

## The Physics-informed Al Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery Milestone 12 Report

Jennifer Sleeman (PI), Ph.D. Jay Brett, Ph.D. Marisa Hughes, Ph.D. Anand Gnanadesikan, Ph.D. Yannis Kevrekidis, Ph.D.

Approved for public release; distribution is unlimited. This material is based upon work supported by the Defense Advanced Research Projects Agency (DARPA) under Agreement No. HR00112290032.

#### Team

- Jennifer Sleeman (APL) PI
- Anand Gnanadesikan (JHU) Co-PI
- Yannis Kevrekidis (JHU) Co-PI
- Jay Brett (APL)
- David Chung (APL)
- Chace Ashcraft (APL)
- Thomas Haine (JHU)
- Marie-Aude Pradal (JHU)
- Renske Gelderloos (JHU)
- Caroline Tang (Duke)
- Anshu Saksena (APL)
- Larry White (APL)
- Marisa Hughes (APL)

#### **Overview**

- This technical report covers the period of April 10, 2023, through June 15, 2023.
- The deliverable for this milestone is this report.

#### **Team Resources**

- Code
  - https://github.com/JHUAPL/PACMANs Public to all (Up to date with all code from start to MS 3 deliverables)
  - https://github.com/JHUAPL/PACMANs\_internal Public to DARPA, JHU, and APL (Hold until internal approvals)
- Documentation
  - https://pacmans.readthedocs.io/en/latest/
- Datasets
  - https://data.idies.jhu.edu/PACMANS/

#### **Goals and Impact**

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

The goal for this milestone includes:

 Deliver final Phase 2 report on comparison of results with conventional models, documenting the established benefits and new capabilities of hybrid models.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Subtask Description: We will report final details of the use case.

- In this report we describe use case modeling related to the global circulation under forcing mechanisms.
- We also describe the research related to CESM2 and GISS box model calibration efforts and its impact on model disagreement research.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Our use cases involve the shutoff of the global overturning circulation under a range of forcing mechanisms associated with global warming. Within the box model this has generated several interesting results.

1. Identification of the role of polar amplification in driving shutoff of the overturning. In the box model, if all latitudes warm at the same rate and freshwater fluxes increase at a rate of 7% the overturning remains stable at very high levels of warming (8-10K). However, when the observed Northern Polar amplification is included in the model, the same physics produces overturning collapse at a much lower value of warming (3-4K). A key here is that as the climate warms, it requires less of a difference in temperature between low and high latitudes to produce the same density difference.

- 2. Identification of mechanisms that allow the overturning to restart. We have found that the deepening of the pycnocline and increasing lateral diffusive salt flux to high latitudes represents a potential mechanism for restarting the overturning not previously recognized in the literature.
- 3. Interbasin tipping points. Our six box model results demonstrate a complicated structure of tipping points between the basins. We find three states of overturning in each basin: a shallow, reversed circulation where the water in the high latitudes is lighter than the low-latitudes due to a freshwater cap, an intermediate circulation similar to the modern Pacific where water sinks in the northern latitudes but returns to low latitudes as intermediate water, and the situation we find in the North Atlantic where water becomes sufficiently dense to sink into the deep. We find that our baseline box model exhibits transitions from a Deep Atlantic/Intermediate Pacific to a Reversed Atlantic/Reversed Pacific state.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- We have identified a particular use case in which some versions of a full coupled model under global warming see an overturning collapse and rapid recovery, while others do not.
- This result is reported by our collaborators at GISS in Romanou et al. (in press).
- As shown in Figure 1, under the scenario of greenhouse gas forcing shown in the top panel, the depth of mixing in the Labrador Sea collapses over the course of the 21st century, but recovers at very different times during the following century. The overturning stream function follows a similar range of paths.



**Figure 1:** Bifurcation in the re-establishment of convection in the Labrador Sea under the SSP2.6 scenario (top panel shows CO2). Bottom panel shows depth of mixing in Labrador Sea from 10 ensemble members. (From Romanou et al., in press).

- We have also begun CESM simulations, but they have not run out far enough to yield robust results further scientific questions remain.
- An important recognition from our work is that this re-establishment of the overturning under constant conditions is not predicted by the classic fold bifurcation theory.
- Under fold bifurcation theory, the forcing must reverse in order to re-establish an overturning. However, this re-establishment behavior is frequently found in our box model results (and indeed represented one of the challenges in exploring the resulting phase space of the box model).

- We are approaching analysis of this use case in two ways. The first is by fitting a box model to the use case and examining whether it produces similar behavior.
- The second is to use modal decomposition to reduce the dimensionality of the space and examine whether the dynamics change as we move into global warming.
- This work has resulted in the finding that one can develop an oscillator mechanism whereby positive anomalies in one mode produce positive tendencies in a second mode, which then produces negative tendencies in the first mode.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- This oscillator is illustrated in Figure 2, which shows the structure of the two modes in the preindustrial climatology.
- A positive value of mode 1 (cooling/freshening in the Labrador Sea) produces a positive trend in mode 2 (southward extension of the subpolar gyre).
- However, positive mode 2 produces a negative trend in mode 1 (warming, salinification of the Labrador Sea).



*Figure 2:* Modal decomposition of SST (left) and SSS (right) modes of variability for model in previous figure. Variability in mode 1 is associated with overturning.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

There are two major items which we have learned from this analysis:

- 1. While the linear analysis is capable of producing an oscillation, the time scales involved are too slow, suggesting an opportunity to use more **nonlinear techniques** such as Koopman operators.
- 2. There are changes in the modal structure as we look at simulations under global warming.

- In particular, in the preindustrial case, changes in the overturning do not result in salinity changes in the Arctic.
- However, as the Arctic warms and more of it melts each summer, it becomes more sensitive to the changes in overturning.
- This change in modal structure may be critical to coupling, as Romanou et al. (2023) suggest that it is freshwater anomalies emanating from the Arctic that determine the timing of shutoff and re-establishment of convection.

#### Task 1.6 Use Case Ocean Modeling - CMIP model disagreement

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

## Sample of time series for multiple global climate models

- 4 CMIP models' SSP5-85 runs processed, showing model disagreement.
  - MPI-ESM1-2-LR: Max Planck Institute for Meteorology Earth System Model
  - ACCESS-CM2: Australian Community Climate and Earth System Simulator
  - CESM2: USA, Community Earth System Model
  - CAN-ESM5: Canadian Earth System Model
- 3 of 4 models show strong decrease in AMOC strength, but pycnocline depth changes are inconsistent shown in Figure 3.



