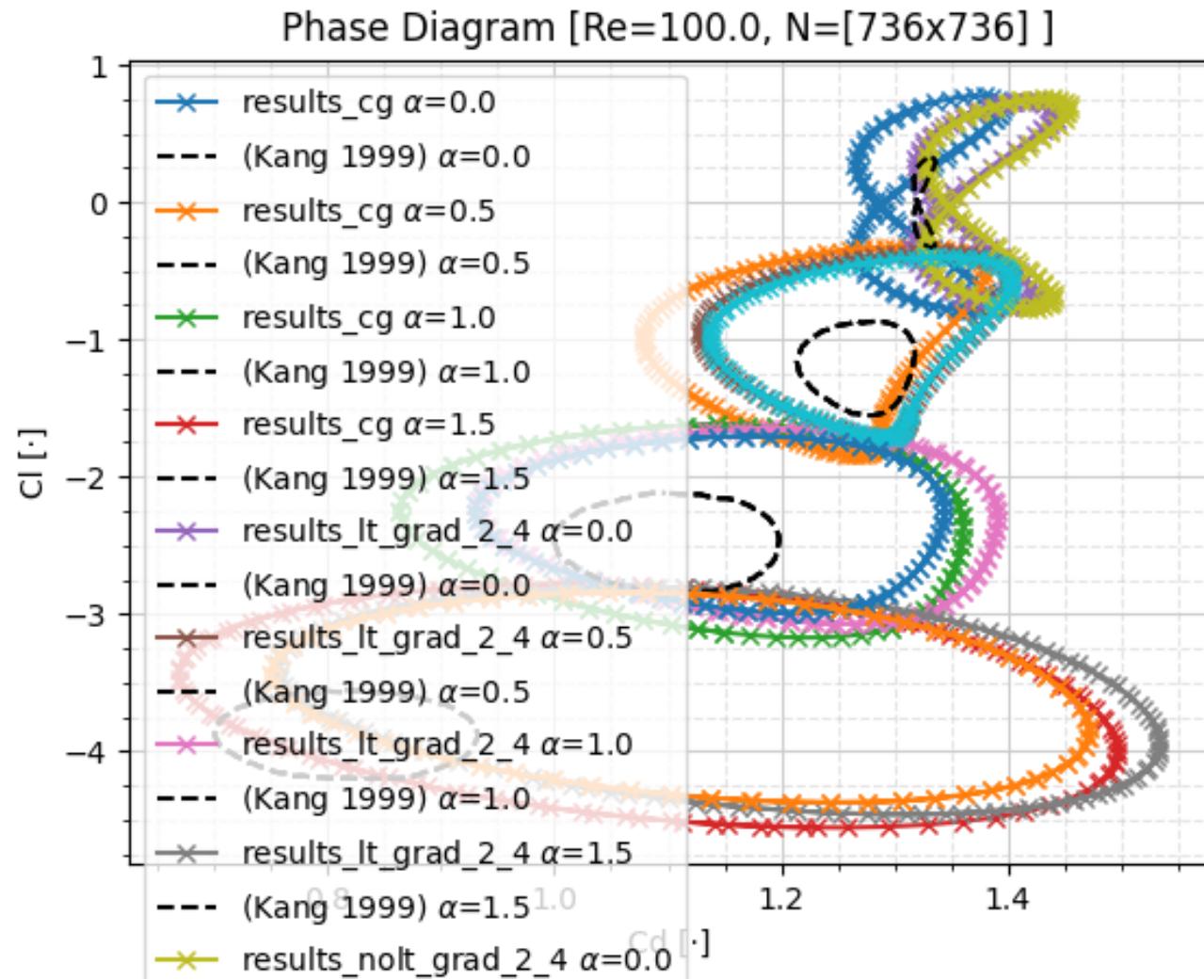
- Next let's check the phase diagram



NeuraSim Error Analysis

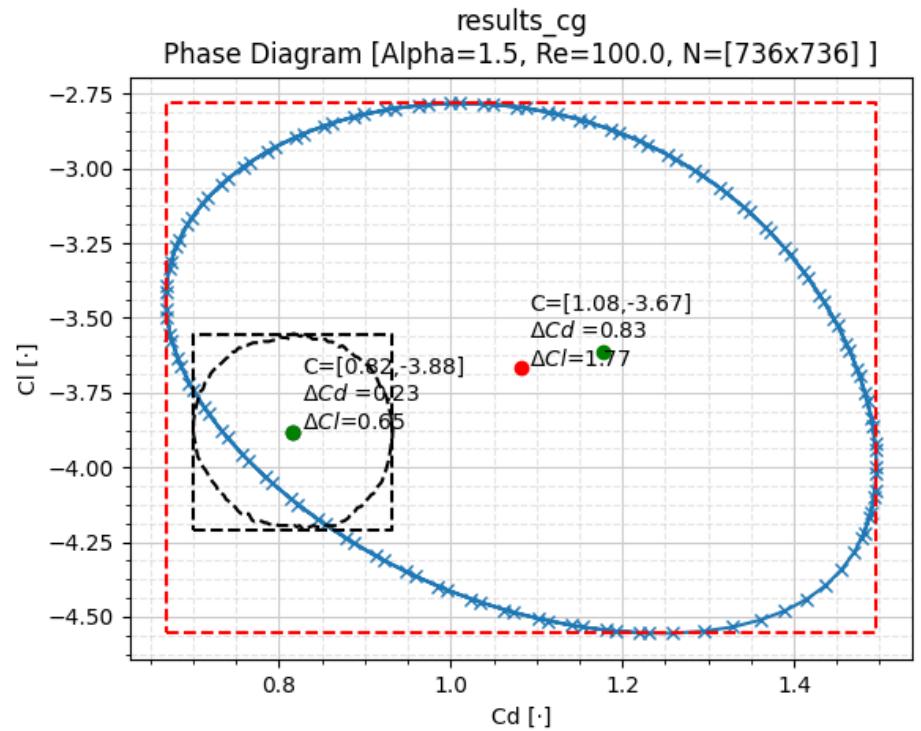
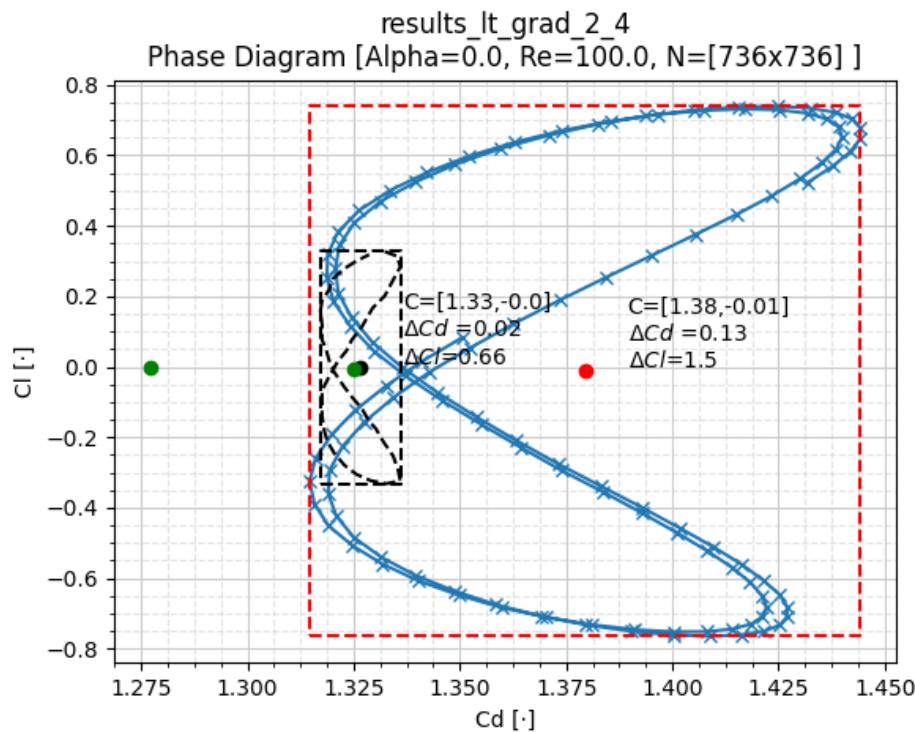
- We can check that the cases for no long term have a much larger error compared with the literature. With the exception of the not long term with grad 2_4. In other words, the addition of the grad 2_4 corrects the error of not having long term. And obtaining a very similar results than the long term case of also with grad 2_4.
- In fact, the cases of grad_2_4 are very similar to what we obtain with the cg. Notice that despite this, we will still have the phase difference. However, in terms of phase space the network has been trained very well to respect to the CG. Even in high ratios of rotation.
- In fact, is for alpha 0 that has some significant error with respect to the CG. This is because the CG is centered always to a smaller Cd than what we obtain with the networks. And maybe since for alpha 0, there is less amplitude the difference is not negligible.

NeuraSim Error Analysis



NeuraSim Error Analysis

- However, how can we quantify the error? The precision?
