Neural networks and reduced models for plasmas

Laurent Navoret

IRMA, Université de Strasbourg and INRIA Nancy-Grand Est, Tonus

Joint work with Léo Bois, Nicolas Crouseilles, Emmanuel Franck, Guillaume Steimer, Vincent Vigon

GDR Emili, Ecole Polytechnique
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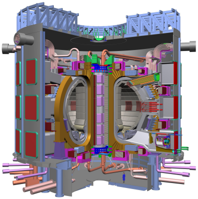
Plasmas dynamics

- distribution function $f(x, v, t)$ in phase space (high-dimension)
- multi-scale (mass ratio, quasineutrality, collisions, anisotropy)



→ full simulations: time and memory demanding
→ need for reduced models for real-time simulations for diagnostics or control

Goal

- reduced models based on neural networks
- study of the stability and accuracy once used numerically
- one-dimensional test

Plan

1. Neural networks
2. Fluid closure
3. Particle reduced model
4. Conclusion

Plan

Neural Network: parametrized function

$$\mathcal{F}_{\hat{\theta}}(X)$$

approximation of a real unknown function $\mathcal{F}(X)$ (ex: physical quantity)

Fit data (supervised learning)

$$\hat{\theta} = \underset{\theta \in \Theta}{\operatorname{argmin}} \sum_i \operatorname{distance}\left(\mathcal{F}(X_i), \mathcal{F}_\theta(X_i)\right)$$

data: $(X_i, \mathcal{F}(X_i))_i$
→ optimization algorithm

Difficulty
→ X: a vector of large dimension (ex: image from simulations)

Neural Network: parametrized function

$$Y = \mathcal{F}_\theta(X) = \sigma\left(W^{(d)}\sigma\left(W^{(d-1)}\sigma\left(\cdots\sigma\left(W^{(0)}X\right)\right)\right)\right)$$

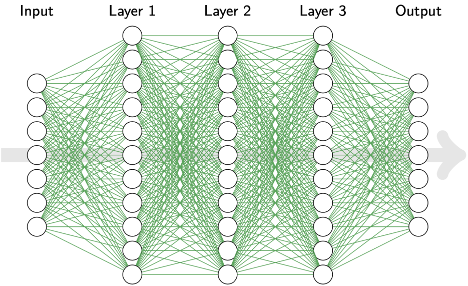
- succession of layers
- one layer: linear combination followed by a non-linear activation function

$$Y^{(p+1)} = \sigma\left(W^{(p)}Y^{(p)}\right)$$

$W^{(p)}$: weights matrices
$\sigma(a) = \max(a, 0)$

- parameters: $\theta = (W^{(p)})_p$

Example: fully connected neural network



A lot of applications in signal analysis

- image classification
- image segmentation
- speech recognition

→ based on GPU implementation
→ large of amount of data
→ user-friendly library (keras)
→ mathematical properties (separation, symmetries, multi-scale) [Mallat, 2015]

Used for the construction of reduced models in physics: 2 examples

1. Fluid closure
2. Particle reduced model

→ specific architecture
→ specific data processing

Plan

Different description

- Kinetic description for collisionless plasma $(\varepsilon > 1)$
  distribution function $f(x, v, t)$, with $x \in [0, L]$, $v \in \mathbb{R}$, $t \geqslant 0$
- Fluid description for collisional plasma $(\varepsilon < 10^{-2})$
  density $\rho(x, t)$, velocity $u(x, t)$, temperature $T(x, t)$

→ Knudsen number ε: mean free path between two collisions / L

→ fluid description are cheaper

→ extend the range of validity of fluid models to weakly collisional plasma

One-dimensionnal Vlasov-Poisson model on $[0, L]$:

$$\partial_t f + v\partial_x f - E\partial_v f = \frac{1}{\varepsilon}(M(f) - f)$$

$$E = -\partial_x \phi, \quad -\partial_{xx}\phi = \frac{1}{L}\int_0^L \rho(t,x)\,dx - \rho$$