*Figure 3:* SSP5-8.5 *Model disagreement across ensemble members.* 

#### Task 1.6 Use Case Ocean Modeling





Figure 4. Four box model



- Four box model has been demonstrated to well represent CESM2 dynamics. (Figure 4)
- Six box model has been developed and analyzed. (Figure 5)

Task 1.6 Use Case Ocean Modeling - Fitted CESM2 to Four Box

• Depth of high-latitude boxes chosen to be 327m for CESM2 and 300m for GISS-E2.1.

Simulator (PACMANS) for Tipping Point Discovery

The Physics-informed AI Climate Model Agent Neuro-symbolic

• Fit  $\epsilon$  from least-squares for AMOC.

Fitting Method

- Fit the Gent-McWilliams diffusivity AI, from leastsquares for the eddy flux.
- Vertical diffusivity  $K_v$  is fit to have the mean upwelling flux match between the theory and the volume flux balance for the low-latitude box.
- Figure 6 shows 11 members simulated using parameters from 1st member.



Figure 6: Comparing the CESM2 data with the fitted four box model. General shape/trend is correct for both AMOC strength and pycnocline depth.

#### Task 1.6 Use Case Ocean Modeling - Fitted CESM2 to Four Box

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Depth of high-latitude boxes chosen to be 327m for CESM2 and 300m for GISS-E2.1.
- Fit  $\epsilon$  from least-squares for AMOC.
- Fit the Gent-McWilliams diffusivity AI, from least-squares for the eddy flux.
- Vertical diffusivity  $K_v$  is fit to have the mean input upwelling flux match between the theory and the volume flux balance for the low-latitude box.
- Figure 7 shows variation in parameters as fitted across 11 members. This represents the uncertainty in the value of these parameters, and is small (2-7%).

By fitting multiple ensemble members, we get a measure of uncertainty on their values for CESM (helpful for model disagreement analysis – see <u>next slide</u>)



**Figure 7:** Variation in the fitted the four box model parameters across the CESM2 ensemble members.

#### Task 1.6 Use Case Ocean Modeling - Fitted CESM2 and GISS-E2.1 to Four Box

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Fitting one member of each

- First ensemble member of CESM2 Large Ensemble.
- Historical and SSP3-7.0 run of GISS-E2.1.
- Table 1 below shows the values.

	CESM2	GISS-E2.1
$\epsilon$	1.74e-4	1.49e-4
AI	1430	1610
$K_{v}$	3.37e-5	3.27e-5

**Table 1.** Comparison between CESM2 andGISS parameter where epsilon and AI forGISS are outside of the uncertainty range ofCESM2 values.

**Question:** can these emergent parameters help explain inter-model differences in AMOC projections under a warming climate?

**Approach:** Examine separatrix of the two for AMOC on/off.

# Task 1.6 Use Case Ocean Modeling Final Report - Differences in AMOC for 2 surrogates

CESM2

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

GISS-E2.1



Figure 8. GISS and CESM2 as a function of Ekman flux and Freshwater flux.

Both represent the same world, both look similar

Difference of 0.2Sv Fwn or 0.5Sv Mek in shutoff GISS AMOC 0.7Sv stronger in 'on' state

#### Task 2.7 Phase 2 Data Final Delivery

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Subtask Description: We will document updates and deliver any new datasets.

• In this report we describe the new datasets that have been developed and shared for both the box models and calibrated CESM2 and GISS models.

#### Task 2.7 Phase 2 Data Final Delivery

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

#### Four box processed CMIP global model data:

11 members of CESM2 large ensemble-- USA, Community Earth System Model.

1 each of:

- GISS-E2.1, USA, NASA Goddard Institute for Space Science
- MPI-ESM1-2-LR: Max Planck Institute for Meteorology Earth System Model
- ACCESS-CM2: Australian Community Climate and Earth System Simulator
- CESM2: CAN-ESM5: Canadian Earth System Model

#### Task 2.7 Phase 2 Data Final Delivery

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

#### Box model datasets used for machine learning:

- Python package of the box models allows one to specify initial conditions and parameter values.
- Produces datasets in netcdf format.

#### Four box model ML dataset:

- Recreates the Gnanadesikan experiments (in Matlab code).
- Generates the same plots.
- Enables creation of labeled training data for training machine learning algorithms and temporal training data for training the AI surrogates.

#### Six box model ML dataset:

- Created using a grid search approach.
- Enables creation of labeled training data for training machine learning algorithms and temporal training data for training the AI surrogates.

#### Task 3.8 AI Physics-Informed Surrogate Model Phase 2 Final Report

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Subtask Description: We will report final details of perceived benefits and capabilities based on the evaluations and benchmarks.

• In this report we highlight the benefits of using the hybrid models and describe the latest results in the bifurcation analysis applied to the six box model.

#### Task 3.8 AI Physics-Informed Surrogate Model Phase 2 Final Report

- The Al/Hybrid model approach has been **extremely effective** in generating new hypotheses which we expect to be the focus of future modeling work.
- In particular, the process of dimensionality reduction forced us to grapple with key shortcomings of theory.
- We describe these shortcomings of theory.

#### Task 3.8 Al Physics-Informed Surrogate Model Phase 2 Final Report

- 1. We had to reconcile the work in the literature about the competing roles of density contrasts between high and low latitudes and northern vs. southern latitudes.
  - Doing this has generated a significant series of hypotheses that can be tested using idealized models.
- 2. The fold bifurcation theories that have dominated discussions of overturning shutoff and collapse do not **spontaneously produce recovery**, which is seen in both the coupled models and the box models.
  - We have framed a number of theories for how such recovery might occur, which will focus future exploration of the CMIP6 models.

#### Task 3.8 AI Physics-Informed Surrogate Model Phase 2 Final Report

- 3. The AI-based hybrids **focus attention on models near tipping points**, which is a very different approach than previously taken in climate modeling.
  - It motivated us to design new experimental designs and model suites.
- 4. The development of a **wider suite of tipping points** than previously recognized offers interesting opportunities from a dynamical systems point of view.

## Task 3.8 Al Physics-Informed Surrogate Model Phase 2 Final Report The Physics-informed Al Climate Model Agent Neuro-symbolic

Simulator (PACMANS) for Tipping Point Discovery





Figure 9. Four box model

Figure 10. Six Box Model

- Recall, this effort began with bifurcation analysis of the four box model shown in Figure 9, with the goal of learning escape times.
- To support continued climate modeling efforts we have also begun bifurcation analysis of the six box model, shown in Figure 10.