- I have created some coefficients or index in the phase space to quantify it. I have try to plot it in some meta way (within case or alpha) but the plot is too noisy, so using some concrete alphas as an example, then the rest will be presented in a table.



NeuraSim Error Analysis

- The following are the coefficients

dir_name	alpha	center	DCd	DCI
results_cg	0	[1.33 -0.01]	0.13	1.56
results_cg	0.5	[1.23 -1.08]	0.3	1.52
results_cg	1	[1.11 -2.4]	0.5	1.55
results_cg	1.5	[1.08 -3.67]	0.83	1.77
results_lt_grad_2_4	0.00	[1.38 -0.01]	0.13	1.5
results_lt_grad_2_4	0.5	[1.27 -1.05]	0.27	1.36
results_lt_grad_2_4	1	[1.16 -2.36]	0.46	1.42
results_lt_grad_2_4	1.5	[1.14 -3.63]	0.78	1.66
results_no_lt	0	[0.83 -0.]	0.01	0.1
results_no_lt	0.5	[0.87 -0.76]	0.04	0.14
results_no_lt	1	[0.97 -1.68]	0.06	0.13
results_no_lt	1.5	[1.25 -2.68]	0.14	0.2
results_nolt_3	0	[1.27 -0.02]	0.11	1.16
results_nolt_3	0.5	[1.11 -0.98]	0.15	0.72
results_nolt_3	1	[1.02 -2.24]	0.14	0.4
results_nolt_3	1.5	[1.09 -3.44]	0.11	0.2
results_nolt_grad_2_4	0	[1.39 -0.01]	0.13	1.53
results_nolt_grad_2_4	0.5	[1.27 -1.06]	0.27	1.32
results_nolt_grad_2_4	1	[1.14 -2.35]	0.41	1.29
results_nolt_grad_2_4	1.5	[1.11 -3.61]	0.72	1.53

