KU LEUVEN

VLAAMS SUPERCOMPUTER CENTRUM

Vlaanderen is supercomputing

ML in traditional HPC simulations

George Miloshevich

CmPA / Dept. Mathematics

MARIE CURIE ACTIONS
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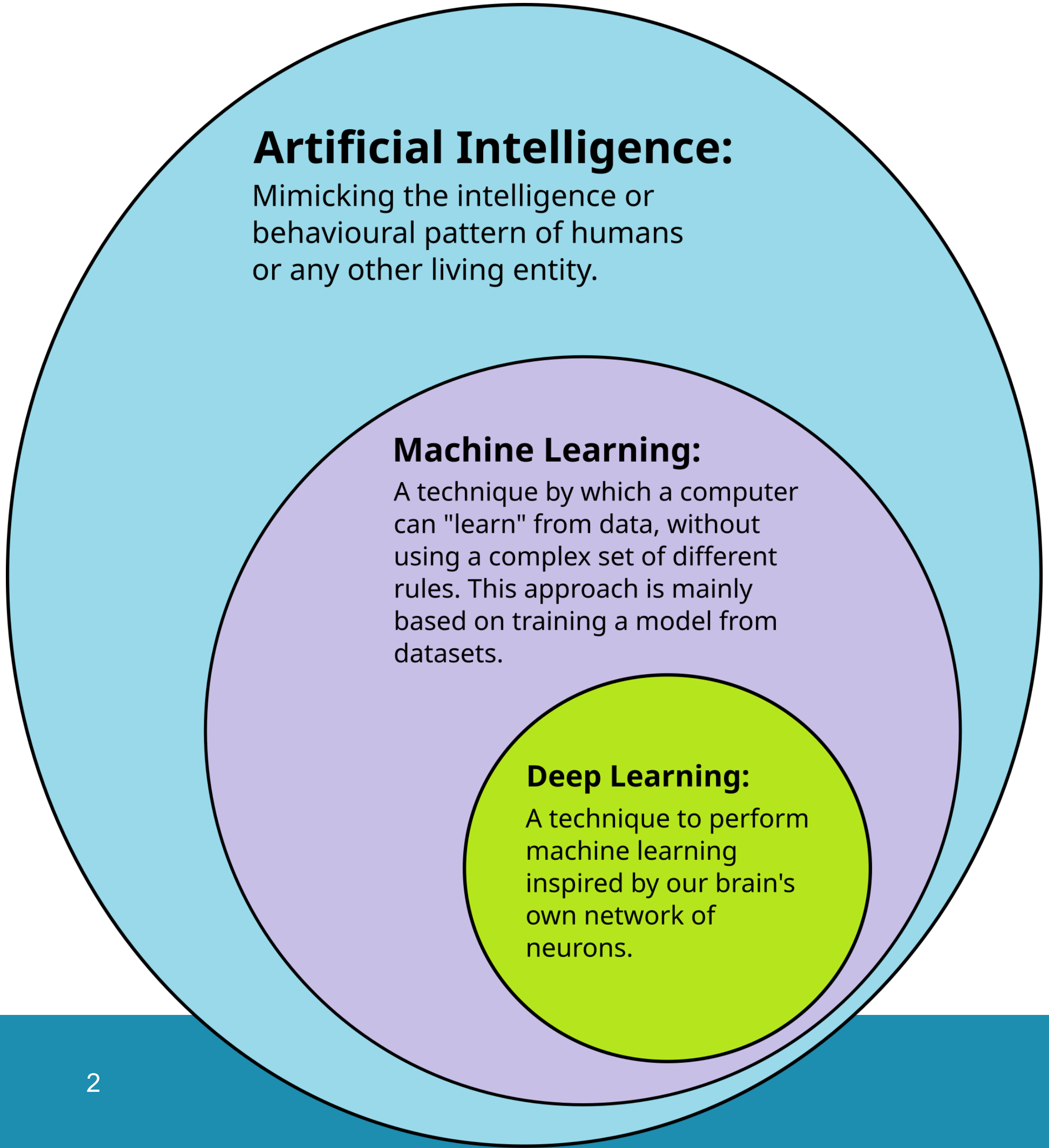
Funded by the European Union
ASAP Automatics in Space Exploration
cpa

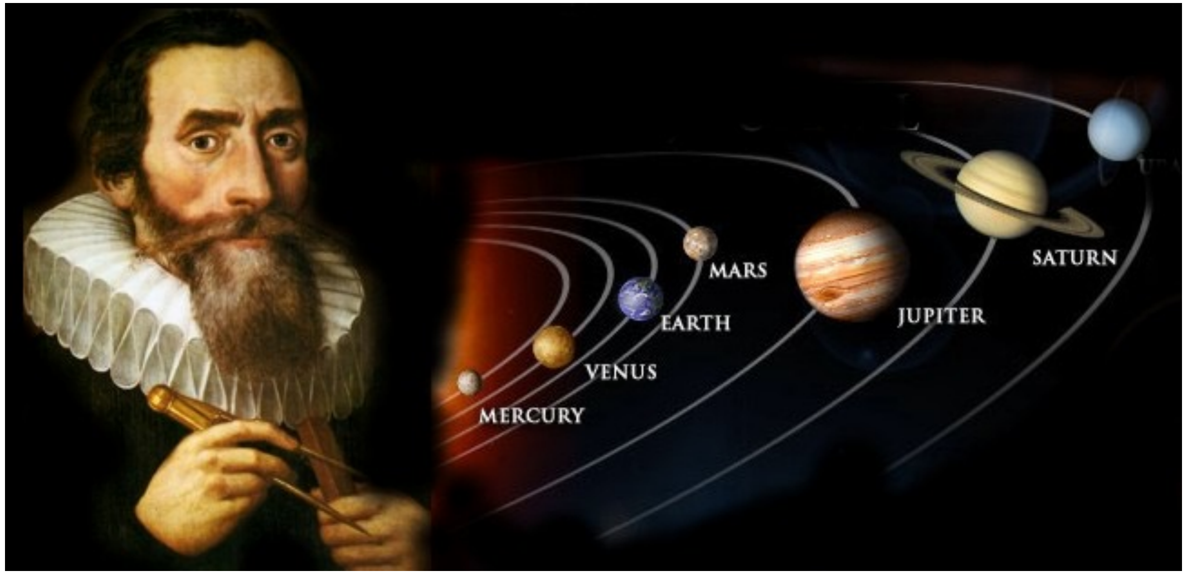
What is Machine Learning/ AI?

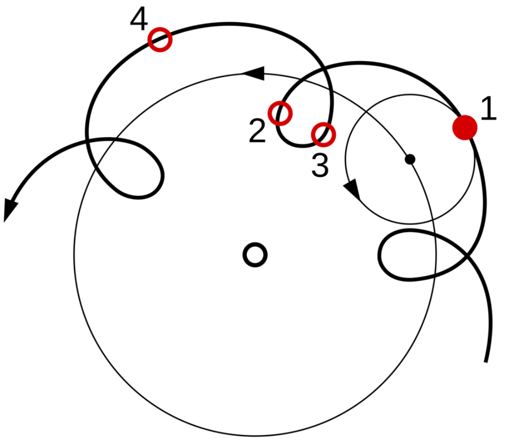


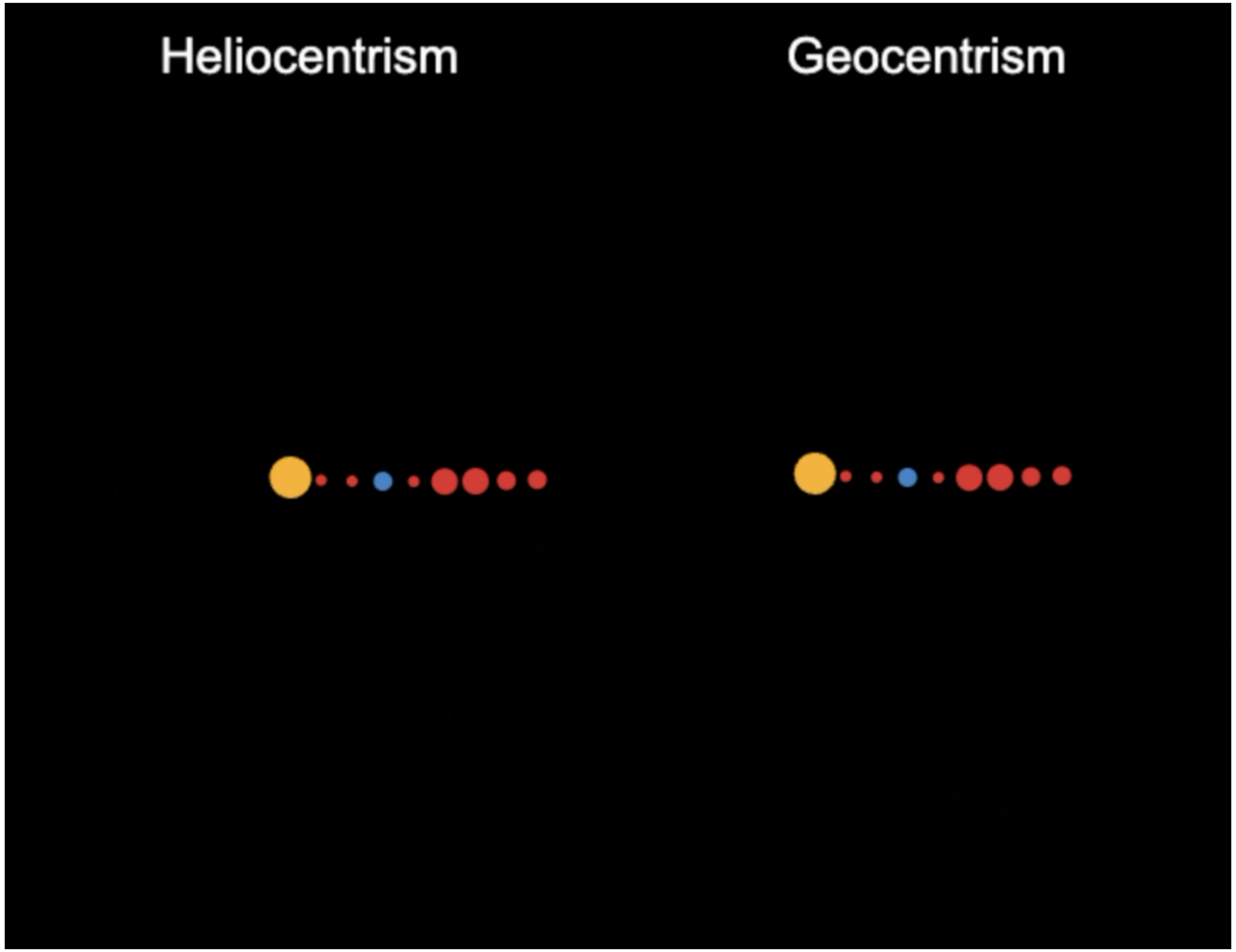
AlphaGo competing against legendary Go player Lee Sedol