#### Task 3.8 Al Physics-Informed Surrogate Model Phase 2 Final Report The Physics-informed Al Climate Model Agent Neuro-symbolic

Simulator (PACMANS) for Tipping Point Discovery

- The bifurcation diagram was analyzed with respect to the nondimensional north freshwater flux.
- Figures 11(a) and 11(b) show the NH overturning  $M_{n^*}$  while Figures 11(c) and 11(d) show the nondimensional depth D<sub>\*</sub>.
- The Hopf at T<sup>n</sup><sub>r FW</sub> =0.0384 is subcritical. The value where the limit cycle seems to "go vertical" is 0.0375. It approaches an unstable homoclinic orbit.



**Figure 11.** a) NH overturning  $M_{n^*}$  b) Nondimensional depth  $D_*$  c-d) Zoom-in close to the Hopf bifurcation point for  $M_{n^*}$  and for  $D_*$ , respectively

#### Task 3.8 Al Physics-Informed Surrogate Model Phase 2 Final Report The Physics-informed Al Climate Model Agent Neuro-symbolic

Simulator (PACMANS) for Tipping Point Discovery

- The bifurcation diagrams seems to reflect the behavior observed in the paper (Gnanadesikan et al. 2018) where initial conditions with D=1 are attracted by the upper branch because there is an early switch activation.
- The "blow up" is given by the upper limit point LP. For D=4 the "blow up" is close to the subcritical Hopf. The solution loses stability before the exact Hopf point because the initial conditions may start outside the unstable limit cycle. Hysteresis behavior is shown below.



**Figure 12.** a) Hysteresis diagram as  $M_{n^*}$  varies; b) Hysteresis diagram as  $D_*$  varies

#### 15 June 2023 31

# Task 3.8 Al Physics-Informed Surrogate Model Phase 2 Final Report The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

#### Additional Dynamics Results:

- The limit cycle approaches an homoclinic bifurcation, with the period blowing up vertically.
- Additional visualizations of this behavior are shown in Figure 13.



*Figure 13.* a) *Limit cycle continuation; b)* Blow-up of the period of the limit cycle; c) Limit cycle on the bifurcation diagram; d) Homoclinic orbit in a three-dimensional state variable projection.

### Task 3.8 AI Physics-Informed Surrogate Model Phase 2 Final Report

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Schematic of three types of circulation in high latitudes:



Figure 14. Schematics of three types of circulation patterns.

- Modern ocean can be described as "DeepNA-IntNP"
- Stommel model, Gnanadesikan et al., 2018 show a transition between DeepNA and SurfNA.
- What about the six box model?

#### **Task 3.8 Al Physics-Informed Surrogate Model Phase 2 Final Report** The Physics-informed Al Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

• After review/obtaining results, we found it was much more complicated



#### Task 3.8 Al Physics-Informed Surrogate Model Phase 2 Final Report – Continued Work

- 1. We used a recently developed deep-learning framework [Dietrich et al., 2021] that identifies effective stochastic differential equations (eSDEs) from data. By using this deep-learning framework we will continue this work to learn a parameter-dependent eSDE for parameter values  $\lambda$  before and after the tipping point.
- 2. We may use the deterministic (drift) component of the eSDE to construct the bifurcation diagram based on this surrogate model. We will illustrate that the drift component of the surrogate eSDE model is capable of discovering the bifurcation point.
- 3. Furthermore, we will then use the surrogate eSDE model to perform rare event computations (exit time/stopping time computation). We start from the identified stable steady state and integrate the eSDE, for a specific value of the parameter, until the first time we reach (and surpass) the saddle. The latter can be performed by using the surrogate models and performing (a) kinetic Monte Carlo (kMC) simulation, (b) solving a partial differential equation boundary value problem arising from the Feynman-Kac formula, (c) and computing the mean exit time numerically with quadrature integration. We also perform kMC simulations of the full model (with added noise) to estimate the mean exit time.
- 4. We will then estimate the total time needed for the escape time computations. Preliminary results, on similar complex systems for epidemiological networks [Gross and Kevrekidis, 2008], suggest that the kMC computations of the surrogate eSDE model need 18 minutes whereas the escape time computation of the full model needs ~ 200 times more. This also takes into account the time needed to sample the data and train the network.
- 5. In the immediate future, we will finalize the six box model computations and obtain targeted tipping point models close to (a) the saddle-node tipping point and (b) the subcritical Hopf tipping point discovered.

#### Task 4.8 AI Simulation Phase 2 Final Report

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

**Subtask Description:** We will report final details of perceived benefits and capabilities based on the evaluations and benchmarks, including the effectiveness of the tipping point causality model as part of conventional workflow and shortcomings/constraints of a simulated approach and necessary constraints.

 In this section we will describe the benefits of using the AI simulation for tipping point discovery. We will describe the role of causality and how it will improve the overall workflow. We will describe shortcoming and constraints of TIP-GAN, the neuro-symbolic model, and the causal model.

#### Task 4.8 Al Simulation Phase 2 Final Report - Benefits

- New type of generative adversarial network **TIP-GAN** for tipping point discovery is able to learn bifurcations in parameter space.
  - Showed we could recreate the Gnanadesikan 2018.
  - Have been able to use the TIP-GAN to make new discoveries and learn more about parameter sensitivities .
- Newly developed **neuro-symbolic deep learning architecture** for scientific discovery using natural language question/answer
  - Have been able to show that the neuro-symbolic model has strong performance translating questions to questions and questions to programs and reasonable performance translating programs to questions.
  - Latest version trained on 2<sup>nd</sup> version of AMOC questions shows similar performance.
- TIP-GAN and neuro-symbolic integration shows tremendous speed-up in scientific discovery process and strong performance answering AMOC-shutoff question.
- The causal model uncovered interesting correlations between parameters. It was not integrated into the process flow with TIP-GAN and the neuro-symbolic model, as it is still being independently evaluated.
Recall the TIP-GAN and neuro-symbolic flow as seen in Figure 16.

> Run Model

Surrogate

**Climate Model** 

answering.



VQE70 – The Physics-informed AI Climate Model Agent Neurosymbolic Simulator (PACMANS) for Tipping Point Discovery

- Showed that the GAN could be used to exploit the area of uncertainty consistent with the separatrix as seen in Figure 17.
- Also showed compelling classification precision, recall, F1 scores.