dir_name	alpha	center_ref	DCd_ref	DCI_ref
kang 1999	0	[1.33 -0.]	0.02	0.66
kang 1999	0.5	[1.27 -1.21]	0.1	0.68
kang 1999	1	[1.1 -2.49]	0.2	0.74
kang 1999	1.5	[0.82 -3.88]	0.23	0.65

NeuraSim Error Analysis

- And the error with respect the literature (kang) are the following.

dir_name	alpha	e_center_x	e_center_y	e_center_100%	e_box_Cl	e_box_Cd	e_box_100%
results_cg	0	0	2.85	142.71	1.37	5.98	367.76
results_cg	0.5	-0.03	-0.11	-6.73	1.22	1.88	154.98
results_cg	1	0.01	-0.04	-1.22	1.1	1.51	130.4
results_cg	1.5	0.33	-0.05	13.55	1.71	2.57	213.91
results_lt_grad_2_4	0.00	0.04	4.24	214.09	1.28	5.88	358.32
results_lt_grad_2_4	0.5	0	-0.14	-6.8	0.99	1.62	130.35
results_lt_grad_2_4	1	0.06	-0.05	0.34	0.93	1.31	111.88
results_lt_grad_2_4	1.5	0.4	-0.06	16.89	1.53	2.36	194.39
results_no_lt	0	-0.38	0.88	24.96	-0.86	-0.66	-75.93
results_no_lt	0.5	-0.32	-0.37	-34.47	-0.8	-0.59	-69.87
results_no_lt	1	-0.11	-0.32	-21.96	-0.82	-0.68	-74.76
results_no_lt	1.5	0.53	-0.31	10.86	-0.7	-0.41	-55.66
results_nolt_3	0	-0.04	7.31	363.48	0.77	4.67	271.83
results_nolt_3	0.5	-0.13	-0.19	-15.8	0.05	0.41	23.22
results_nolt_3	1	-0.07	-0.1	-8.56	-0.45	-0.29	-37.32
results_nolt_3	1.5	0.33	-0.11	10.93	-0.7	-0.52	-60.85
results_nolt_grad_2_4	0	0.05	1.92	98.57	1.32	5.87	359.6
results_nolt_grad_2_4	0.5	0	-0.13	-6.18	0.92	1.56	124.05
results_nolt_grad_2_4	1	0.03	-0.06	-1.08	0.75	1.09	91.55
results_nolt_grad_2_4	1.5	0.36	-0.07	14.5	1.34	2.11	172.37

NeuraSim Error Analysis

- And rearranged.

e_center_100%	0	0.5	1	1.5
results_cg	143	-7	-1	14
results_lt_grad_2_4	214	-7	0	17
results_no_lt	25	-34	-22	11
results_nolt_3	363	-16	-9	11
results_nolt_grad_2_4	99	-6	-1	15

e_box_100%	0	0.5	1	1.5
results_cg	368	155	130	214
results_lt_grad_2_4	358	130	112	194
results_no_lt	-76	-70	-75	-56
results_nolt_3	272	23	-37	-61
results_nolt_grad_2_4	360	124	92	172

- Which in terms of mean values (center) with the exception of alpha 0, already commented, are relatively good. Specially with grad.
- Regarding the amplitude (box) is very big. But being that a good thing, since the nets have a very similar error to the CG. (With exception of no long term, already commented). With a slight more similar amplitude error for the case of the Unet with long term and grad.

NeuraSim Error Analysis

- So if we see the error with respect the CG, to better asses the networks learning.

dir_name	alpha	e_center_x	e_center_y	e_center_100%	e_box_Cl	e_box_Cd	e_box_100%
results_cg	0	0	0	0	0	0	0
results_cg	0.5	0	0	0	0	0	0
results_cg	1	0	0	0	0	0	0
results_cg	1.5	0	0	0	0	0	0
results_lt_grad_2_4	0	0.04	0.36	19.9	-0.04	-0.01	-2.6
results_lt_grad_2_4	0.5	0.03	-0.03	-0.2	-0.1	-0.09	-9.71
results_lt_grad_2_4	1	0.04	-0.01	1.51	-0.08	-0.08	-8.07
results_lt_grad_2_4	1.5	0.06	-0.01	2.37	-0.07	-0.06	-6.25
results_no_lt	0	-0.38	-0.51	-44.61	-0.94	-0.95	-94.54
results_no_lt	0.5	-0.29	-0.3	-29.75	-0.91	-0.86	-88.52
results_no_lt	1	-0.12	-0.3	-21.21	-0.91	-0.87	-89.23
results_no_lt	1.5	0.15	-0.27	-5.92	-0.89	-0.84	-86.25
results_nolt_3	0	-0.04	1.16	55.73	-0.25	-0.19	-22.14
results_nolt_3	0.5	-0.1	-0.09	-9.71	-0.53	-0.51	-51.77
results_nolt_3	1	-0.08	-0.06	-7.41	-0.74	-0.72	-72.9
results_nolt_3	1.5	0	-0.06	-2.86	-0.89	-0.87	-87.68
results_nolt_grad_2_4	0	0.04	-0.24	-9.81	-0.02	-0.02	-1.89
results_nolt_grad_2_4	0.5	0.03	-0.02	0.48	-0.13	-0.11	-12.26
results_nolt_grad_2_4	1	0.02	-0.02	0.09	-0.17	-0.17	-16.87
results_nolt_grad_2_4	1.5	0.03	-0.02	0.48	-0.14	-0.13	-13.29