Learning from Data

Understanding optimal coordinates in data



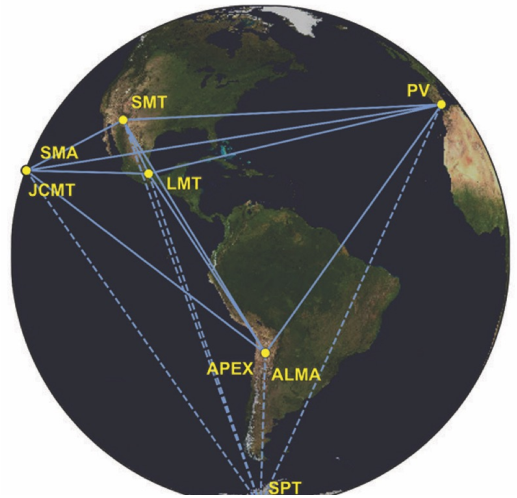


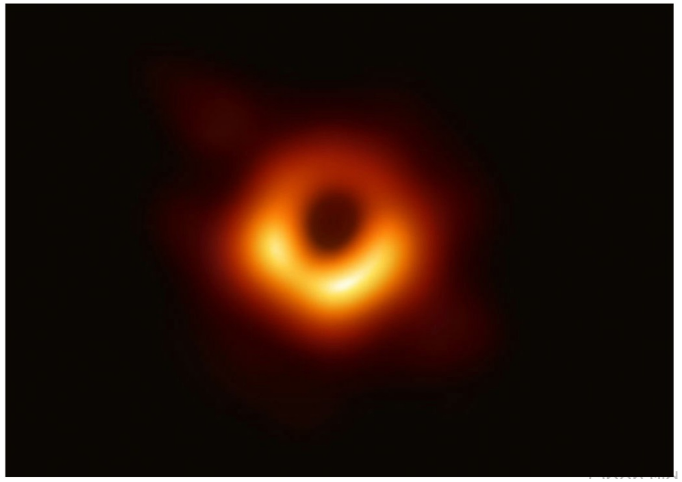


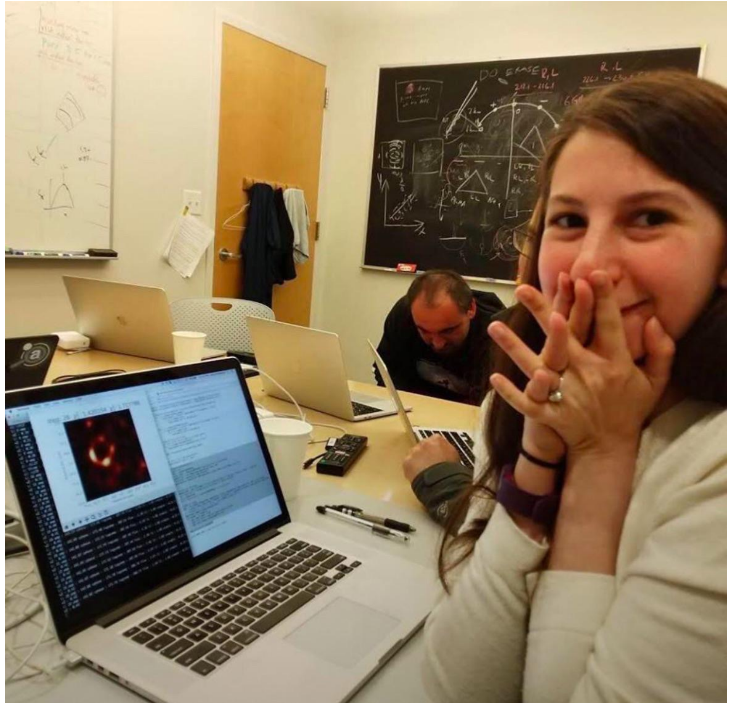
Big Data Requires Automated Analysis

In the last century, you could publish your observation data as a part of your manuscript and analyze them using pen and paper.

- Recent projects might generate Petabytes of data that needs to shipped across the globe.



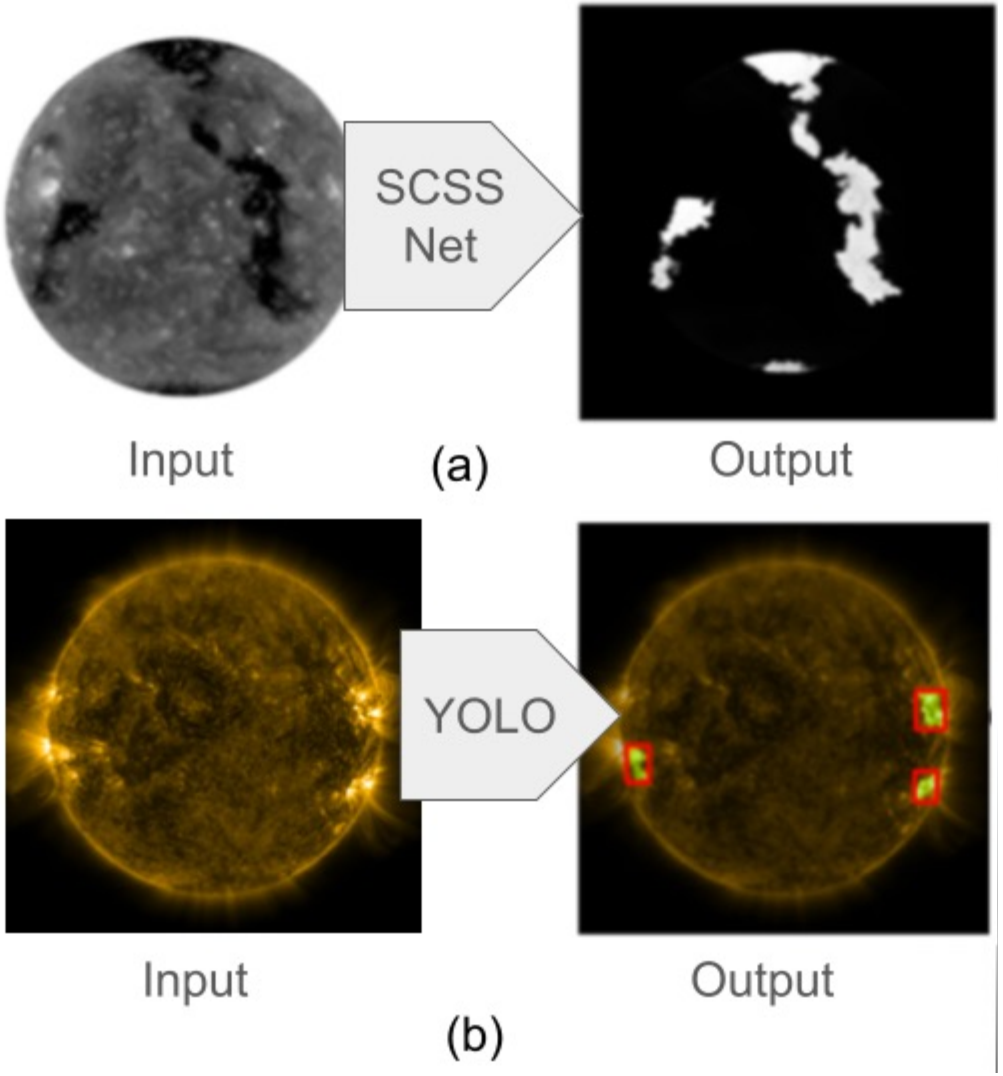


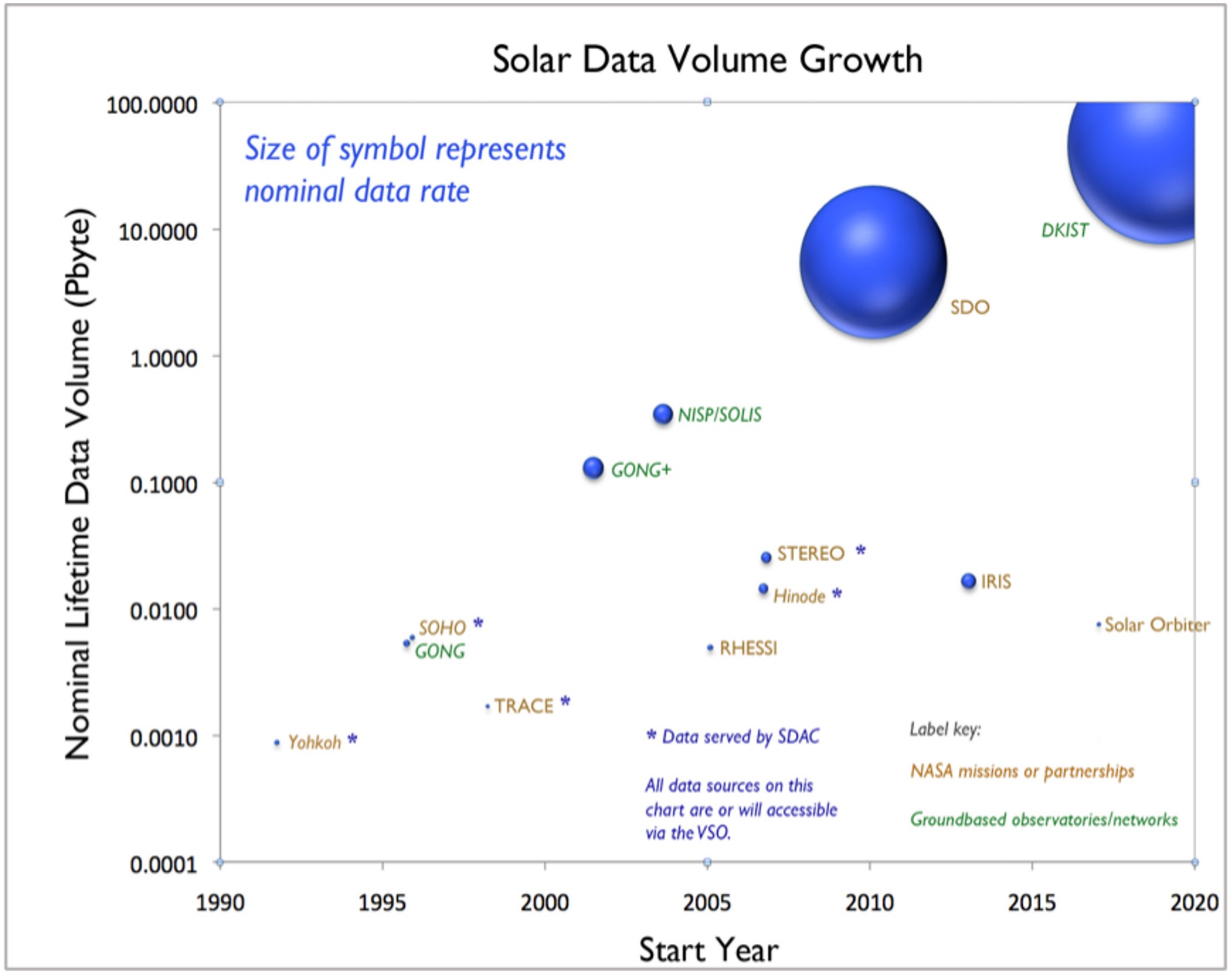


CHIRP (**Continuous High-resolution Image Reconstruction using Patch priors**) is a Bayesian algorithm used to perform a deconvolution on images created in radio astronomy. The acronym was coined by lead author Katherine L. Bouman in 2016

K. Bouman et al 2016 IEEE

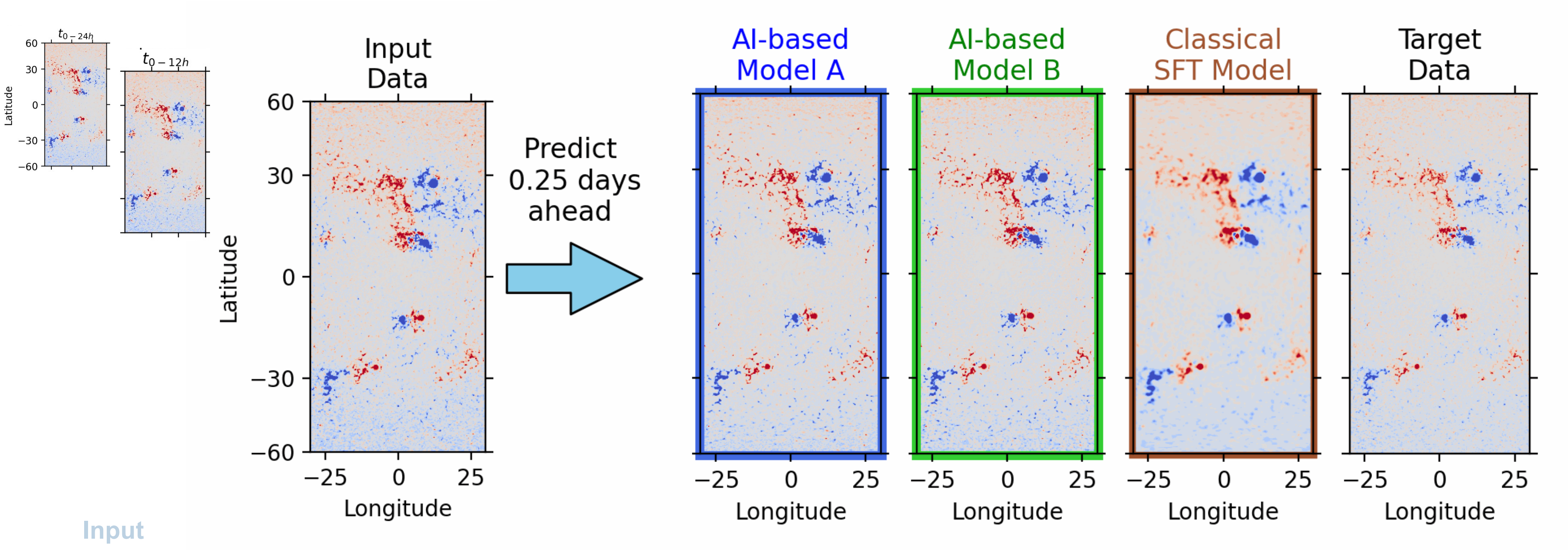
ML Applications in science: Detection of events