Dlow0 - Thermocline depth of lower latitudes Mek - Ekman flux from the southern ocean Fwn - Fresh water flux (North)



Sleeman, Jennifer, David Chung, Chace Ashcraft, Jay Brett, Anand Gnanadesikan, Yannis Kevrekidis, Marisa Hughes et al. "Using Artificial Intelligence to aid Scientific Discovery of Climate Tipping Points." AAAI Fall Symposium – Knowledge Guided ML (Nov 2022), arXiv preprint arXiv:2302.06852 (2023)

VQE70 – The Physics-informed Al Climate Model Agent Neuro-

symbolic Simulator (PACMANS) for Tipping Point Discovery





*Figure 18.* Recreated collapses using Python-generated tools for machine learning dataset creation from the four box model (Gnanadesikan 2018)

Dataset	F1 Discriminator Score	% in uncertainty region
Test		35.5
1 Generator GAN	.971	67.4
2 Generator GAN	.927	91.4
3 Generator GAN	.925	98.7









**Figure 19.** Comparing GAN-generated results for N = (1, 2, 3) with the test set.

By increasing the number of generators, the GAN is better able to target the area of the bifurcation consistent with the 2018 experiments.

15 June 2023 39

**Table 2.** F1 scores and % of uncertainty region.





### TIP-GAN is also able to learn AMOC recoveries as shown in Figures 20-22.

Simulator (PACMANS) for Tipping Point Discovery

The Physics-informed AI Climate Model Agent Neuro-symbolic

Task 4.8 Al Simulation Phase 2 Final Report - Benefits



Figure 21. Test set with new recovery label included.



40

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery



*Figure 23. t*-SNE TIP-GAN (*n*=2) generator embeddings Timestep 0.



Figure 24. t-SNE TIP-GAN (n=2) generator embeddings Timestep 10.



t-SNE embeddings shows TIP-GAN learning more structure over time and in particular becoming more biases towards AMOC models with shutoffs consistent with the training loss function objectives

Figure 25. t-SNE TIP-GAN (n=2) generator embeddings Timestep 20.



The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Figure 27. t-SNE TIP-GAN (n=2) generator embeddings Timestep 40 for GISS Calibrated Model.



#### source

- Gen 1 shutoff
- Gen 1 nonshutoff
- Gen 2 shutoff
- Gen 2 nonshutoff

#### Figure 28. t-SNE TIP-GAN (n=2) generator embeddings Timestep 40 for CESM2 calibrated model.



t-SNE embeddings of the GISS calibrated and CESM2 calibrated show that TIP-GAN finds fewer shutoffs for GISS than CESM2.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Using TIP-GAN we perturbed both together and separate:

- the initial depth of the pycnocline *D\_low*
- the Northern Hemisphere freshwater flux *F\_wn*
- Ekman flux

#### Research discovery:

- Ekman flux appears to create states that are more spread out and not all collapsing to the manifold as shown in Figure 29.
- Tells us there is still more work to be done to understand how southern ocean fluxes are influencing the AMOC.



**Figure 29.** Shows AMOC on/off as a function of Freshwater Flux and Overturning colorcoded in terms of parameters that were generated a-priori where a single parameter was randomly generated in isolation or two parameters were randomly generated together.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Using TIP-GAN we perturbed both together and separate:

- the initial depth of the pycnocline *D\_low*
- the Northern Hemisphere freshwater flux  $F_wn$
- Eddy Mixing Coefficient A\_Redi

### Research discovery:

 By varying the initial conditions and eddy mixing coefficient together, we can extend the "off" state to much lower levels of freshwater flux than if we vary only one of the parameters as shown in Figure 30. This has implications for how easily the overturning recovers from shutoff.



**Figure 30.** Shows AMOC on/off as a function of Freshwater Flux and Overturning colorcoded in terms of parameters that were generated a-priori where a single parameter was randomly generated in isolation or two parameters were randomly generated together.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Findings: High temperatures in the northern high latitude box can shut off AMOC, consistent with the expected density dependence. Interestingly, a link to the southern ocean is suggested by a more moderate *Tnorth* temperature and high *Ssouth* salinity shown in Figure 31. This suggests that AMOC shutoff could be by density differences affected between the north and south highlatitude boxes rather than just the direct north and low-latitude box density difference from the governing equations.

GENERATOR 2 (red off) Thorth being high is a shutoff; clear vs Dlow0 and S\_south, where it is insensitive to them. Also, Thorth high and Tlow low is a shutoff; that's the density difference we'd expect.Generator 1 (blue off) shows up in high Thorth and Dhigh and medium Thorth high Ssouth

*Figure 31.* Shows a pair plot of CESM2 model parameters for understanding relationships between pairs of parameters.

300 - 50 - 50 - 50 - 50 - 150 - 100 -					
500 - 400 - 6, 300 - 200 100 -					
20- 0115- 111- 5-				•	
25 80 81 100 11 10 5					
20 20 5 15 10 5					
28 - 70 - 0 - 115 - 1 - 10 - 5 -					
37 . 000000 . 38 . 34 . 33 .					
37 - 36 001005 5 34 - 33					
37 - 36 - 000015 - 34 - 33 -					
37 - 60 - 60 - 90 - 90 - 90 - 90 - 90 - 90 - 90 - 9					



The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

*Findings:* Although we find many shutoffs at high *Fwn* in human exploration, the GAN has also found many shutoffs at low *Fwn* shown in Figure 32. These are a new area for future exploration by scientists.

Surprising and intriguing that the low Fwn shutoffs (in Gen 2)

*Figure 32.* Shows a pair plot of CESM2 model parameters for understanding relationships between pairs of parameters.





Snorth

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

*Findings: Aredi*, the along-isopycnal mixing coefficient controlling **MLS** and **MLN**, covaries with **Dlow** (flux between Low and highlat boxes, makes dynamical sense) and Snorth (suggests isopycnal mixing important for salinity in the north box, interesting that this shows up more clearly than for **Slow**, **Thorth**, or **Tlow**) shown in Figure 33.

> Figure 33. Shows a pair plot of CESM2 model parameters for understanding relationships between pairs of parameters.



### Task 4.8 AI Simulation Phase 2 Final Report - Early Causal Results Benefits

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

**Generator 1** 

**Generator 2** 

**Generator 1**: *Mn* and *Mek* have linear relationship. This has been observed in the GCMs and in the four box model. The *Dlow Mek* off state linear relationship is interesting and novel. The low *Fwn* off states tend to have low *Mek* and moderate *Dlow*—that's a great **hypothesis** to be tested in the future.

*Hypothesis:* There is an AMOC-off condition that can occur with low *Mek*, moderate *Dlow*, and low-to-moderate *Fwn*. Test with global ocean model.

<u>Generator 2:</u> Found fewer AMOC-off states at high *Fwn* than generator 1.

Correlation plots show stronger correlations between *Mn* and *Mek* in Generator 2 than Generator 1.



The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

General TIP-GAN discoveries:

- TIP-GAN is more sensitive to freshwater flux changes as opposed to temperature changes.
- TIP-GAN shows that varying the eddy mixing coefficient would make sense when moving from the box models to the global models.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Neuro-symbolic translation final findings.
- Using the bi-directional translations enables scientific discovery by allowing scientists to ask questions of the trained TIP-GAN.