+ spatial periodic boundary conditions

BGK collision operator

- relaxation to a Maxwellian $M(f)(x,v,t) = \frac{\rho(x,t)}{\sqrt{2\pi T(x,t)}}\, e^{-\frac{(v-u(x,t))^2}{2T(x,t)}}$
- ρ, u, T: moments of the distribution function f

[density]

$$\rho(x,t) = \int_{\mathbb{R}} f(x,v,t)dv$$

[pressure]

$$p(x,t) = \int_{\mathbb{R}} f(x,v,t)(v-u(x,t))^2 dv$$

[momentum]

$$\rho(x,t)u(x,t) = \int_{\mathbb{R}} f(x,v,t)v dv$$

[temperature]

$$\rho(x,t)T(x,t) = p(x,t)$$

Fluid equations satisfied by the moments $(\rho, \rho u, w)$:

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = -E\rho \\ \partial_t w + \partial_x(wu + pu + q) = -E\rho u \end{cases}$$

$w = \rho u^2/2 + p/2$: energy

→ heat flux: $q(x,t) = \int_{\mathbb{R}} \frac{1}{2} f(x,v,t)(v - u(x,t))^3 dv$

→ system not closed

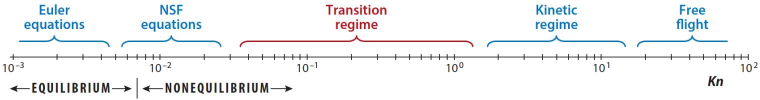
→ **Closure: expression of q as a function of the other moments**

$$\boxed{\hat{q} = \mathcal{C}(\varepsilon, \rho, u, T)}$$

→ **first possibilities**

- [Euler closure] $f = M(f) + O(\varepsilon)$ $\Rightarrow$ $\hat{q} = 0$
- [Navier-Stokes closure] $f = M(f) + \varepsilon g + O(\varepsilon^2)$ $\Rightarrow$ $\hat{q} = -\frac{3}{2}\varepsilon\, p\, \partial_x T$

Validity model [Torrilhon, 2016]



Extend range of validity of fluid models

- higher order terms in Chapman-Enskog
- higher order moments (Grad 13 model)
- higher order moments based on entropic closure (Levermore 14 moment)

→ ill-posed systems

Add specific kinetic

- Landau damping effect
- Hammett-Perkins closure [Hammett, Perkins 90, 92]
  - → fitting dispersion relation of the linearized equation
  - → q as Hilbert transform of the temperature

$$\hat{q}_k = -in_0\sqrt{\frac{8}{\pi}}i\ \mathrm{sign}(k)\hat{T}_k$$

  - → non-local closure
- Many extensions in the case of magnetized plasmas

Neural network closures:

- turbulent flows [Zhou et al. 2020]
- higher moments for neutral fluid [Han et al, 2019]
- learning known plasma closures [Ma et al. 2020] [Maulik et al. 2020]

Goal : insert a data driven closures into fluid solvers for $\varepsilon \in [0.01, 1]$

$\rightarrow$ Off-line phase: supervised learning from kinetic simulations

$\rightarrow$ On-line phase: compute the closure at each time step of the fluid solver

Non-local Neural Network closure

$$X = (\varepsilon, \rho, u, T) \in (\mathbb{R}^{N_x})^4 \quad \longrightarrow \quad \hat{q} = C_{\hat{\theta}}(\varepsilon, \rho, u, T) \in (\mathbb{R}^{N_x})^4$$

$\hat{\theta} \in \Theta$: set of parameters

Training: solve the optimization problem (gradient method)

$$\hat{\theta} = \underset{\theta \in \Theta}{\operatorname{argmin}} \frac{1}{|\mathcal{D}|} \sum_{(X;q) \in \mathcal{D}} \frac{1}{N_x} \sum_{i=1}^{N_x} |C_\theta(X)_i - q_i|$$