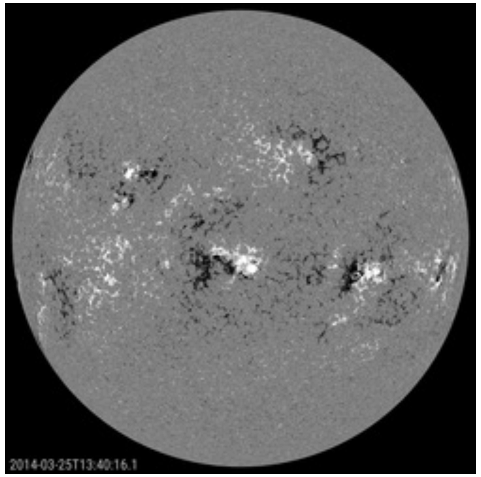




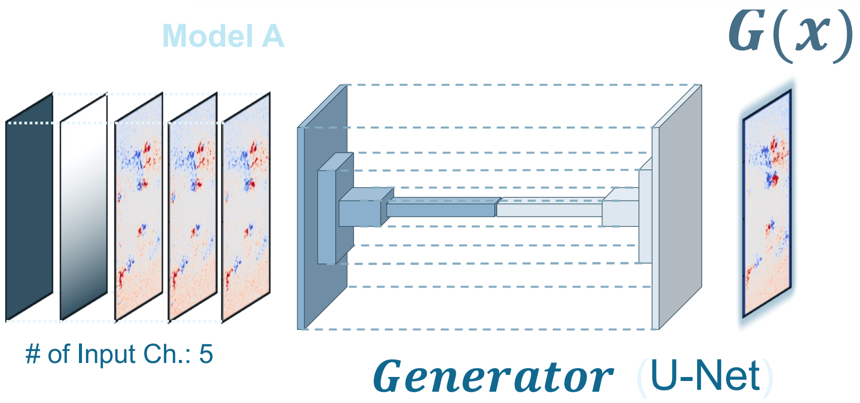
P. Gonidakis, F. Carella, E. Dineva, H-J. Jeong, P. Antunes, A. Podobas, S. Raptis, V. Toy-Edens, M. Jin, S. Poedts, J. Magdalenic, **G. Miloshevich**: submitted to JGR: ML & Comp

Machine learning in magnetogram prediction





Solar magnetogram

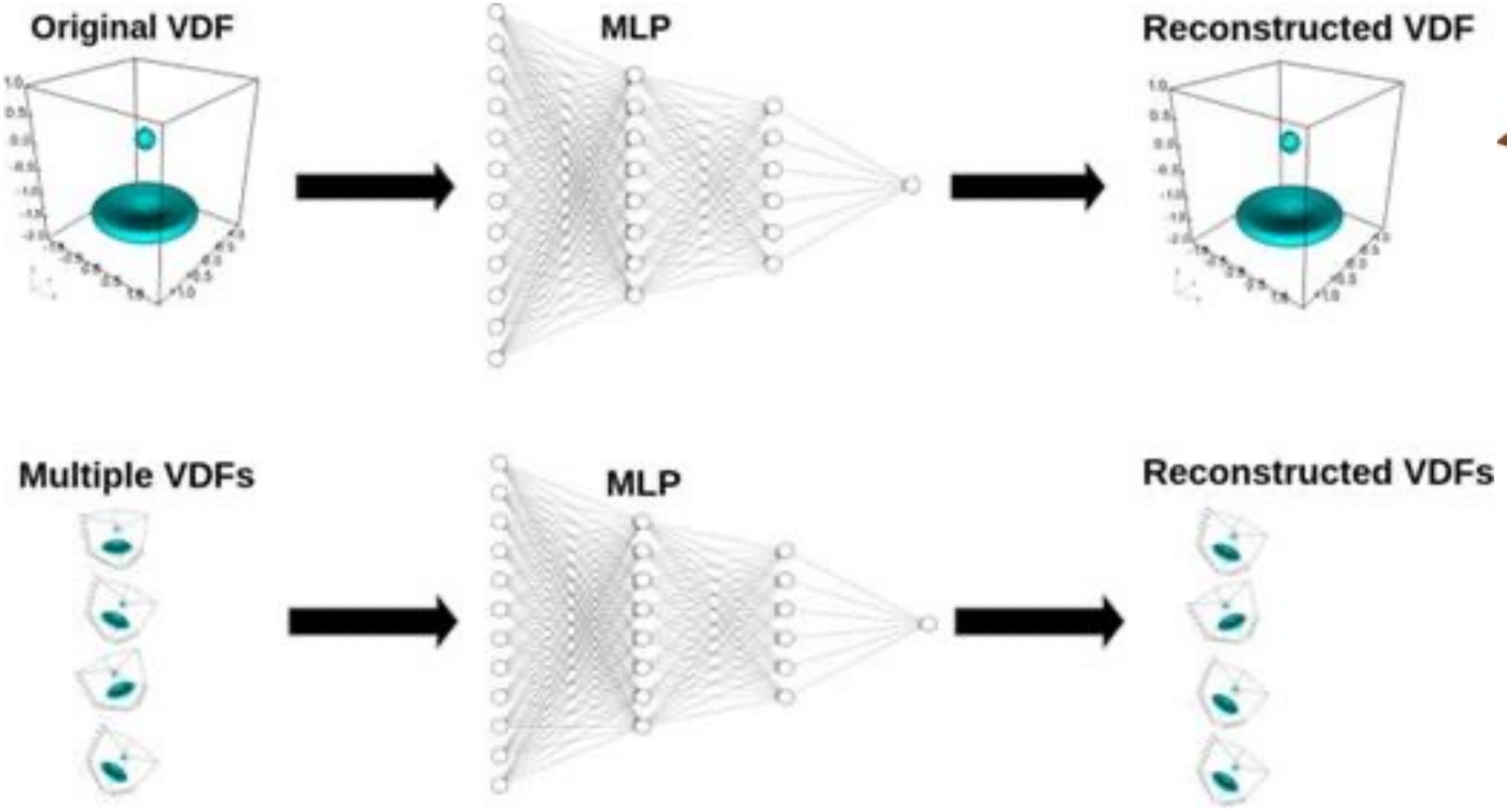


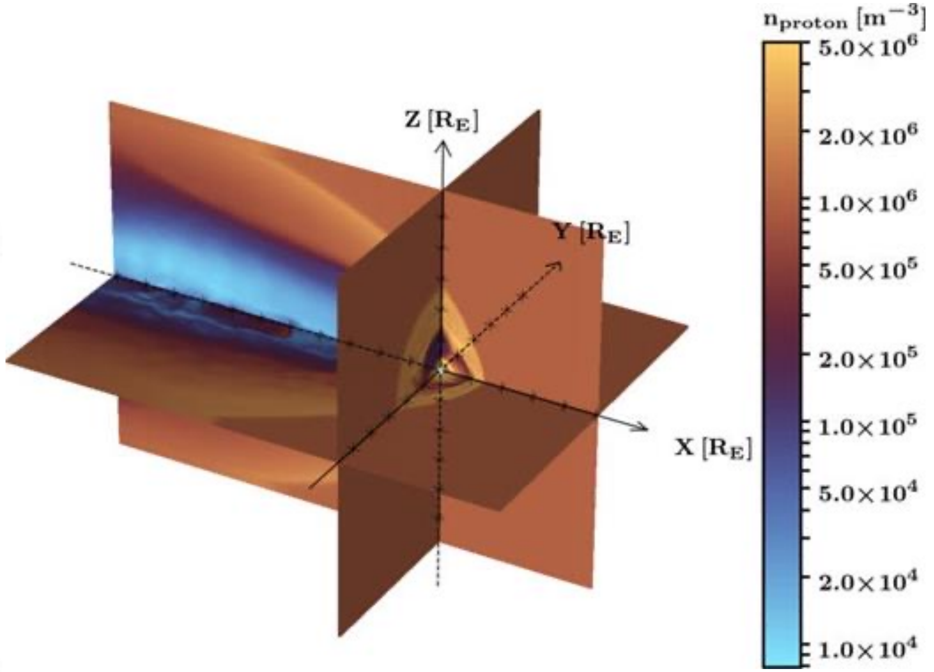
Surface Flux Transport Model:

$$\frac{\partial B_r}{\partial t} + \nabla_h \cdot (\mathbf{u}_h B_r) = \eta \nabla_h^2 B_r + S,$$

Smart checkpointing: compressing saved sims

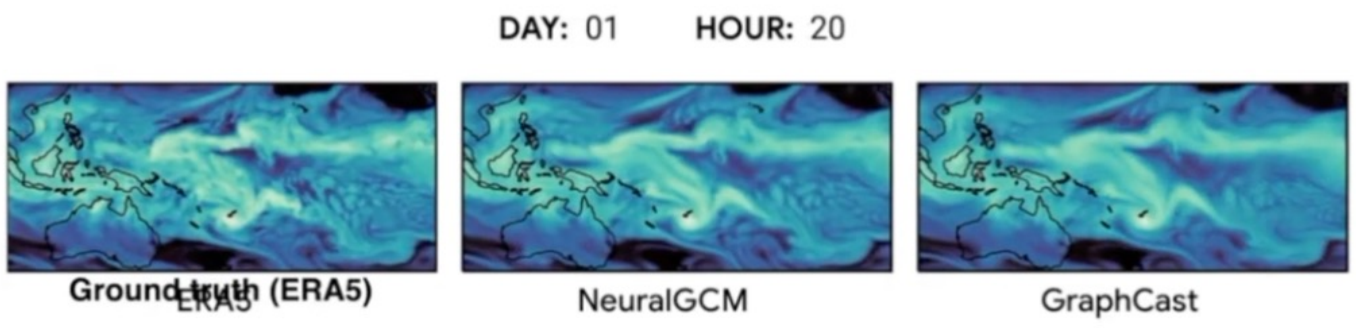
$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \frac{\partial f_s}{\partial \mathbf{x}} + \frac{e_s}{m_s} \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \cdot \frac{\partial f_s}{\partial \mathbf{v}} = 0,$$