*Figure 38.* Neuro-symbolic translation questions to programs for GAN consumption and GAN output to NL questions for human consumption – \*first of its kind\*

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Early work evaluated using a well-known benchmark CLEVR.
- Adapted to evaluate our model with promising results.



*Figure 39.* Normalized mean Levenshtein distance by sequence length. Great performance on all three translations.

CDF of	f Normaliz	zed Leve	enshtei	n Distan	ces for 1	L1 toker	n mode	I
1.0 -						J[		Text to Text Text to Program Program to Text
0.8 -								Overall
0.6 -								
0.4 -				F				
0.2 -				<b></b>				
0.0 🖵 🥌								
30	40	50	60	70	80	90	100	
		Normali	zed Leve	enshtein D	istance			
	CDF of 1.0 - 0.8 - 0.6 - 0.4 - 0.2 - 0.0 - 30	CDF of Normalia	CDF of Normalized Level 1.0 - 0.8 - 0.6 - 0.4 - 0.2 - 0.0 30 40 50 Normali	CDF of Normalized Levenshtei	CDF of Normalized Levenshtein Distant	CDF of Normalized Levenshtein Distances for 1	CDF of Normalized Levenshtein Distances for 11 toker	CDF of Normalized Levenshtein Distances for 11 token mode 1.0 0.8 0.6 0.4 0.2 0.0 30 40 50 60 70 80 90 100

*Figure 40.* CDF of normalized mean Levenshtein distance by sequence length. Great performance on all three translations.

	Quest to Question	Question to Program	Program to Question	Overall
Distance	99.78	99.78	66.10	88.55

#### Table 3. Levenshtein results - using CLEVR dataset

Questions in CLEVR test various aspects of visual reasoning including attribute identification, counting, comparison, spatial relationships, and logical operations.



Q: Are there an equal number of large things and metal spheres?
Q: What size is the cylinder that is left of the brown metal thing that is left of the big sphere?
Q: There is a sphere with the same size as the metal cube; is it made of the same material as the small red sphere?
Q: How many objects are either small cylinders or red things?

*Figure 41. Example questions from the CLEVR dataset.* 

$$\operatorname{lev}_{a,b}(i,j) = \begin{cases} \max(i,j) & \text{ if } \min(i,j) = 0\\ \min \begin{cases} \operatorname{lev}_{a,b}(i-1,j) + 1\\ \operatorname{lev}_{a,b}(i,j-1) + 1\\ \operatorname{lev}_{a,b}(i-1,j-1) + 1_{(a_i \neq b_j)} \end{cases} & \text{ otherwise.} \end{cases}$$

Levenshtein Distance Used to Measure Performance

### Task 4.8 AI Simulation Phase 2 Final Report – Shortcomings/Constraints

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

### <u>TIP-GAN:</u>

- There are challenges in using a full GCM with TIP-GAN.
  - $\circ~$  Models tend not to have AMOC collapse.
  - $\circ~$  No real ground truth.
- TIP-GAN becomes unstable without thorough analysis of bounding parameter values.
- Proving the TIP-GAN made new discoveries is hard to quantify due to the high dimensional space.
- Moving from a deterministic to a stochastic model also proves to be challenging as TIP-GAN is trained with the surrogate model as the oracle, so the question with a stochastic model is, "Given the stochasticity, how many runs of the model is enough to calculate an accurate probability of the likelihood of a shut-off?"
  - We don't see this as a limitation, but more as an interesting extension to the current TIP-GAN.

### Task 4.8 AI Simulation Phase 2 Final Report – Shortcomings/Constraints

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

#### Neuro-symbolic Translations:

- Bi-directionally translating scientific questions and programs is challenging.
  - Question to program translation is straightforward, newer complex questions yielded results that were comparable with the simpler question.
  - However, program to question translation is challenging due to the one-to-many relationship and the consideration of semantics.
  - Again, we see this as an opportunity to really push the research into this area of AI-assisted scientific discovery by using GPT and other large language models to help reduce question complexity and to perform automatic question generation.

#### Causal Learning:

- Is showing causal paths across TIP-GAN generators enough for explainability?
- Causal graphs to represent generative learning were hard to construct and interpret.
  - $_{\odot}\,$  Establishing causality is challenged by feedback loops across parameters.

### Task 5.3 Phase 2 Evaluation

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

**Subtask Description:** We will evaluate the full AI hybrid approach and benchmark with conventional models comparing performance of tipping point identification. We will evaluate new capabilities in terms identifying locations of importance and processes that differ shapely between models, motivating the requirement for more direct measurements and additional observable data.

- In this report we describe a study used to evaluate and benchmark the AI hybrid approach with conventional models.
- Part of this study is to understand the effects of global warming using the Al-Simulator, which may inform the need for additional observational data.
- We also include final results related to the performance integration.

### Task 5.3 Phase 2 Evaluation – Warming Scenario

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

• In this study, we understand the effects of global warming using the AI-Simulator to assist with better understanding the outcomes given a set of scenarios. We run the same scenarios using the box model and compare the outcomes.

**Experiment 1**: Starting from an AMOC-on condition and following a warming and hydrologic cycle increasing pattern, when does AMOC turn off? In this case, we include more warming at high latitudes, representative of polar amplification.

#### Parameter Setup for AMOC On Model: T0n=2; T0s=4;T0d=3; T0l=17; Fws=1e6 (1Sverdrup) Fwn 0.5e6

<u>Warming Scenario 1</u>: T0n=4; T0s=6;T0d=3; T0l=18; Fws=1.07e6 (1Sverdrup) Fwn 1.07\*0.5e6 <u>Warming Scenario 2</u>: T0n=6; T0s=8;T0d=3; T0l=19; Fws=1.14e6 (1Sverdrup) Fwn 1.14\*0.5e6 <u>Warming Scenario 3</u>: T0n=8; T0s=10;T0d=3; T0l=20; Fws=1.21e6 (1Sverdrup) Fwn 1.21\*0.5e6

### Task 5.3 Phase 2 Evaluation – Warming Scenario

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

• TIP-GAN with high confidence predicts no shut-off for all scenarios, warming 3 resulted in a shut-off for warming 3 using the box model.

Scenario	Box Model	<b>Tip-GAN Prediction</b>	Confidence
On Point	No	No	.985
Warming 1	No	No	.983
Warming 2	No	No	.979
Warming 3	Yes	No	.972

**Table 4.** Results of the three warming scenarios comparing the box model with TIP-GAN predictions. TIP-GAN and the box model are in disagreement for warming scenario 3.