NeuraSim Error Analysis

- And rearranged

<i>e_center_100%</i>	0	0.5	1	1.5	<i>e_box_100%</i>	0	0.5	1	1.5
results_cg	0	0	0	0	results_cg	0	0	0	0
results_lt_grad_2_4	19.9	-0.2	1.51	2.37	results_lt_grad_2_4	-2.6	-9.71	-8.07	-6.25
results_no_lt	-44.61	-29.75	-21.21	-5.92	results_no_lt	-94.54	-88.52	-89.23	-86.25
results_nolt_3	55.73	-9.71	-7.41	-2.86	results_nolt_3	-22.14	-51.77	-72.9	-87.68
results_nolt_grad_2_4	-9.81	0.48	0.09	0.48	results_nolt_grad_2_4	-1.89	-12.26	-16.87	-13.29

- As stated before in several times. We confirm in this way what we have said in a quantitative manner.
- And so, having a UNET with long term and grad. We have an acceptable error (<10%) with the exception of the mean values for alpha 0, for what has been mentioned before.

NeuraSim Error Analysis

- Having quantify the precision, now we have to asses the performance.

case_name	alpha	Total Time [min]	Iteration Time Total [min]	Iteration Time [s/ite]	Iteration Time % of total sim	Poisson Time Total [min]	Poisson Time [s/ite]	Poisson Time % of inference	UNET Inference Time Total [min]	UNET Inference Time [s/ite]	UNET Inference Time % of poisson sim	CG Inference Time Total [min]	CG Inference Time [s/ite]	CG Inference Time % of poisson sim
results_cg	0	1100.72	1100.5	6.6	100	1094.56	6.57	99.5	0	0	0	1092.44	6.55	99.8
results_cg	0.5	1128.03	1127.7	6.77	100	1121.73	6.73	99.5	0	0	0	1119.48	6.72	99.8
results_cg	1	1168.79	1168.56	7.01	100	1162.82	6.98	99.5	0	0	0	1160.66	6.96	99.8
results_cg	1.5	1190.05	1189.81	7.14	100	1184.11	7.1	99.5	0	0	0	1181.95	7.09	99.8
results_lt_grad_2_4	0	13.42	13.13	0.08	97.8	6.02	0.04	45.9	1.91	0.01	31.8	0	0	0
results_lt_grad_2_4	0.5	11.64	11.4	0.07	97.9	5.58	0.03	48.9	1.67	0.01	29.9	0	0	0
results_lt_grad_2_4	1	11.9	11.63	0.07	97.7	5.68	0.03	48.8	1.68	0.01	29.5	0	0	0
results_lt_grad_2_4	1.5	11.61	11.34	0.07	97.7	5.53	0.03	48.8	1.67	0.01	30.2	0	0	0
results_no_lt	0	26.82	26.45	0.16	98.6	11.7	0.07	44.3	4.42	0.03	37.8	0	0	0
results_no_lt	0.5	25.45	25.09	0.15	98.6	10.99	0.07	43.8	4.29	0.03	39.1	0	0	0
results_no_lt	1	25.59	25.16	0.15	98.3	10.91	0.07	43.4	4.23	0.03	38.8	0	0	0
results_no_lt	1.5	25.54	25.11	0.15	98.3	10.96	0.07	43.6	4.25	0.03	38.8	0	0	0
results_nolt_3	0	27.22	26.77	0.16	98.4	12.07	0.07	45.1	4.37	0.03	36.2	0	0	0
results_nolt_3	0.5	12.65	12.39	0.07	98	6	0.04	48.4	1.7	0.01	28.3	0	0	0
results_nolt_3	1	26.02	25.59	0.15	98.3	11.49	0.07	44.9	4.28	0.03	37.3	0	0	0
results_nolt_3	1.5	11.97	11.68	0.07	97.6	5.7	0.03	48.8	1.68	0.01	29.5	0	0	0
results_nolt_grad_2_4	0	25.81	25.38	0.15	98.3	11.34	0.07	44.7	4.2	0.03	37.1	0	0	0
results_nolt_grad_2_4	0.5	11.59	11.35	0.07	97.9	5.56	0.03	49	1.67	0.01	30	0	0	0
results_nolt_grad_2_4	1	11.82	11.55	0.07	97.7	5.65	0.03	48.9	1.68	0.01	29.7	0	0	0
results_nolt_grad_2_4	1.5	11.81	11.53	0.07	97.6	5.64	0.03	48.9	1.74	0.01	30.8	0	0	0

The big difference between network time and alphas might be needed to be further studied. Maybe was some interference of the hardware.