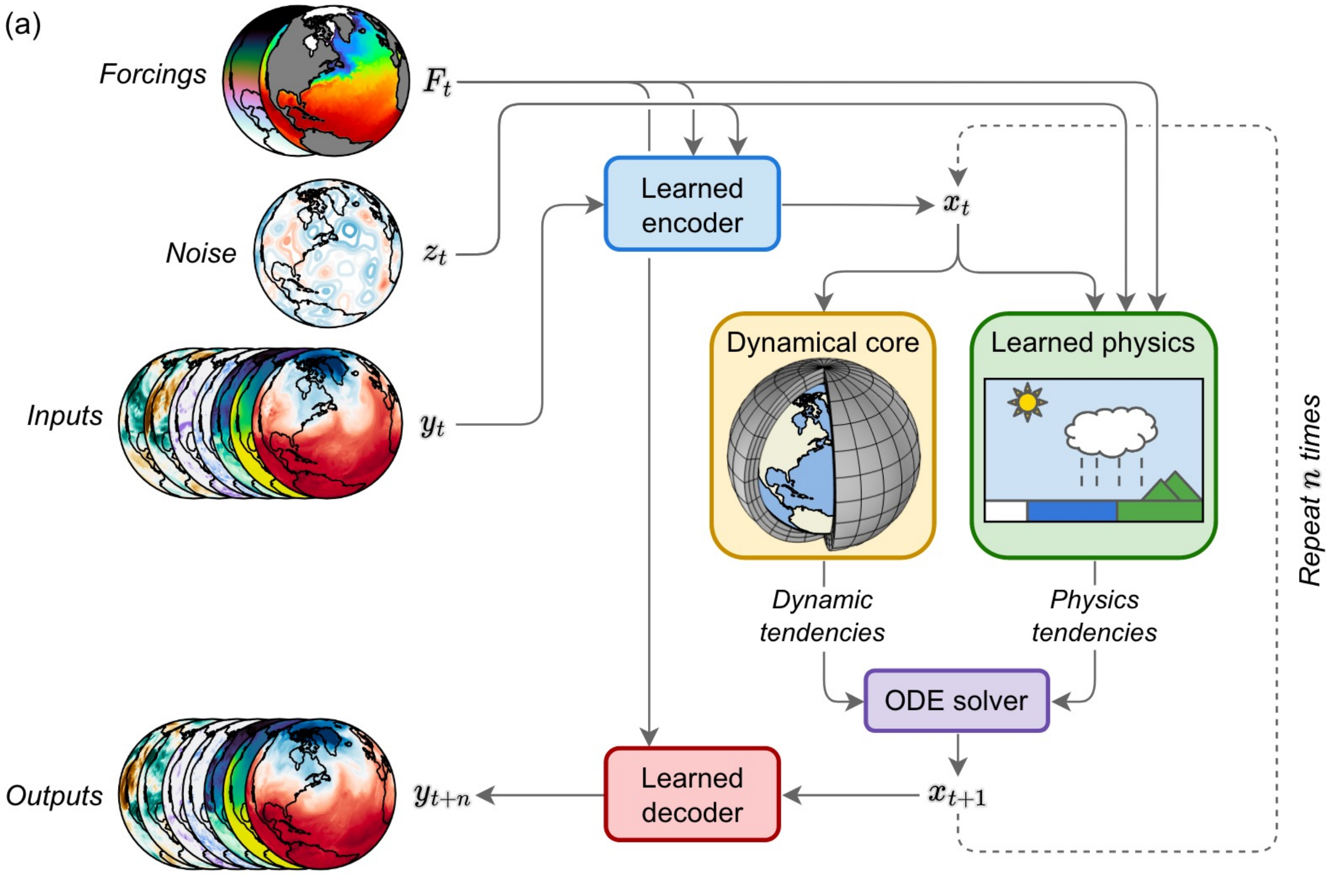


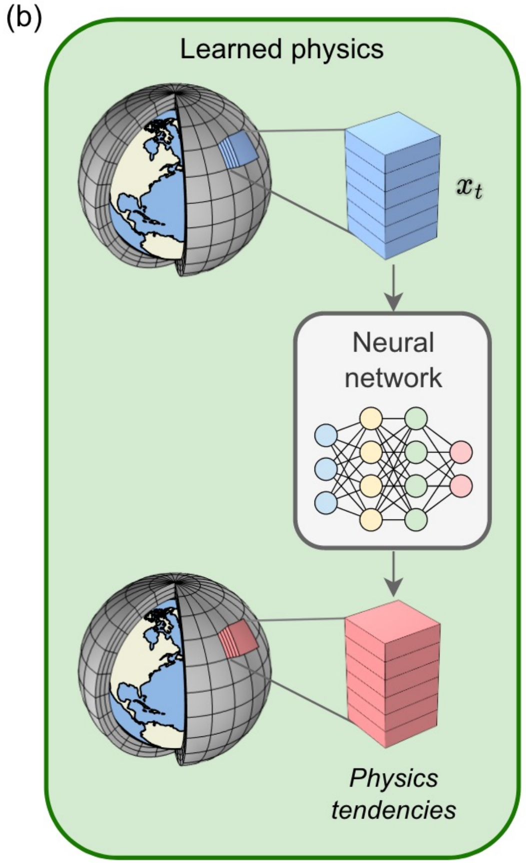


 K. Papadakis, M. Alho, J. Kataja, I. Bouri, A. Kit, J. Heikonen, M. Palmroth, Phys. Plasmas 32 (2025) 113905.

Subgrid closure

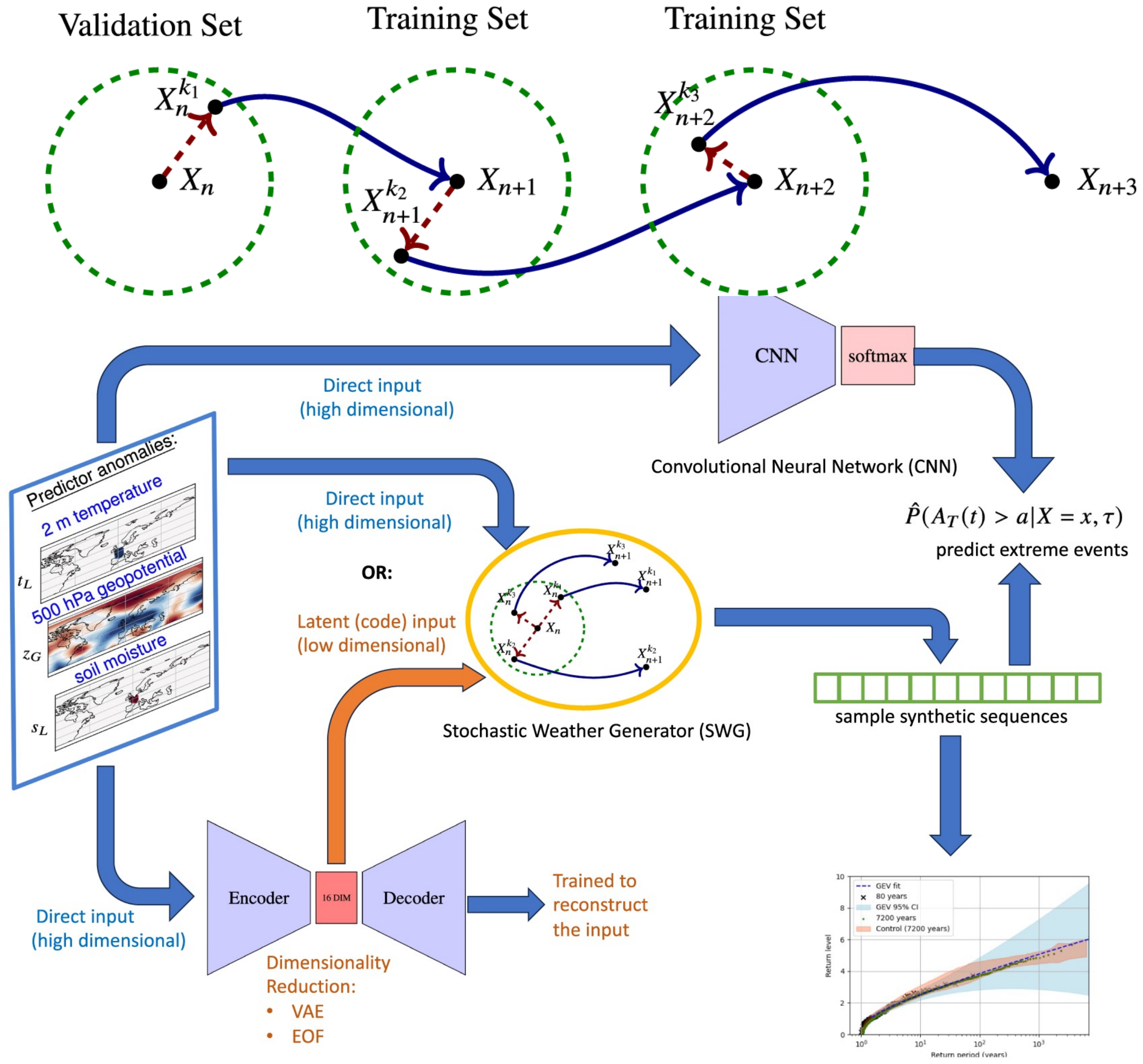


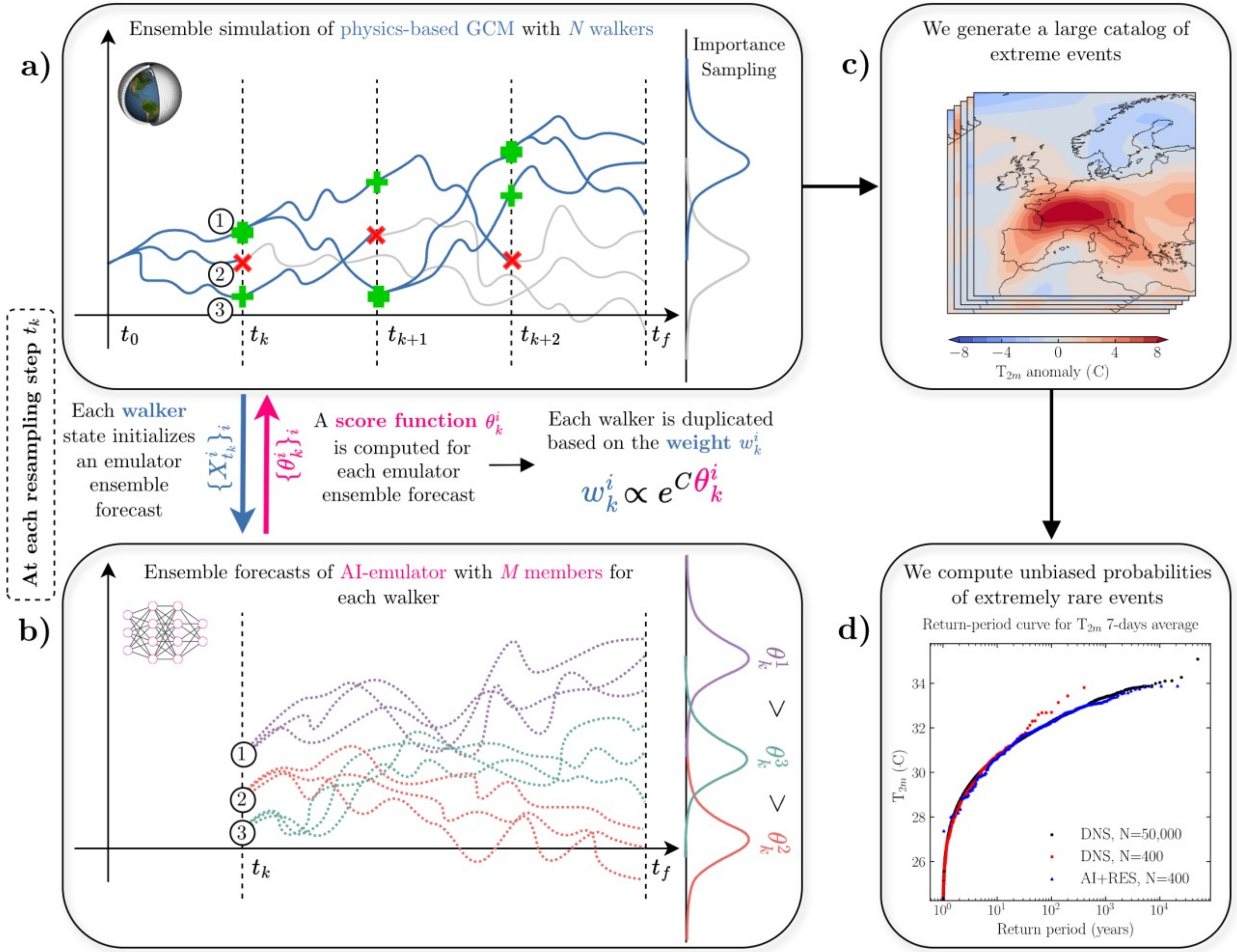




 Kochkov, D. et al *Neural General Circulation Models for Weather and Climate*. ***Nature* 2024**, *632* (8027)

Using surrogates for extreme value analysis





G. Miloshevich, D. Lucente, P. Yiou, F. Bouchet, Environmental Data Science 3 (2024) e9.
A. Lancelin, A. Wikner, L. Dubus, C.L. Priol, D.S. Abbot, F. Bouchet, P. Hassanzadeh, J. Weare, (2026).

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations

M Raissi, P Perdikaris, GE Karniadakis - Journal of Computational **physics**, 2019 - Elsevier

… We introduce **physics-informed neural networks** – **neural networks** that are trained to solve supervised learning tasks while respecting any given laws of **physics** described by general …

Forward Problem:

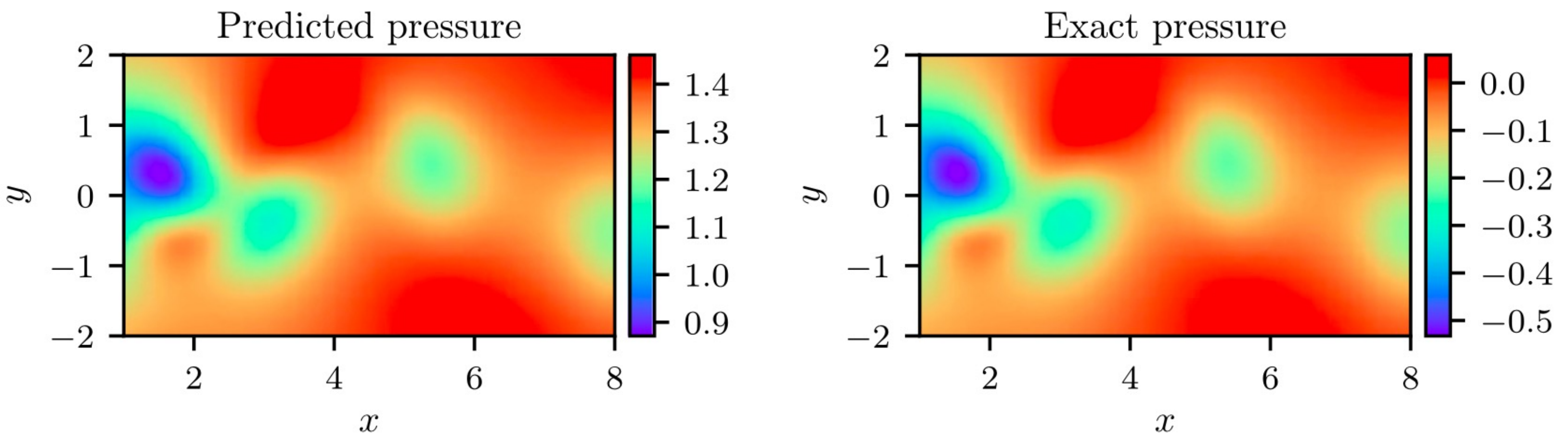
$$u_t + \mathcal{N}[u] = 0,\ x \in \Omega,\ t \in [0, T]$$

$$MSE = MSE_u + MSE_f$$

$$MSE_u = \frac{1}{N_u}\sum_{i=1}^{N_u} |u(t_u^i, x_u^i) - u^i|^2,$$

$$MSE_f = \frac{1}{N_f}\sum_{i=1}^{N_f} |f(t_f^i, x_f^i)|^2.$$

Inverse Problem:



Correct PDE	$u_t + (uu_x + vu_y) = -p_x + 0.01(u_{xx} + u_{yy})$ $v_t + (uv_x + vv_y) = -p_y + 0.01(v_{xx} + v_{yy})$
Identified PDE (clean data)	$u_t + 0.999(uu_x + vu_y) = -p_x + 0.01047(u_{xx} + u_{yy})$ $v_t + 0.999(uv_x + vv_y) = -p_y + 0.01047(v_{xx} + v_{yy})$
Identified PDE (1% noise)	$u_t + 0.998(uu_x + vu_y) = -p_x + 0.01057(u_{xx} + u_{yy})$ $v_t + 0.998(uv_x + vv_y) = -p_y + 0.01057(v_{xx} + v_{yy})$

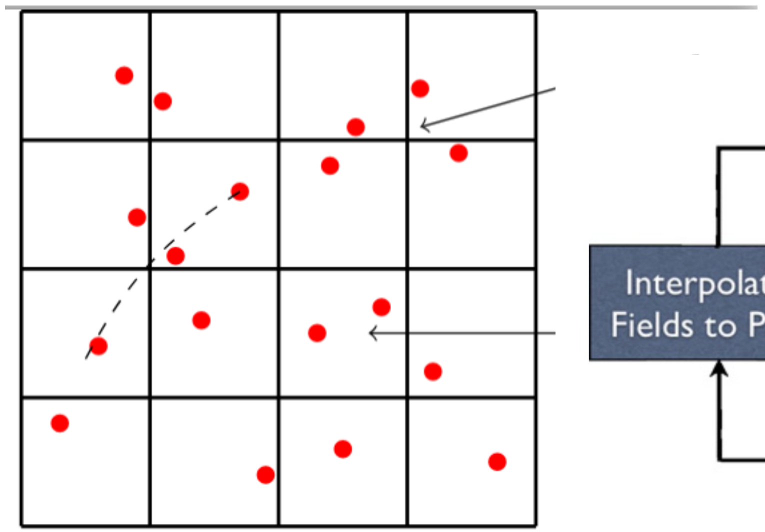
 M. Raissi, P. Perdikaris, G.E. Karniadakis, Journal of Computational Physics 378 (2019) 686–707.

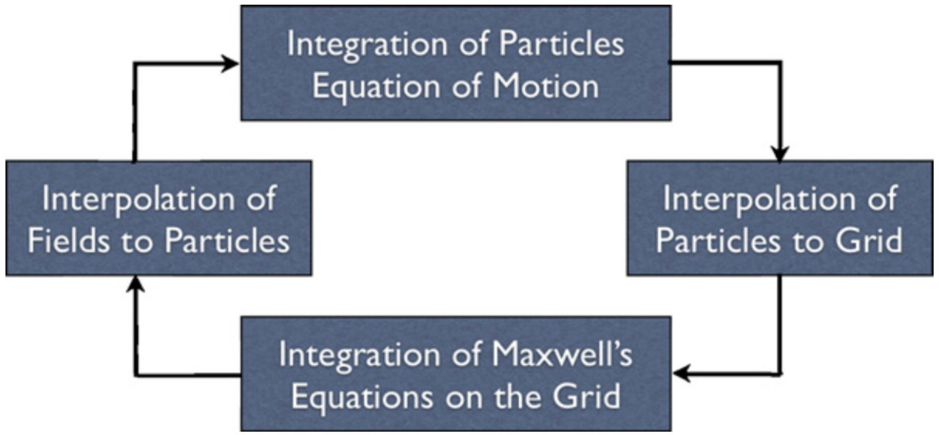
The model hierarchy in collisionless plasmas

$k > d_i, \rho_i$

- Kinetic Modelling, Particle in Cell (PIC)

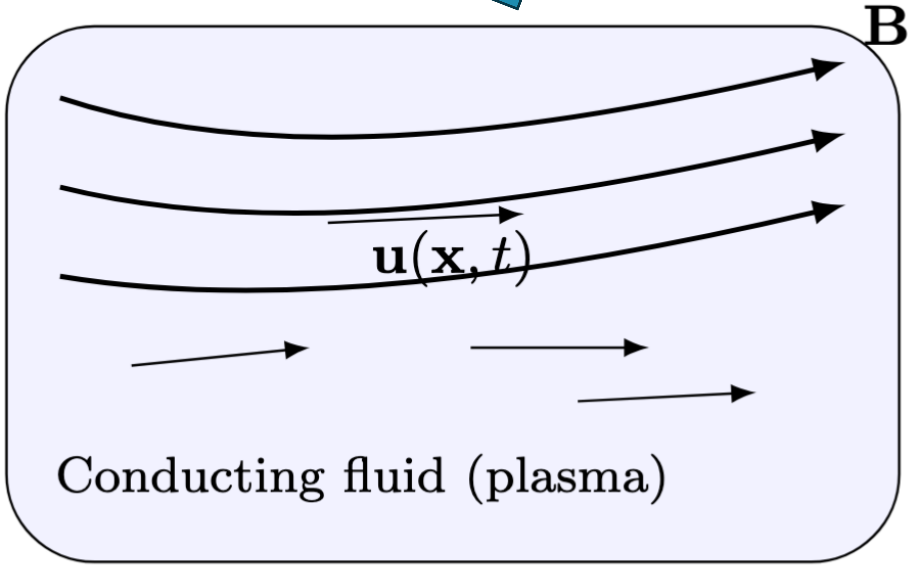
$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \frac{\partial f_s}{\partial \mathbf{x}} + \frac{e_s}{m_s}\left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c}\right) \cdot \frac{\partial f_s}{\partial \mathbf{v}} = 0,$$





- MHD (fluid modelling)

$$\rho\left[\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V}\nabla)\mathbf{V}\right] = -\nabla P + \mathbf{j} \times \mathbf{B},$$



S. Markidis, G. Lapenta, Rizwan-uddin, Mathematics and Computers in Simulation 80 (2010) 1509–1519.

Magnetic reconnection

Magnetohydrodynamics

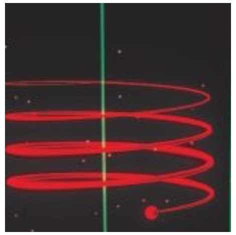
ions as particles **but** electrons fluid

ions **and** electrons as particles

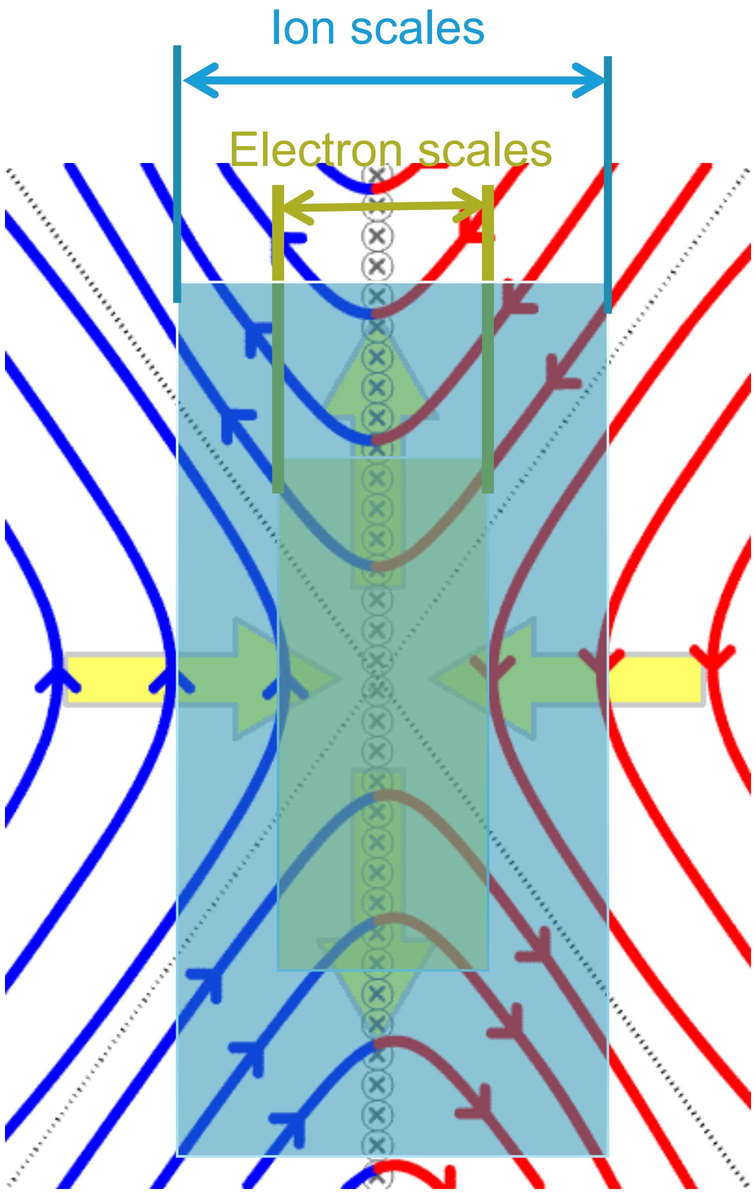
global scales
10 000 km

ion scales
1000 km

electron
10 km



Gyro (Larmor) radius



Turbulence

Reconnection

VSWMC models (operational (17) and operational soon (5))

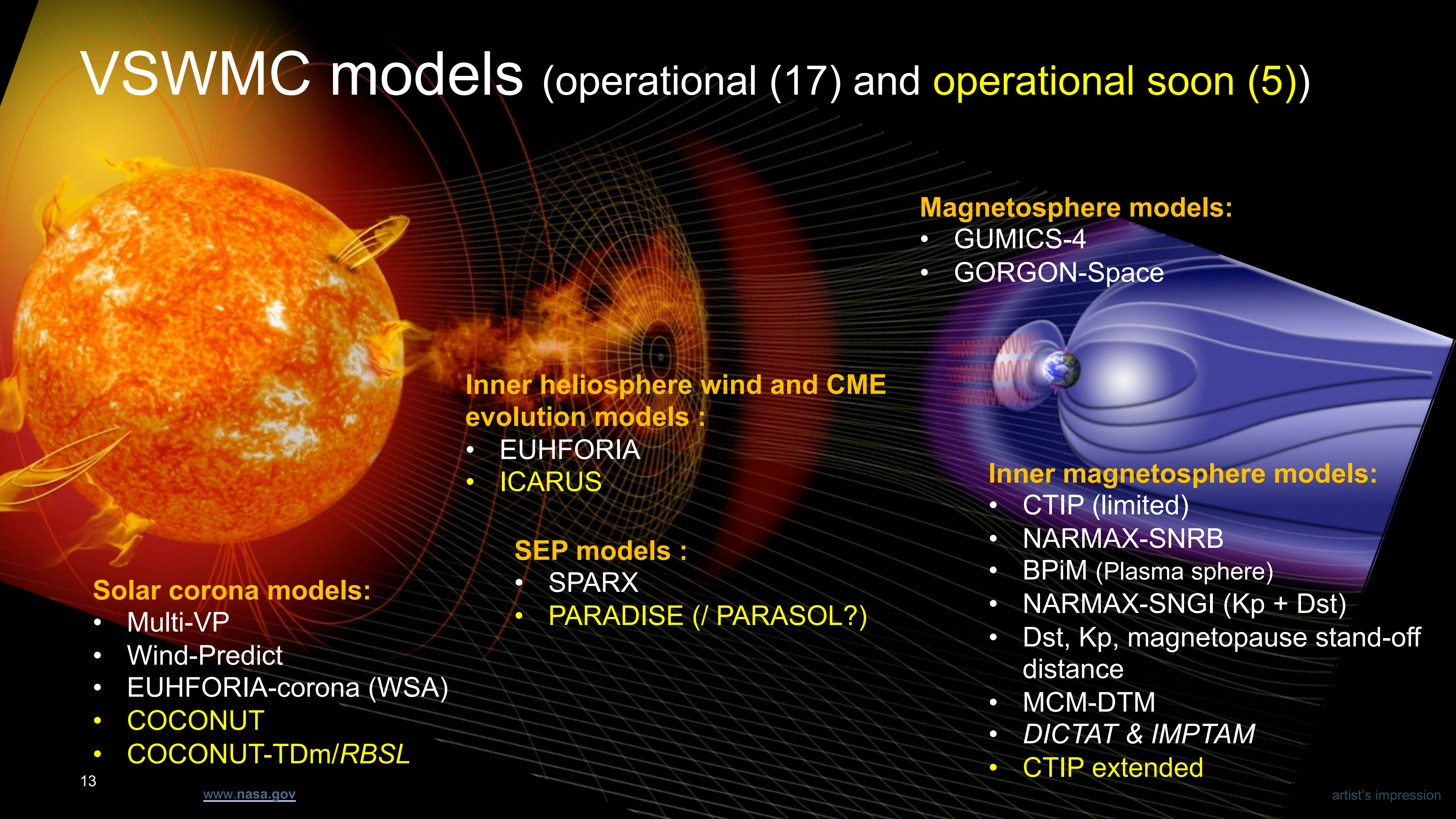
Magnetosphere models:
- GUMICS-4
- GORGON-Space

Inner heliosphere wind and CME evolution models :
- EUHFORIA
- ICARUS

SEP models :
- SPARX
- PARADISE (/ PARASOL?)