### Task 5.3 Phase 2 Evaluation – CESM-2 Warming Scenario

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

• Running the same example, but instead using CESM-2 Calibrated Model and removing polar amplification, there was even higher confidence that warming 3 will not result in a shutoff. This is consistent with the box model results.

<u>Warming Scenario 1</u>: T0n=3; T0s=5;T0d=3; T0l=18; Fws=1.07e6 (1Sverdrup) Fwn 1.07\*0.5e6 <u>Warming Scenario 2</u>: T0n=4; T0s=6;T0d=3; T0l=19; Fws=1.14e6 (1Sverdrup) Fwn 1.14\*0.5e6 <u>Warming Scenario 3</u>: T0n=5; T0s=7;T0d=3; T0l=20; Fws=1.21e6 (1Sverdrup) Fwn 1.21\*0.5e6

Scenario	Shutoff?	Prediction	Confidence
Warming 1	No	No	.996
Warming 2	No	No	.993
Warming 3	No	No	.987

**Table 5.** Results of the three warming scenarios for CEMS2 Calibrated model comparing the box model with TIP-GAN predictions. TIP-GAN and the box model are in full agreement.

## Task 5.3 Phase 2 Evaluation – GISS Warming Scenario

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Ran the same examples, but instead used the GISS Calibrated Model. Both result in similar predictions. Removing polar amplification did not result in higher confidence that warming 3 will not result in a shutoff, but it was still consistent with the box model results.
- When increasing *Fwn* and keeping *Fws* and temperatures constant, TIP-GAN predicts an off state when *Fwn* is ~3x the default value (0.5e6).

Scenario	Shutoff?	Prediction	Confidence
Default	No	No	.987
Warming 1	No	No	.990
Warming 2	No	No	.992
Warming 3	Yes	No	.994

**Table 6.** Results of the three warming scenarios for the GISS calibrated model, comparing the box model with TIP-GAN predictions. TIP-GAN and the box model are in agreement.

Scenario	Shutoff?	Prediction	Confidence
Warming 1	No	No	.994
Warming 2	No	No	.993
Warming 3	No	No	.992

**Table 7.** Results of the three warming scenarios with polar amplification removed for the GISS calibrated model, comparing the box model with TIP-GAN predictions. TIP-GAN and the box model are in agreement.

### Task 5.3 Phase 2 Evaluation – Conclusions

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- In the CESM-2 model TIP-GAN predicts a shutoff when *Fwn* is nearly double (1.91x) the default value (0.5e6).
- If *T* and *Fwn* are incrementally increased to produce a shutoff prediction, TIP-GAN still does not predict a shutoff when *Fwn* is fixed and temperature is steadily increased.
- TIP-GAN's decision boundary is significantly more sensitive to changes in *Fwn* than temperature.
- TIP-GAN was trained on temperatures bounded from 2-24 Celsius. The GAN doesn't identify an off state for the warmest case (*T\_low0* = 20) or for any cases where *T\_low0* approaches 25 C.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

In this experiment:

- 1. 2000 natural language questions were randomly generated pertaining to the AMOC collapsing based on the value of 3 changing parameters (using a uniform distribution for each parameter).
- 2. Questions were translated into TIP-GAN programs.
- 3. TIP-GAN answered programs based on trained models (previously trained using the four box model).
- 4. Answers were returned to simulated researcher.
- 5. Process was compared to an actual researcher.
- 6. Total time was computed for each process.
- 7. Performance on question to program translations were computed.
- 8. Performance on answers to questions were computed.

61

### Task 5.3 Phase 2 Evaluation – Al Simulation Integration

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

• The neuro-symbolic translation from question to program was evaluated on translating the 2000 questions. The neuro-symbolic translation was able to translate every question correctly shown in Table 8. Example questions shown in Table 9.

**Note:** The questions were similar in structure, with *D***\_low0**, *Fwn*, and *M***\_ek** as the parameters that could be involved in the question (all other parameters held constant). Any combination of 1 to 2 parameters formulated the question.

	Precision	Recall	F-Measure
AMOC Off	100%	100%	100%
AMOC ON	100%	100%	100%

**Table 8**. Neuro-symbolic performance in translating natural language questions to programs. Evaluated on how accurately it translated the question to the correct program structure - it appears to have performed very well.

Example Question	<b>Program Translation</b>
if D_low0 is 142.2005075375089 and Fwn is 1020814.0505557163, does the AMOC collapse?	ChangeSign(four_box_mode I(SetTo(D_low0,142.200507 5375089),SetTo(Fwn,10208 14.0505557163)),M_n)

Table 9. Example question and TIP-GAN ProgramTranslation. (Note: **D\_low0** is the parameter forthermocline depth of the lower latitudes and **Fwn** is theparameter for freshwater flux in the North.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- The TIP-GAN was trained using the four box model. The trained TIP-GAN was then used to answer the questions provided by the neuro-symbolic model.
- Results are shown in Table 10 and Figure 42.

	Precision	Recall	F-Measure
AMOC Off	99.602%	100%	99.8%
AMOC ON	100%	99.600%	99.8%

**Table 10.** TIP-GAN Prediction Performance for the 2000 questions translated into programs.

**Note:** The programs were used to directly predict AMOC On/Off for each question, as opposed to running the four box model to obtain the answer.



*Figure 42.* TIP-GAN Prediction Performance Confusion Matrix for the 2000 questions translated into programs.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

	Neuro-symbolic Translation	<b>TIP-GAN Prediction</b>	Full AI Simulation
Total Average Time in seconds	0.04	0.0000054	0.045

**Table 11.** In this table we show the average time in seconds to perform the translation from question to program and to obtain an answer to the program. The final column is the overall AI Simulation total time.

	Four Box Model Run (Python)	<b>TIP-GAN Prediction</b>
Total Average Time in seconds	0.96	0.0000054

**Table 12.** In this table we show the average time in seconds, comparing running the four box model to obtain an answer to a question as opposed to getting the prediction from the TIP-GAN.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

Oceanographer simulating answering a question.