NeuraSim Error Analysis

- Or the UNETS to respect the CG:

case_name	alpha	Total relative time %	Inference relative % time
results_lt_grad_2_4	0	-98.78	-99.82
results_lt_grad_2_4	0.5	-98.97	-99.85
results_lt_grad_2_4	1	-98.98	-99.86
results_lt_grad_2_4	1.5	-99.02	-99.86
results_no_lt	0	-97.56	-99.59
results_no_lt	0.5	-97.74	-99.62
results_no_lt	1	-97.81	-99.64
results_no_lt	1.5	-97.85	-99.64
results_nolt_3	0	-97.53	-99.6
results_nolt_3	0.5	-98.88	-99.85
results_nolt_3	1	-97.77	-99.63
results_nolt_3	1.5	-98.99	-99.86
results_nolt_grad_2_4	0	-97.65	-99.62
results_nolt_grad_2_4	0.5	-98.97	-99.85
results_nolt_grad_2_4	1	-98.99	-99.86
results_nolt_grad_2_4	1.5	-99.01	-99.85

- So, we have pretty much for all UNETS a reduction of almost the 100% of the inference time.

NeuraSim Error Analysis

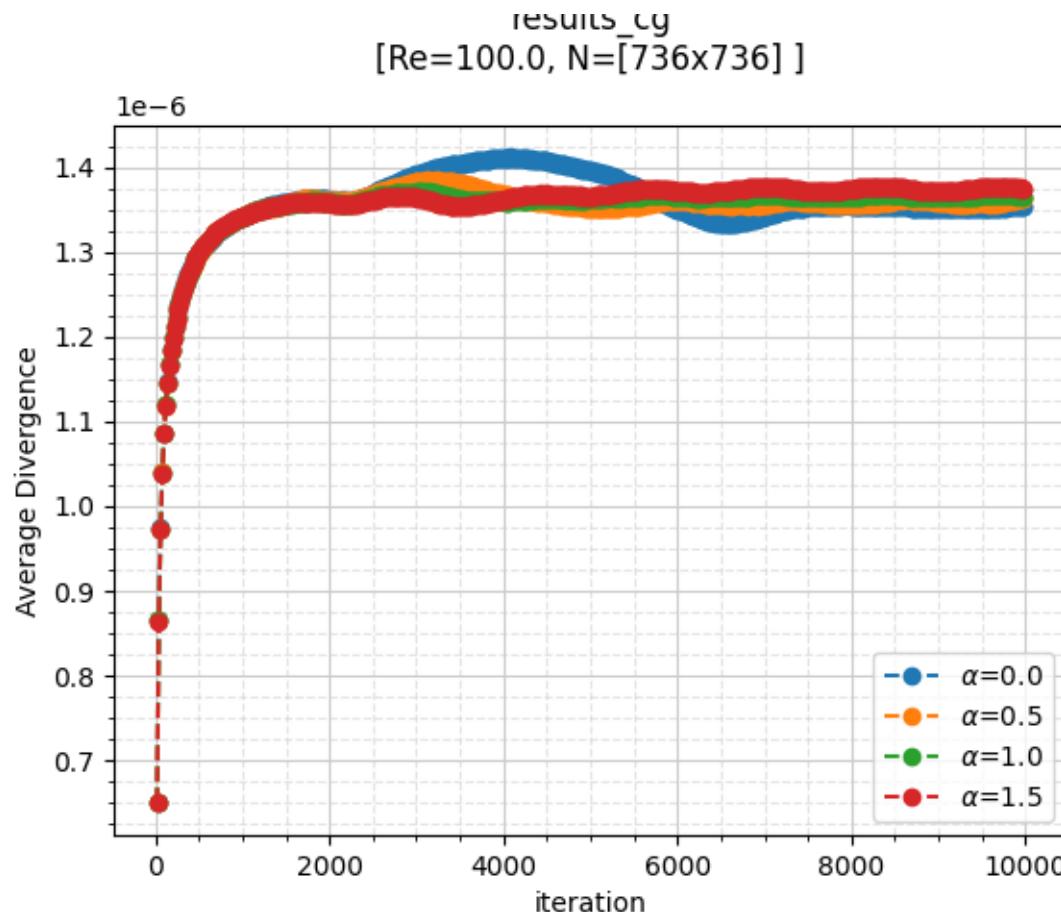
- To sum up what we have just seen.
 - The precision of both the CG and the UNETS are somewhat very low compared with the literature. However, if we compare the precision of the networks to the CG. We see that the networks without long term are very bad. But in exchange, the networks with backpropagation (grad) are remarkably similar. Being slightly better the network with grad and long term.
 - In that case, we have a precision error inferior to 10% for all alphas with the exception of alpha 0, where the small amplitude range makes the error non negligible.
 - At the same time. The CG present a smaller mean Cd than the networks.
 - And there is a small phase difference between the CG and the networks.
-
- On the other hand, the performance improvement of the networks is remarkable. Reducing the pure inference time almost a 100%.
 - Passing, for this case, from 19 hours to 12 minutes more or less.