Inner magnetosphere models:
- CTIP (limited)
- NARMAX-SNRB
- BPiM (Plasma sphere)
- NARMAX-SNGI (Kp + Dst)
- Dst, Kp, magnetopause stand-off distance
- MCM-DTM
- *DICTAT & IMPTAM*
- CTIP extended

Solar corona models:
- Multi-VP
- Wind-Predict
- EUHFORIA-corona (WSA)
- COCONUT
- COCONUT-TDm/*RBSL*



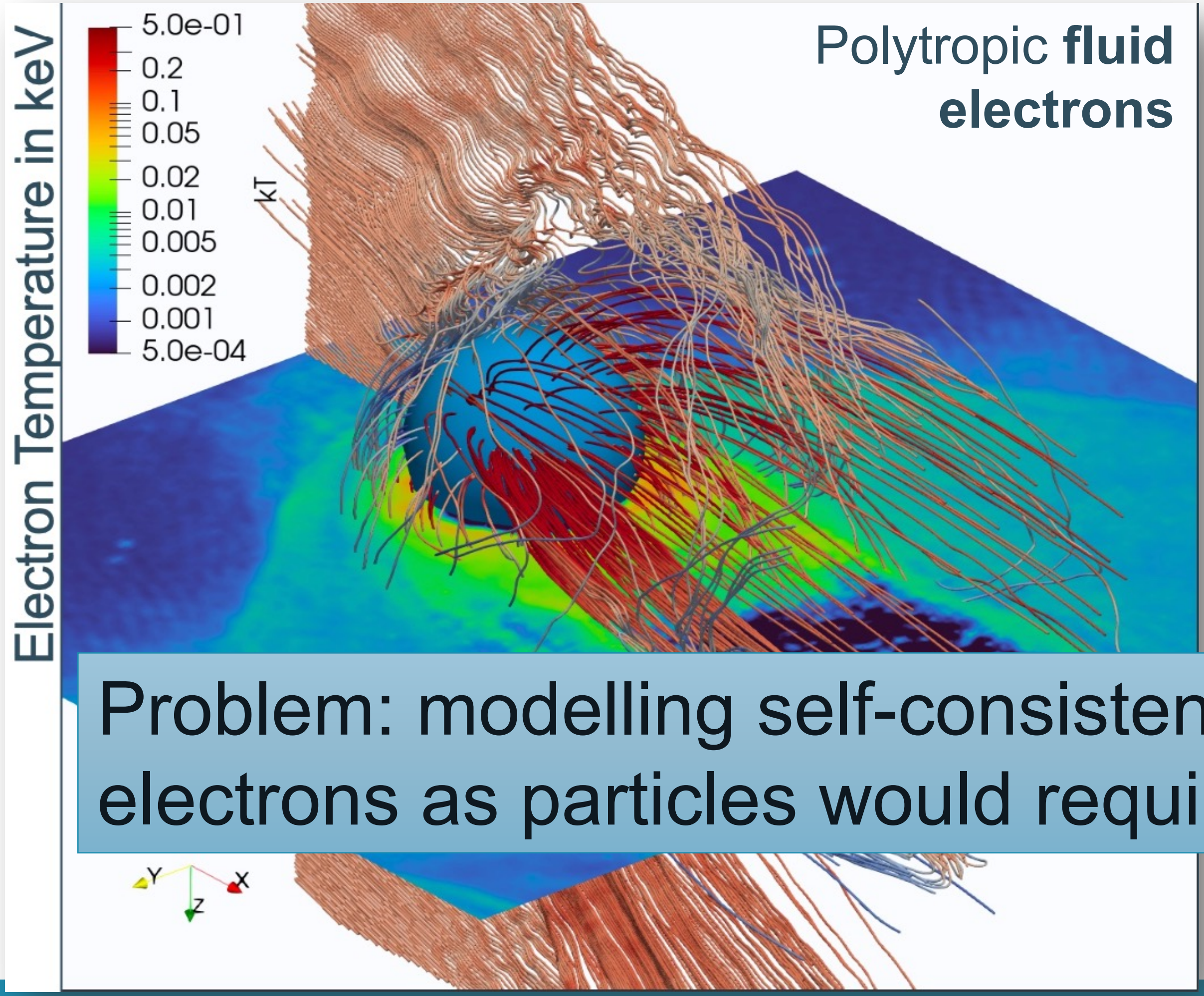
www.nasa.gov

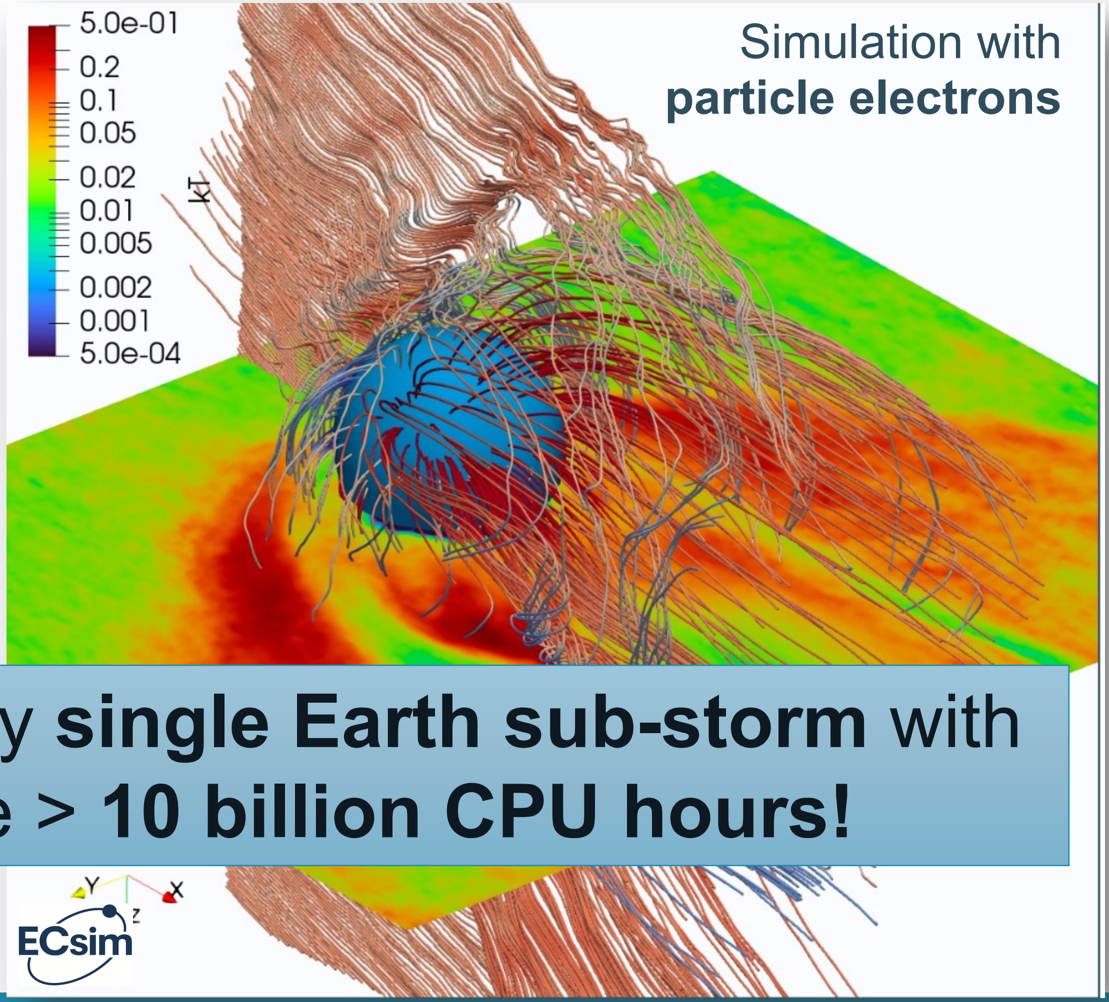
artist's impression

Problem: How are particles energized in magnetospheres?

Giovanni Lapenta

ECsim = Energy Conserving PIC





Problem: modelling self-consistently **single Earth sub-storm** with electrons as particles would require > **10 billion CPU hours!**

G. Lapenta, D. Schriver, R.J. Walker, J. Berchem, N.F. Echterling, M. El Alaoui, P. Travnicek, Journal of Geophysical Research: Space Physics 127 (2022) e2021JA030241.

From kinetic to fluid: moment closure problem

Conservation of mass:

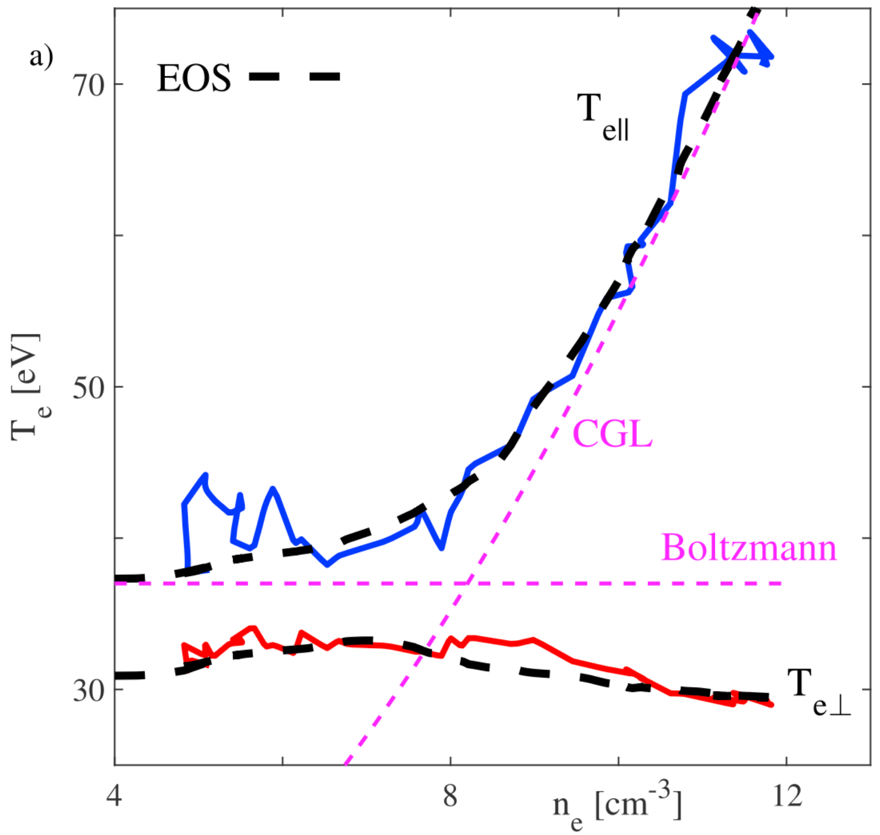
$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \boldsymbol{V}_s) = 0$$

Conservation of momentum:

$$\rho_s \left(\frac{\partial \boldsymbol{V}_s}{\partial t} + (\boldsymbol{V}_s \cdot \nabla) \boldsymbol{V}_s \right) = -\nabla \cdot \mathbf{P}_s + n_s q_s (\boldsymbol{E} + \boldsymbol{V}_s \times \boldsymbol{B})$$

$$\mathbf{P}_s = m_s \int (\boldsymbol{v} - \boldsymbol{V})(\boldsymbol{v} - \boldsymbol{V}) f_s d\boldsymbol{v};$$