**Question**: If Ekman Flux is 28226923.55 and Northern Hemisphere Freshwater Flux is 840575.51, does the AMOC collapse?

Answer: Yes

	Human Question to Program translation	Running the Four Box Model in Matlab	Human Interpretation of answer
Total Time in seconds	360	0.32	180

**Table 13.** Estimated Time Performance for a single example question to program translation and execution of four box model to obtain an answer.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- We extended the complexity of the questions used and generated 19 different question types.
- We performed a 90/10 split for training and test sets
  - $\circ$  250,000 train samples
  - o 12,500 test samples



*Figure 43. Distribution of Questions Used for Training the Neuro-symbolic Networks.* 

Question Type	Example
1	What is the value of the overturning in the north latitudes at time step 3441 if the freshwater flux in the north latitude is 54785.814174809064?
2	If the Redi coefficient is 966.1041715067744 and the lower latitude initial thermocline depth is 367.03168813434985, does the AMOC collapse?
3	What is the final value of the AMOC when the initial salinity of the northern box is 31.90016602053442?
4	What is the nearest point to the current configuration with the AMOC off?
5	Find the nearest point to the current configuration with the AMOC off.
6	Does Fwn collapse the AMOC at 47887.43025295444?
7	Find the nearest point to the current configuration with the AMOC on, only varying the following parameters: the value of epsilon, the interface height diffusion coefficient, the initial temperature of the shallow ocean, the initial salinity of the shallow ocean, the initial salinity of the deep ocean, the area of the northern box.
8	If I set M_SD to 16376895.649532888, the freshwater flux in the southern latitude to 998459.5946592593, and the total model area to 371951331002107.25, will the overturning in the parth latitudes increase?
0	If I decrease the initial temperature of the deep ocean by 0.42685610126021595, will the north atlantic deep water formation rate decrease 2
9	By increasing the initial temperature of the northern box by 0.20513786641511758, will salinity in the southern latitudes decrease?
11	Given the starting vector, with Fws now allowed to vary from 0.0 to 1500000.0, does increasing Fws increase AMOC according to the GAN?
12	Find the nearest 4 points to the current configuration with the AMOC on.
13	Given the starting vector, vary epsilon between 0.00017769398928617632 and 0.00018038463322936978. For what values is AMOC "OFF"?
14	Given the starting vector, vary the initial temperature of the southern ocean between 2.5798667083604157 and 11.195587818693213, and the freshwater flux in the southern latitude between 500565.1088961287 and 871885.0115239422. For what values is AMOC "ON"?
15	Given the starting vector, vary the resistance to overturning between 0.0001860342067503932 and 0.00019679077103575926. For what values is AMOC "ON"? What are the largest 29 values for which the AMOC is an?
15	From the given point, what fraction of the neighbors within plus or minus 55 percent of each variables current value have AMOC off
17	From the nearest point to the starting vector where the AMOC is on, find the nearest point increasing M_SD where the AMOC is on. Use the GAN to determine AMOC state.
18	From the starting vector, and according to the GAN, does decreasing the initial salinity in the north or decreasing the time step produce a closer AMOC on state?
19	From the nearest point to the starting vector where the AMOC is off, and according to the four box model, does hosing or climate warming get us to a AMOC on point closer to the starting vector?
Table 14. E	xample Questions Based on Templates Used for Training the
Neuro-symb	polic Networks

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery



The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery



*Figure 46.* Combined mean cosine similarity by translation type Great performance on all three translations.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery



*Figure 48.* Combined mean Bleu score by translation type. Great performance on all three translations.

*Figure 49.* CDF of combined mean Bleu score by translation type. Great performance on all three translations.

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery



*Figure 50.* Combined mean equality score by translation type. Great performance on all three translations.

*Figure 51.* CDF of combined mean equality score by translation type. Great performance on all three translations.

### Final Remarks and Conclusions – TIP-GAN

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- In a short period of time we formed a **multi-disciplinary team** that had never worked together prior to this effort.
- We developed a new **TIP-GAN** AI-based assisted climate modeling approach that includes a **neuro-symbolic translation** model for translating between natural questions and programs.
- We showed that the TIP-GAN can in fact learn bifurcations in parameter space and that together a substantial speedup can be obtained when compared with a typical scientific discovery process flow both in converting questions to programs and in answering questions.

### **Final Remarks and Conclusions - Insights and Six Box Model** The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- We showed how TIP-GAN could be trained using the four box model as an oracle, and that the Al approach to discovering tipping points can lead to new insights and shortcomings in existing models. This motivated the effort to develop the six box model.
- The six box model models the overturning behavior in terms of the Atlantic and Pacific. It reflects more of the **complexities of the AMOC** than in the four box model.
- Bifurcation analysis applied to six box model show high degrees of complexity in terms of the bifurcations.

### **Final Remarks and Conclusions – Large GCMs**

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- By calibrating box models to large GCMs, there is a path forward in applying PACMANs to the large GCMs.
- We showed that the box models reasonably represent the **dynamics of the CESM2** model when calibrated to the box model.
- We were able to obtain a **measure of uncertainty** regarding the ensemble member spread across three key parameters. This will provide additional insights of model disagreement.
### Final Remarks and Conclusions – Al Simulator

The Physics-informed AI Climate Model Agent Neuro-symbolic Simulator (PACMANS) for Tipping Point Discovery

- Evaluations shows that the AI Simulator is **both efficient and accurate** in terms of predicting AMOC collapse.
- Benchmarks shows that the AI Simulator uncovers interesting sensitivities to model parameters that could inform how large modeling efforts should be conducted.
- **Causal models** showed correlations between parameters that warrant further investigation.