NeuraSim Error Analysis

- However, from where it comes the error remaining? And, really the error of the CG as well?
- From the residual divergence that the solver doesn't cancels. Since remember is a compressible solver, i.e. the divergence of velocity should be zero.
- Therefore, the divergence study will allow us to see the “error source” of the networks compared with the CG. And the CG itself. It should be zero. Obviously there would be an acceptable value.

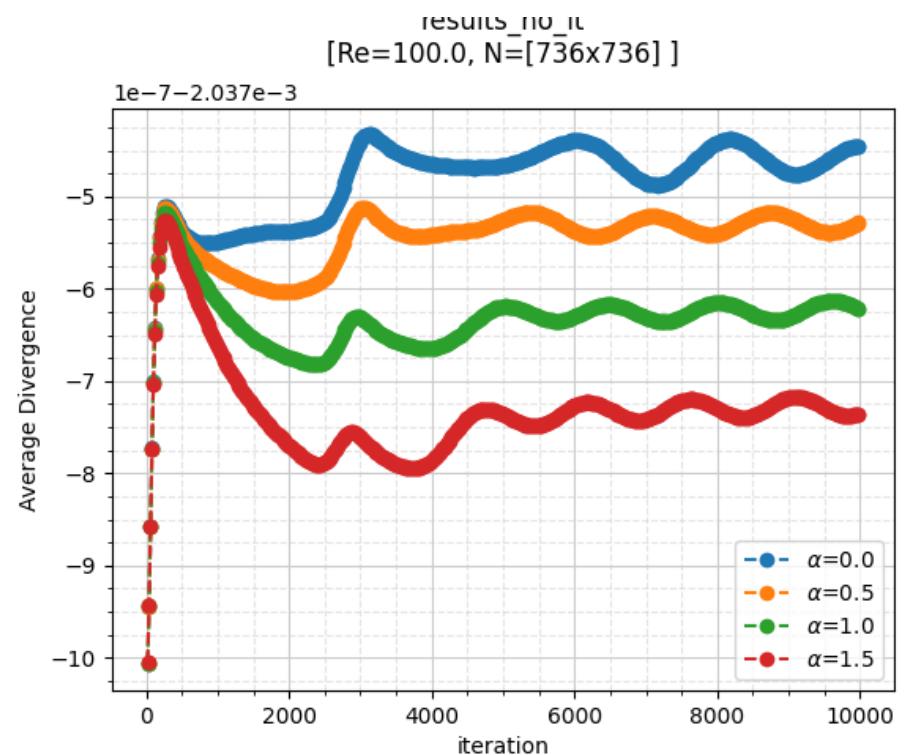
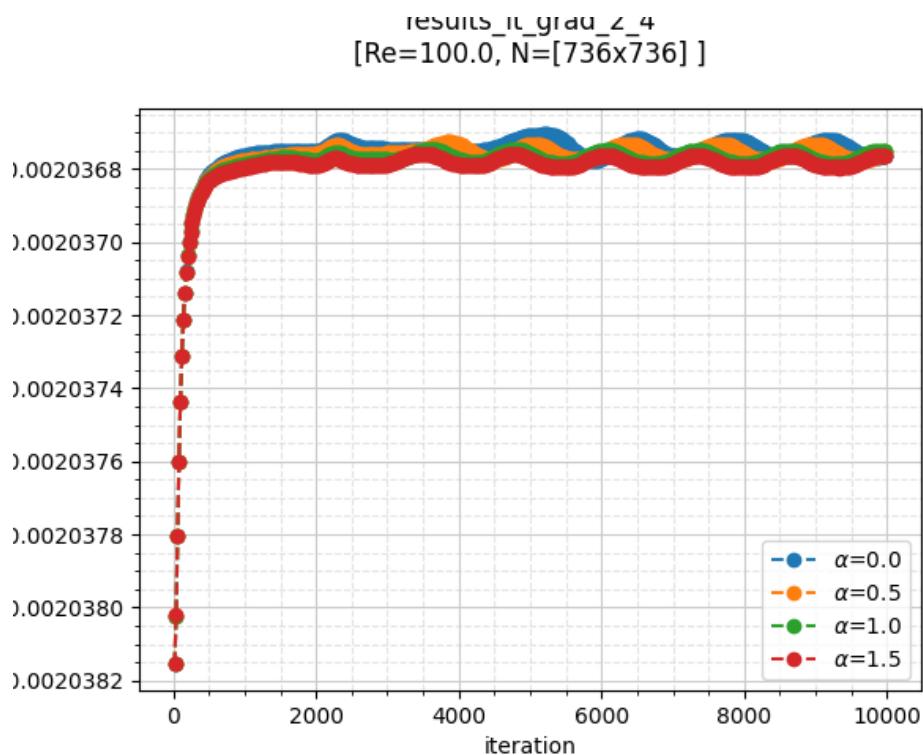
NeuraSim Error Analysis

- Let's see the average divergence over time.