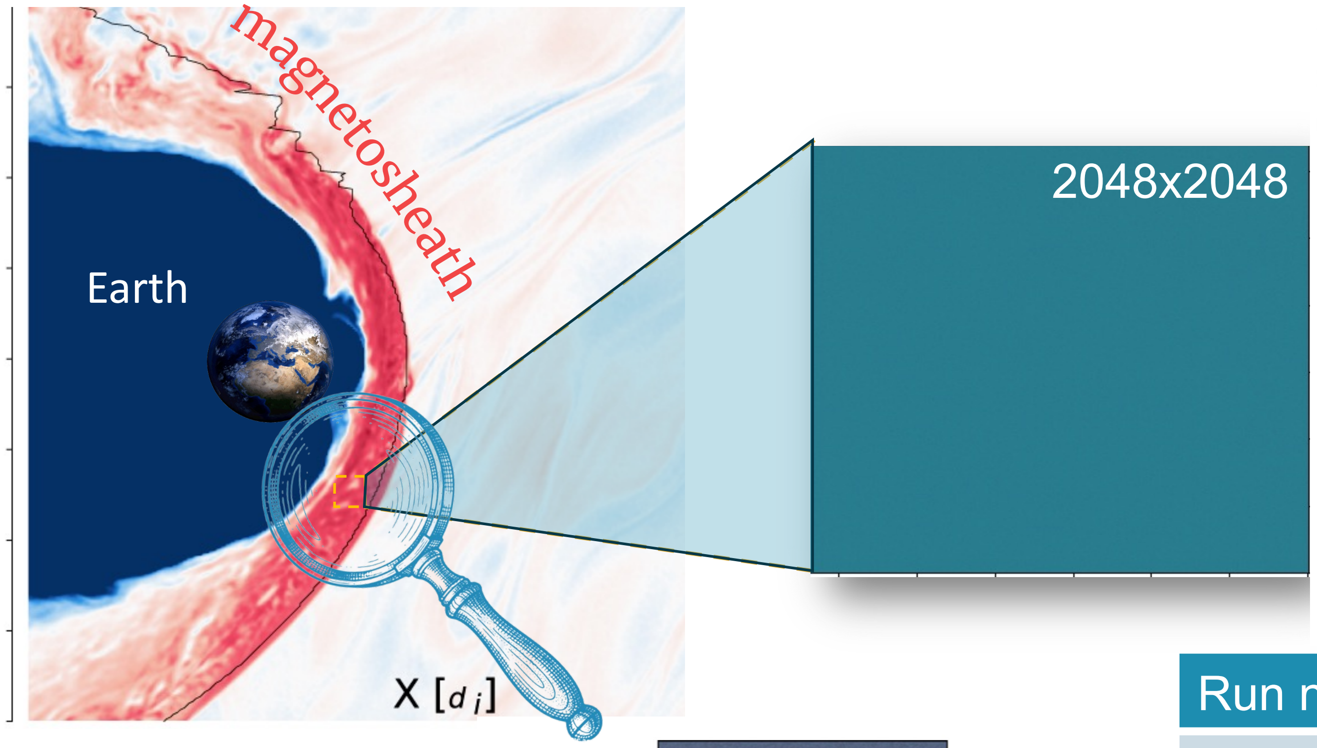
$$\mathbf{Q}_s = m_s \int (\boldsymbol{v} - \boldsymbol{V})(\boldsymbol{v} - \boldsymbol{V})(\boldsymbol{v} - \boldsymbol{V}) f_s d\boldsymbol{v}.$$

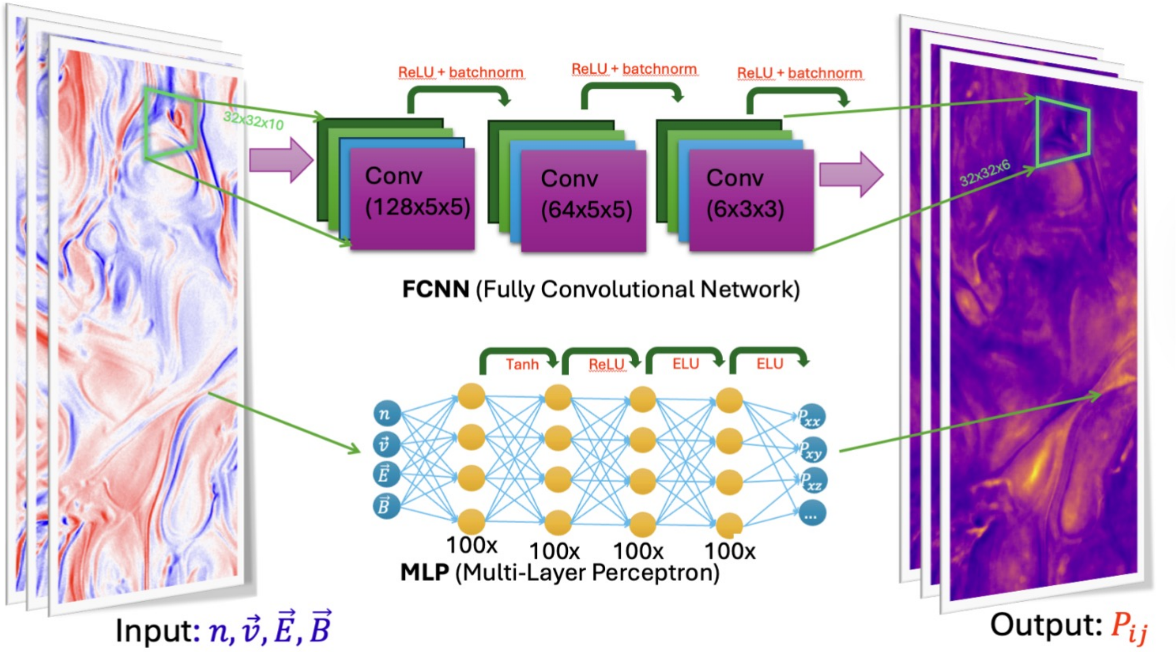


Empirical evidence for pressure equation of state in-situ

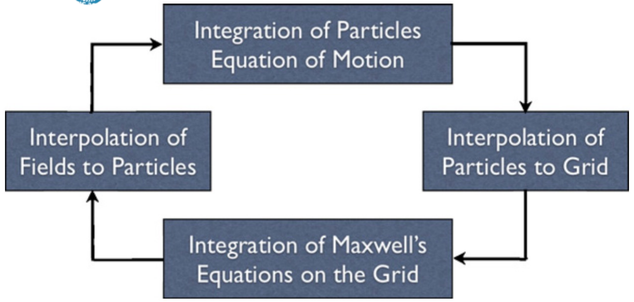
B.A. Wetherton, J. Egedal, A. Lê, W. Daughton, Geophysical Research Letters 46 (2019) 6223–6229.

Magnetosheath simulation of 2D decaying turbulence





ECsim – Energy conserving, semi-implicit particle in cell code (fully kinetic)



Run name	$\delta B/B$	β_e	β_i	Particles per cell
1 (generalization)	0.5	2	8	5000
4 (training)	0.5	2	8	256
1 (validation)	0.5	2	8	256
1 (testing)	0.5	2	8	256

G. Miloshevich, et al, (featured) Phys. Plasmas 33 (2026) 012901.

Funded by the European Union
Los Alamos NATIONAL LABORATORY
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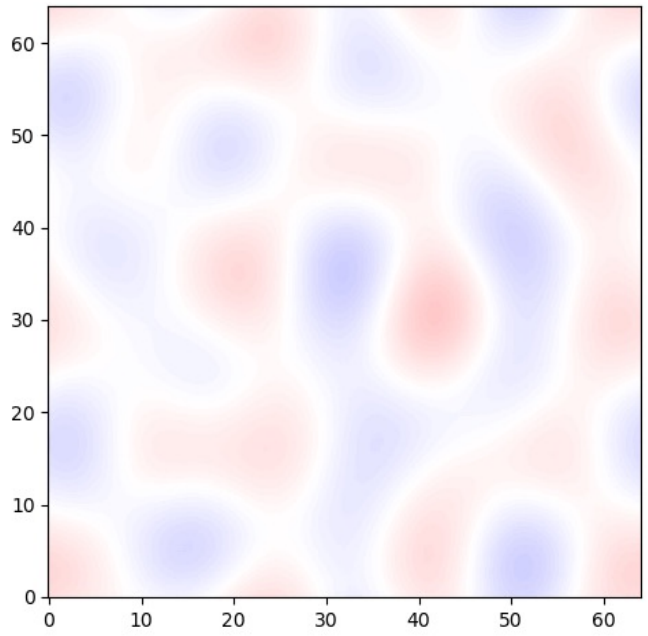
Hybrid PIC (Menura) with electron closure

C++ → PyTorch → CUDA C++

e + i modelled as particles

i: particles; e: neural fluid



Fully Kinetic PIC

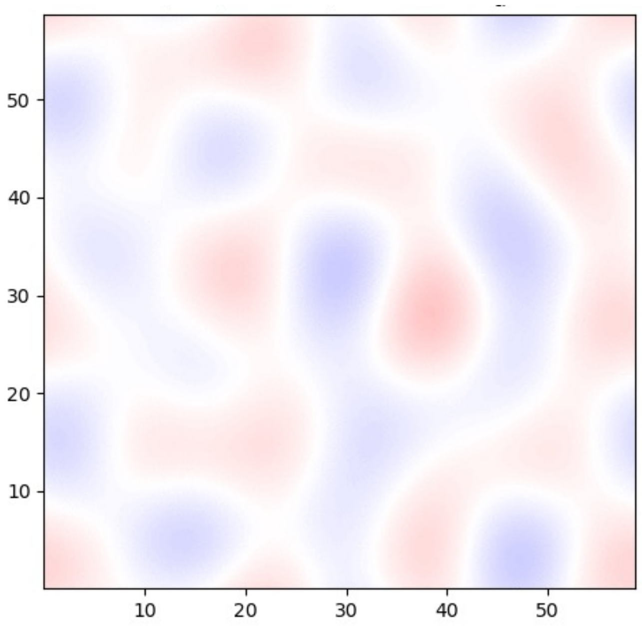
Computation time: **3 days on 128 nodes**

$$\mathbf{P} = \mathbf{P}_{NN}(n_e, \mathbf{v}_e, \mathbf{B})$$

$$\mathbf{P} \to \mathcal{G}^3 \, \nabla \cdot \mathbf{P}$$

$$\mathbf{B} \to \mathcal{G}^1 \, \mathbf{B}$$

$$\mathbf{E} \to \mathcal{G}^1 \, \mathbf{E}$$



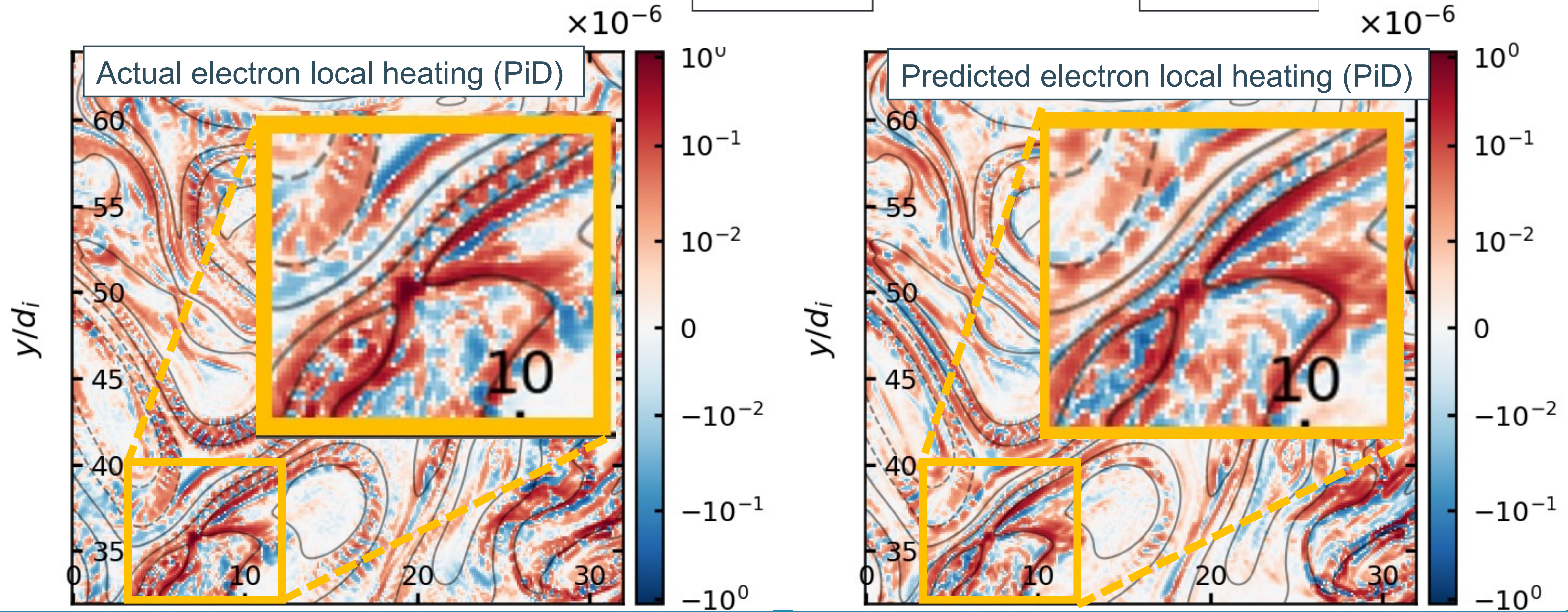
Hybrid PIC with neural closure

Computation time: **30 minutes on 1 node**

Generalization to 5000 particles/cell

PiD: Incompressible pressure-strain:

$$\langle E_\alpha^{th} \rangle \underset{}{\overset{-\langle (\boldsymbol{P}_\alpha \cdot \nabla) \cdot \boldsymbol{u}_\alpha \rangle}{\rightleftarrows}} \langle E_\alpha^{f} \rangle$$