$\mathcal{D}$ data set
$C_\theta(X)$: prediction of the neural network
q: true heat flux

→ Define the architecture of the network
→ Generate data

Convolutional neural network

→ sparse neural networks

→ very efficient for structured data (image, signals)

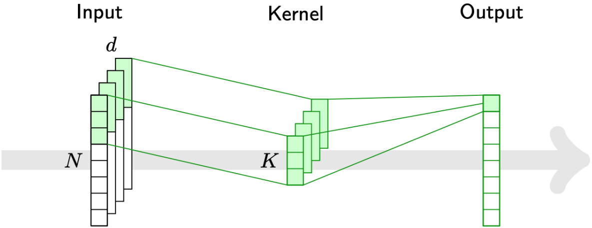
→ each layer: several 1D convolutions with small kernels followed by activation functions

input: X of shape (N, d)
output: Y of shape (N, d')

kernel: K of shape (p, d, d') size p

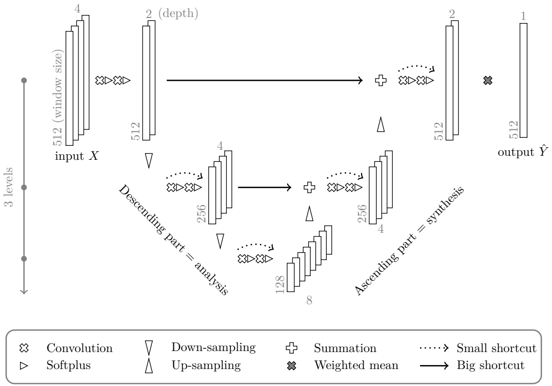
$$Y_{i,k} = \sigma\left(\sum_{j=1}^{d}\sum_{di=1}^{p} X_{i+di,j} K_{di,j,k}\right)$$

→ scalar product with the kernel: measure of similarity



One-dimensional V-net architecture [Ronneberger et al., 2015] [Milletari et al., 2016]

- multi-scale analysis (like in wavelet analysis)
- based on up-samplings and dow-samplings
  - → down-sampling: decrease the size of the signals / increase the number of channels
  - → up-samping: increase the size of the signals / decrease the number of channels
- shortcut: add the input to output for accelarating the training process



Choice of the hyperparameters:

Hyper-parameter	Value
size of the input window (N)	512
number of levels (ℓ)	5
depth (d)	4
size of the kernels (p)	11
activation function	softplus

softplus: $\sigma(x) = \ln(1 + \exp(x))$

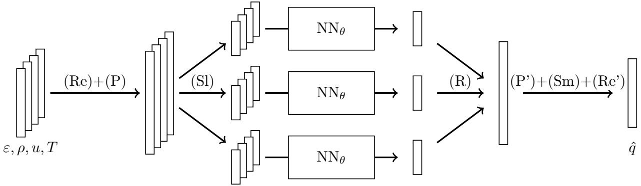
$\rightarrow$ 15 layers

Neural network parameters to learn

- $O(2^\ell d^2 pN)$
- Here: $161\,937$ parameters

For learning and flexibility:

1. Resampling to a given resolution N_x' and preprocessing (standardization of the data)
2. Slicing into overlapping "windows" of size $N = 512$
3. Neural network
4. Reconstructing
5. Post-processing, smoothing and resampling



$$C_\theta : \quad X \overset{\text{(Re)+(P)}}{\longmapsto} X^{(P)} \overset{\text{(Sl)}}{\longmapsto} (X_j^{(P)})_j \overset{(\text{NN}_\theta)}{\longmapsto} (\hat{Y}_j^{(P)})_j \overset{\text{(R)}}{\longmapsto} \hat{Y}^{(P)} \overset{\text{(P')+(Sm)+(Re)}}{\longmapsto} \hat{Y}.$$