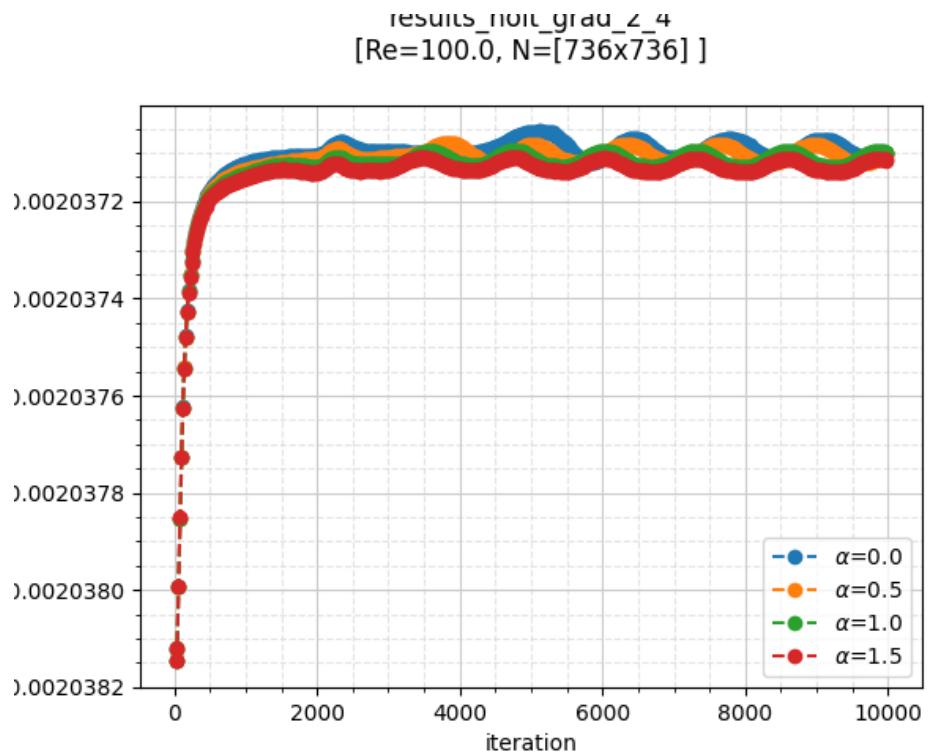
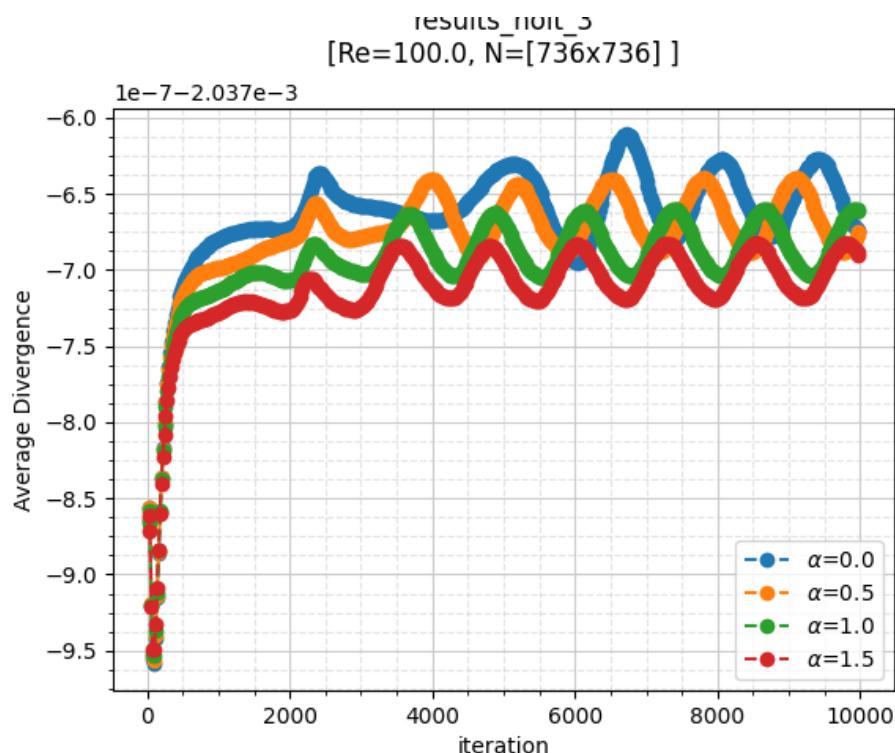
NeuraSim Error Analysis

- Let's see the average divergence over time.