G. Miloshevich; L. Vranckx, F. N. de Oliveira Lopez, P. Dazzi, **G. Lapenta**†. *(featured) Physics of Plasmas* **2026**

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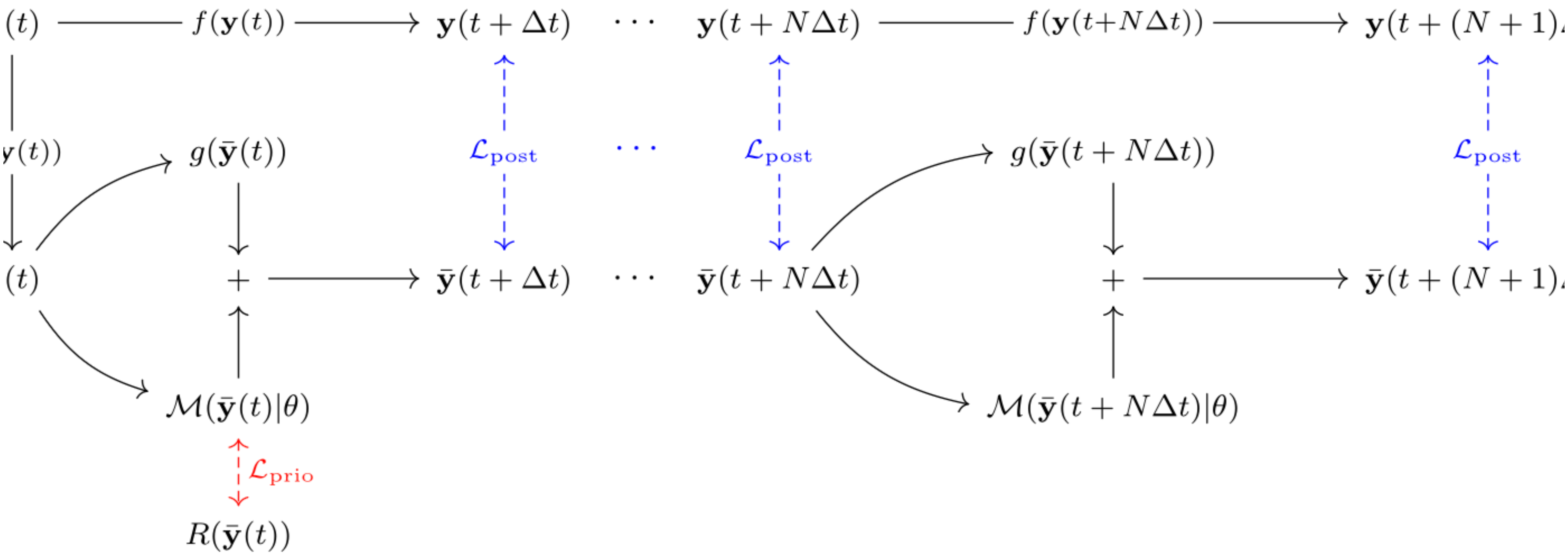
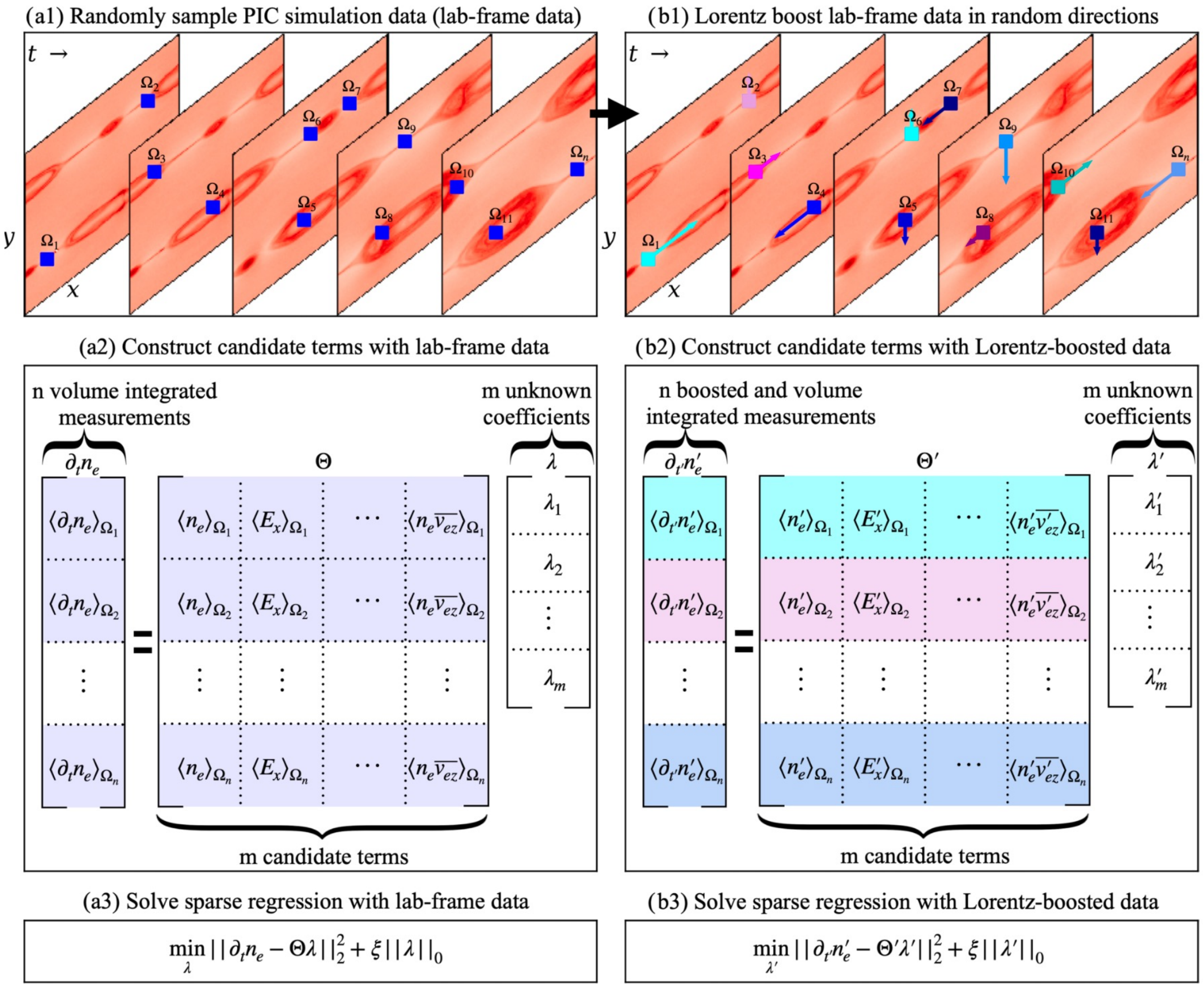
Online stability: Online training



H. Frezat, J. Le Sommer, R. Fablet, G. Balarac, R. Lguensat, Journal of Advances in Modeling Earth Systems 14 (2022) e2022MS003124.

Interpretability: Symbolic and Sparse regression



Identified in Lab frame:

$$P_{e\|\mathrm{Lab}} = -0.069 + 0.113 n_e + 0.370 \overline{v_{ex}}^2 - 0.291 \overline{v_{ez}}^2 - 0.078 B_x^2 + 0.065 B_z^2 - 0.075 B_z n_e.$$

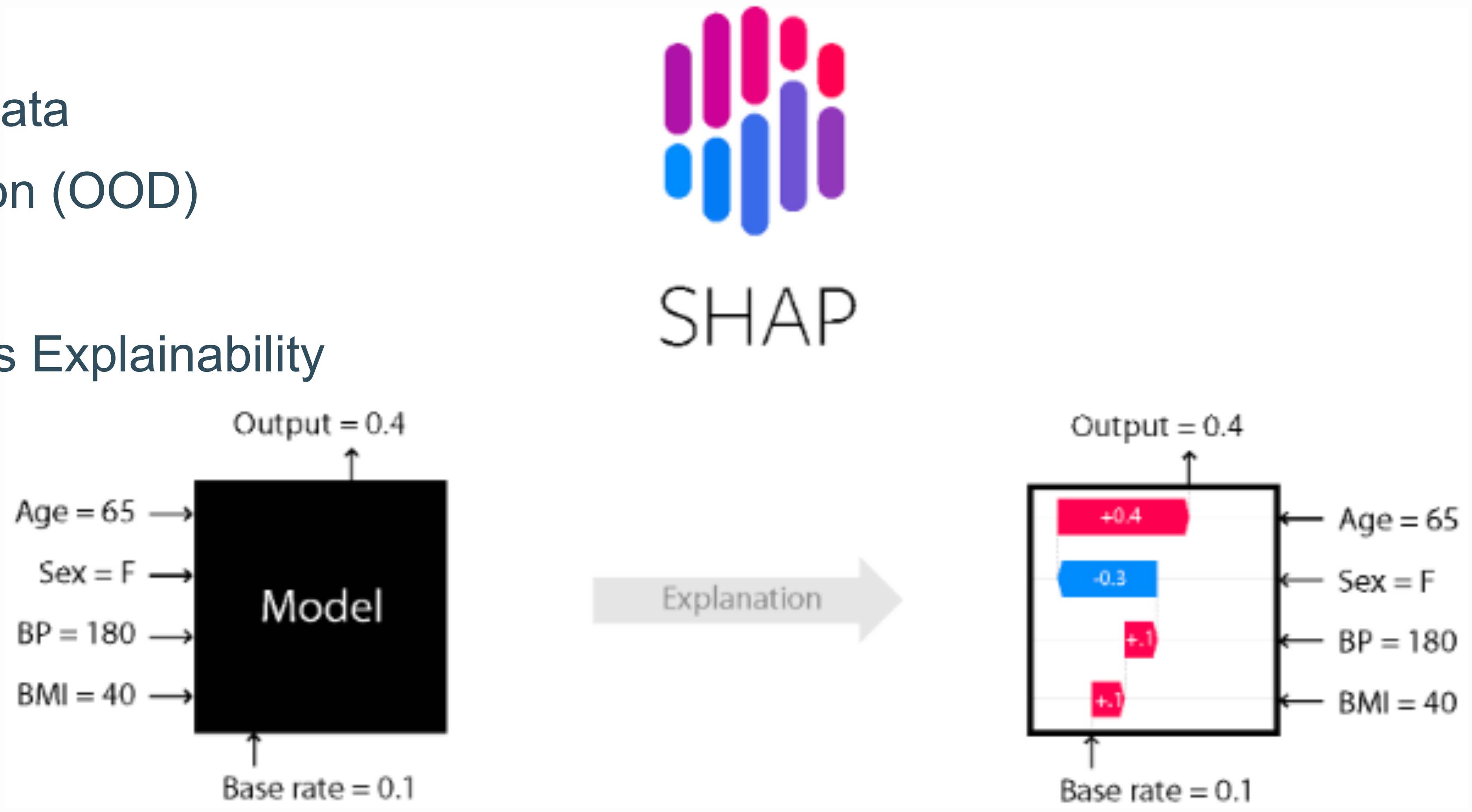
Identified with Galiliean boost augmentations

$$P_{e\|\mathrm{Boost}} = -0.071 + 0.103 n_e - 0.040 B_x^2 + 0.193 B_y^2 + 0.062 B_z^2 - 0.062 B_z n_e$$

M.C. McGrae-Menge, J.R. Pierce, F. Fiuza, E.P. Alves, Phys. Rev. Res. 8 (2026) 013200.

Main limitations: when to be careful

- Poor quality of data
- Out-of-distribution (OOD)
- Rare events
- Interpretability vs Explainability



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ASAP Automatics in Space Exploration

Use cases for AI in simulations:

- Detection of events
- Forecasting outcome
- Surrogate modelling
- Checkpoint management
- Data-driven discovery
- Subgrid closure

WE ARE HIRING SOON

Fall 2026: D-SURGE

Data-driven **S**imulations for **U**nderstanding **R**econnection in **GE**omagnetism