### JOHNS HOPKINS APPLIED PHYSICS LABORATORY

#### Citations

- 1. Boers, Niklas. "Observation-based early-warning signals for a collapse of the Atlantic Meridional Overturning Circulation." Nature Climate Change 11, no. 8 (2021): 680-688.
- 2. Gnanadesikan, A., A simple model for the structure of the oceanic pycnocline, Science., 283:2077-2079, (1999).
- 3. Forget, G., J.-M. Campin, P. Heimbach, C. N. Hill, R. M. Ponte, C. Wunsch, ECCO version 4: An integrated framework for non-linear inverse modeling and global ocean state estimation. Geosci. Model Dev. 8, 3071–3104 (2015)
- 4. Gnanadesikan, A., R. Kelson and M. Sten, Flux correction and overturning stability: Insights from a dynamical box model, J. Climate, 31, 9335-9350, https://doi.org/10.1175/JCLI-D-18-0388.1, (2018).
- 5. Kaufhold, John Patrick, and Jennifer Alexander Sleeman. "Systems and methods for deep model translation generation." U.S. Patent No. 10,504,004. 10 Dec. 2019.
- 6. Garcez, Artur d'Avila, and Luis C. Lamb. "Neurosymbolic AI: the 3rd Wave." arXiv preprint arXiv:2012.05876 (2020).
- 7. Stommel, H. Thermohaline convection with two stable regimes of flow. Tellus 13, 224–230 (1961).
- 8. Karniadakis, George Em, Ioannis G. Kevrekidis, Lu Lu, Paris Perdikaris, Sifan Wang, and Liu Yang. "Physics-informed machine learning." Nature Reviews Physics 3, no. 6 (2021): 422-440.
- 9. Sleeman, Jennifer, Milton Halem, Zhifeng Yang, Vanessa Caicedo, Belay Demoz, and Ruben Delgado. "A Deep Machine Learning Approach for LIDAR Based Boundary Layer Height Detection." In IGARSS 2020-2020 IEEE International Geoscience and Remote Sensing Symposium, pp. 3676-3679. IEEE, 2020.
- 10. Patel, Kinjal, Jennifer Sleeman, and Milton Halem. "Physics-aware deep edge detection network." In Remote Sensing of Clouds and the Atmosphere XXVI, vol. 11859, pp. 32-38. SPIE, 2021.
- 11. Brulé, Joshua. "A causation coefficient and taxonomy of correlation/causation relationships." arXiv preprint arXiv:1708.05069 (2017).
- 12. Rasp, Stephan, Michael S. Pritchard, and Pierre Gentine. "Deep learning to represent subgrid processes in climate models." Proceedings of the National Academy of Sciences 115, no. 39 (2018): 9684-9689.
- 13. Bolton, Thomas, and Laure Zanna. "Applications of deep learning to ocean data inference and subgrid parameterization." Journal of Advances in Modeling Earth Systems 11, no. 1 (2019): 376-399.
- Kurth, Thorsten, Sean Treichler, Joshua Romero, Mayur Mudigonda, Nathan Luehr, Everett Phillips, Ankur Mahesh et al. "Exascale deep learning for climate analytics." In SC18: International Conference for High Performance Computing, Networking, Storage and Analysis, pp. 649-660. IEEE, 2018.

# **Citations cont.**

- 15. Weber, Theodore, Austin Corotan, Brian Hutchinson, Ben Kravitz, and Robert Link. "Deep learning for creating surrogate models of precipitation in Earth system models." Atmospheric Chemistry and Physics 20, no. 4 (2020): 2303-2317.
- 16. Matsubara, Takashi, Ai Ishikawa, and Takaharu Yaguchi. "Deep energy-based modeling of discrete-time physics." arXiv preprint arXiv:1905.08604 (2019).
- 17. Kleinen, T., Held, H. & Petschel-Held, G. The potential role of spectral properties in detecting thresholds in the Earth system: application to the thermohaline circulation. Ocean Dyn. 53, 53–63 (2003).
- 18. Kocaoglu, Murat, Christopher Snyder, Alexandros G. Dimakis, and Sriram Vishwanath. "Causalgan: Learning causal implicit generative models with adversarial training." arXiv preprint arXiv:1709.02023 (2017).
- 19. Feinman, Reuben, and Brenden M. Lake. "Learning Task-General Representations with Generative Neuro-Symbolic Modeling." arXiv preprint arXiv:2006.14448 (2020).
- 20. Yi, Kexin, Chuang Gan, Yunzhu Li, Pushmeet Kohli, Jiajun Wu, Antonio Torralba, and Joshua B. Tenenbaum. "Clevrer: Collision events for video representation and reasoning." arXiv preprint arXiv:1910.01442 (2019).
- 21. Nowack, Peer, Jakob Runge, Veronika Eyring, and Joanna D. Haigh. "Causal networks for climate model evaluation and constrained projections." Nature communications 11, no. 1 (2020): 1-11.
- 22. Andersson, Tom R., J. Scott Hosking, María Pérez-Ortiz, Brooks Paige, Andrew Elliott, Chris Russell, Stephen Law et al. "Seasonal Arctic sea ice forecasting with probabilistic deep learning." Nature communications 12, no. 1 (2021): 1-12.
- 23. Storchan, Victor, Svitlana Vyetrenko, and Tucker Balch. "MAS-GAN: Adversarial Calibration of Multi-Agent Market Simulators." (2020).
- 24. De Raedt, Luc, Robin Manhaeve, Sebastijan Dumancic, Thomas Demeester, and Angelika Kimmig. "Neuro-symbolic=neural+ logical+ probabilistic." In NeSy'19@ IJCAI, the 14th International Workshop on Neural-Symbolic Learning and Reasoning. 2019.
- 25. Eyring, V., Bony, S., Meehl, G. A., Senior, C. A., Stevens, B., Stouffer, R. J., and Taylor, K. E.: Overview of the Coupled Model Intercomparison Project Phase 6 (CMIP6) experimental design and organization, Geosci. Model Dev., 9, 1937-1958, doi:10.5194/gmd-9-1937-2016, 2016.
- Swingedouw, Didier, Chinwe Ifejika Speranza, Annett Bartsch, Gael Durand, Cedric Jamet, Gregory Beaugrand, and Alessandra Conversi.
  "Early warning from space for a few key tipping points in physical, biological, and social-ecological systems." Surveys in geophysics 41, no. 6 (2020): 1237-1284.
- 27. Reichstein, Markus, Gustau Camps-Valls, Bjorn Stevens, Martin Jung, Joachim Denzler, and Nuno Carvalhais. "Deep learning and process understanding for data-driven Earth system science." Nature 566, no. 7743 (2019): 195-204.

## **Citations cont.**

- 28. Sleeman, Jennifer, Ivanka Stajner, Christoph Keller, Milton Halem, Christopher Hamer, Raffaele Montuoro, and Barry Baker. "The Integration of Artificial Intelligence for Improved Operational Air Quality Forecasting." In AGU Fall Meeting 2021. 2021.
- 29. Bellomo, K., Angeloni, M., Corti, S. *et al.* Future climate change shaped by inter-model differences in Atlantic meridional overturning circulation response. *Nat Commun* **12**, 3659 (2021). <u>https://doi.org/10.1038/s41467-021-24015-w</u>
- 30. Sgubin, G., Swingedouw, D., Drijfhout, S. *et al.* Abrupt cooling over the North Atlantic in modern climate models. *Nat Commun* **8**, 14375 (2017). <u>https://doi.org/10.1038/ncomms14375</u>
- Swingedouw, D., Bily, A., Esquerdo, C., Borchert, L. F., Sgubin, G., Mignot, J., & Menary, M. (2021). On the risk of abrupt changes in the North Atlantic subpolar gyre in CMIP6 models. *Annals of the New York Academy of Sciences*, 1504(1), 187-201. <u>https://doi.org/10.1111/nyas.14659</u>
- 32. Mao, Jiayuan, Chuang Gan, Pushmeet Kohli, Joshua B. Tenenbaum, and Jiajun Wu. "The neuro-symbolic concept learner: Interpreting scenes, words, and sentences from natural supervision." *arXiv preprint arXiv:1904.12584* (2019).