NeuraSim Error Analysis

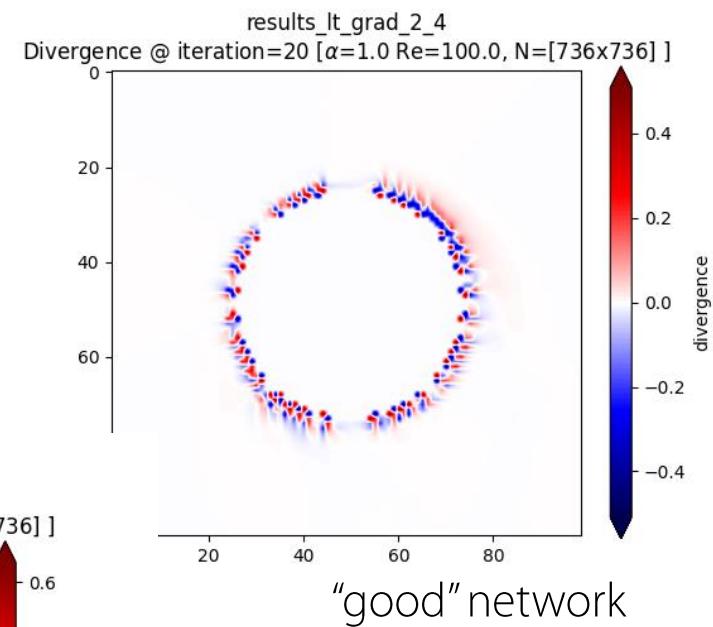
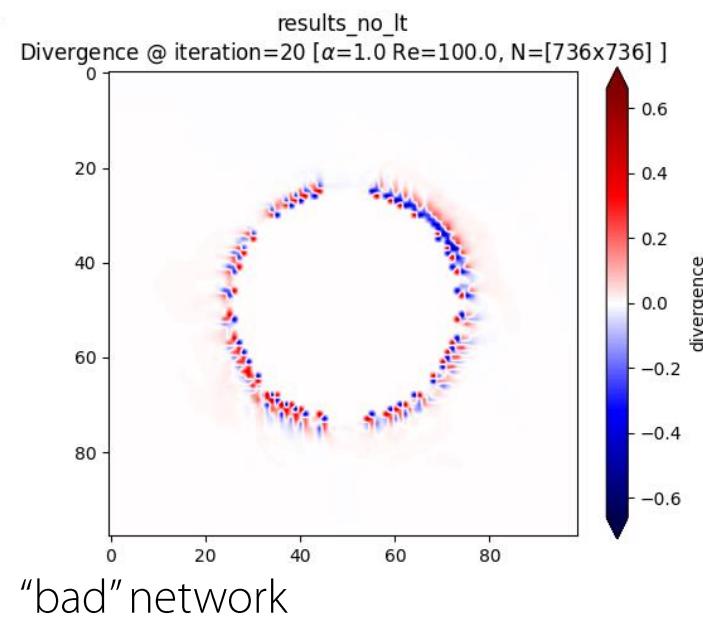
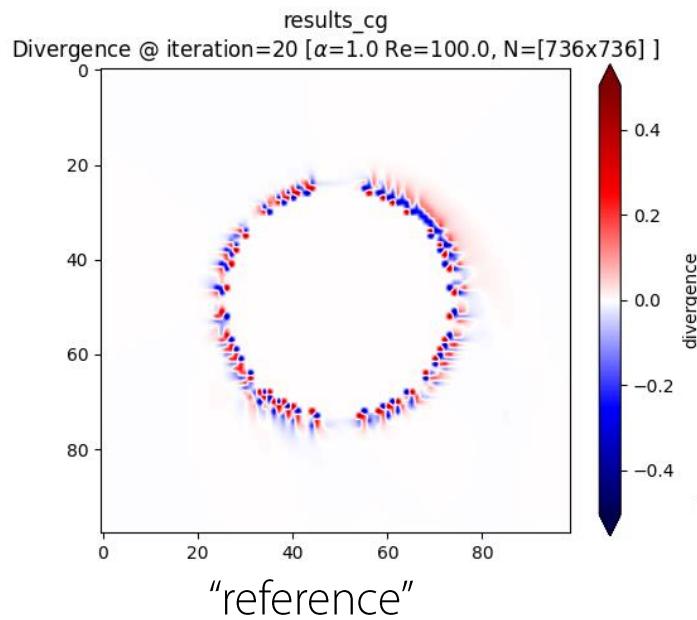
- Let's see the average divergence over time.



NeuraSim Error Analysis

- As we can see, there is a 3 order of magnitude between the CG and the networks. Notice the small difference between the “good” networks and the “bad”. A small difference in divergence has an extreme difference in precision.
- And the main source of this divergence is the cylinder. Even though it is true that with the network it may appear some line at the end of the domain (exit) but the main difference is the cylinder. Following are some snaps of the cylinder area. We will only depict some as an example.
- But it can been appreciated that for the “good” network case, the divergence is much more similar to the CG case. Then, it may be the case that the average difference is a result of the before mentioned line at the exit or similar not the cylinder area itself.

NeuraSim Error Analysis



NeuraSim Error Analysis

- Therefore, to conclude. The network is quiet similar to the CG. But the error source is the same as with the CG. The divergence remaining. For the network is due to the architecture or training. Since the training is base on the CG. And for the CG, and therefore the network also, the numerical schemes.
- Then, I will suggest first of all, to improve the numerical schemes of the solver. Retrain the networks and evaluate if further improvements have to be done.
- However, as presented in previous reports. Using the old trained network using fluidnet. The results for alpha 0 with the network and with the CG were remarkably the same. And I think it is because the numerical schemes of fluidnet were better.
- Then, if the numerical schemes are corrected, I believe we can obtain some remarkable results with the network.

Institut Supérieur de l'Aéronautique et de l'Espace

10, avenue Édouard-Belin – BP 54032

31055 Toulouse Cedex 4 – France

T +33 5 61 33 80 80

www.isae-sup Aero.fr