Data generation by kinetic solver: for each simulation

- initialization: $f_0(x) = M(\rho, u, T)$, with ρ, u and T as Fourier series :

$$\alpha \times \left(\frac{a_0}{2} + 0.5 \sum_{n=1}^{20} (a_n \cos(nx) + b_n \sin(nx)) \right), \quad x \in [0, 2\pi].$$

  a_n, b_n: random

- $\varepsilon \in [0.01, 1]$: non-uniform distribution
- 20 recording time $t_1, t_2, \ldots, t_{20} \in [0.1, 2]$

→ discretization parameters: $N_x = 1024$, $N_v = 141$

→ Finite Volume in space / Finile Element method in velocity [Helluy et al., 2014]

$20 \times$ **500** $= 10\,000$ different spatial data for training
$20 \times$ **500** $= 10\,000$ different spatial data for validation

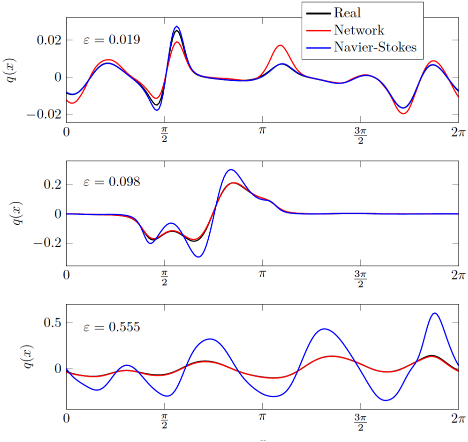
Data generation by kinetic solver: for each simulation

Output normalization

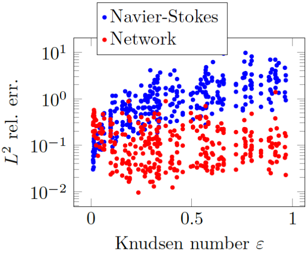
- avoid too small values of the heat flux prediction
- normalisation with the Navier-Stokes heat flux:

$$q^{k_0}_{\text{norm}} = \begin{cases} q^{k_0} \times \dfrac{\theta}{q^{k_0}_{NS}}, & \text{if } 0 < q^{k_0}_{NS} \leqslant \theta, \\ \\ q^{k_0}, & \text{otherwise}, \end{cases}$$

Examples from the validation set:



L^2 relative error on the validation set:



→ For large ε: neural network closure better than Navier-Stokes one

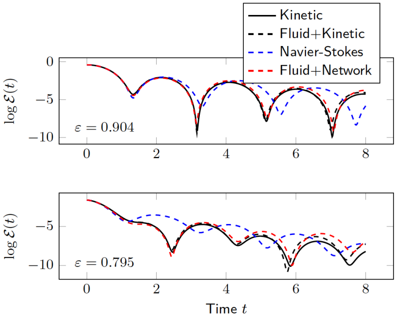
→ relative error independent of the Knudsen number $\approx 10^{-1}$

Fluid model with neural network

Fluid solver+Network: $\hat{q} = C_\theta(\varepsilon, \rho, u, T)$
compared with:

- Fluid +Kinetic ($\hat{q} = q$)
- Fluid +Navier-Stokes ($\hat{q} = -\frac{3}{2}\varepsilon p\, \partial_x T$)

Electric energy



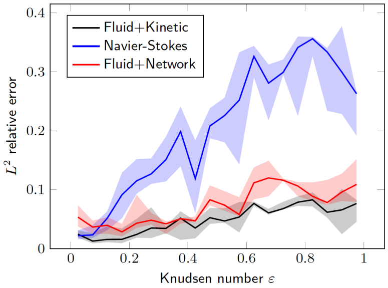
→ for large ε: good results for Fluid+Network
→ error on Fluid+Kinetic due to numerical approximations

Fluid model with neural network

L^2 error on density, momentum, energy on 200 simulations

Fluid solver+Network: $\hat{q} = C_\theta(\varepsilon, \rho, u, T)$
compared with:

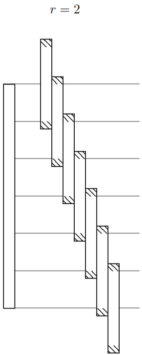
- Fluid +Kinetic ($\hat{q} = q$)
- Fluid +Navier-Stokes ($\hat{q} = -\frac{3}{2}\varepsilon p\, \partial_x T$)



→ cannot expect better than Fluid+Kinetic
→ relative error ≈ 0.2
→ Fluid+Network errors vary like the Fluid+Kinetic one

Stability

Stability
→ no guarantee of stability
→ instabilities triggered by irregular reconstruction of the heat flux due to slicing

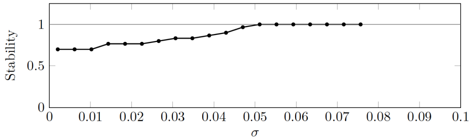


Smoothing of the output

$$\tilde{q}(x) = \int_{-3\sigma}^{3\sigma} q(x+t)w(t)\,dt.$$

w: Gaussian kernel with standard deviation σ

Numerical results: proportion of simulations reaching final time

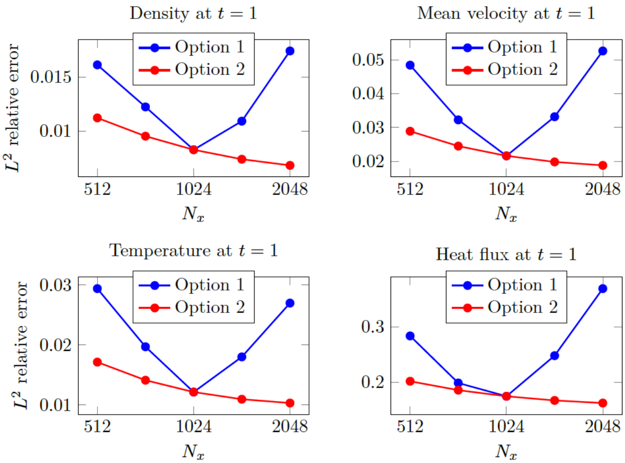


→ $\sigma = 0.06$ leads to stable numerical simulations

Two options for considering refined grids

→ option 1: use slicing

→ option 2: use downsampling to the refinement used for learning



→ keep close to the data used in training set (same resolution)

Particle In Cell method: N macro-particles $(X_j, V_j) \in \mathbb{R}^2$

$$\forall j \in \{1, \dots, N\}, \qquad \begin{aligned} \frac{dX_j}{dt} &= V_j \\ \frac{dV_j}{dt} &= \frac{q}{m}(E_h + E_{\mathsf{ext}})(X_j) \end{aligned}$$

$E_h = -\nabla \phi_h$: approximated **self-consistent** electric field
$E_{\mathsf{ext}} = -\nabla \phi_{\mathsf{ext}}$: external electric field

→ Hamiltonian dynamics
→ costly numerical simulations

→ Goal: describe the dynamics locally around a given trajectory with $K \ll N$ reduced "particles"

1. Find out reduced variables:

$$u = (X, V) \in \mathbb{R}^{2N} \underset{\text{compression}}{\longrightarrow} \bar{u} = (\bar{X}, \bar{V}) \in \mathbb{R}^{2K} \underset{\text{decompression}}{\longrightarrow} u = (X, V) \in \mathbb{R}^{2N}$$

→ fast compression / decompression

Linear reduction: $\bar{u} = Au$

- Proper orthogonal decomposition (POD)
- Proper symplectic decomposition (PSD) [Tyranowski, Krauss, 2019]
- analytical dynamics on the reduced variables

→ valid on linear regime
→ but electric field computed from original variables
→ back and forth between reduced and original variables

Non-linear reduction: neural networks
→ Auto-encoder architecture

Neural network Encoder/Decoder

$\bar{u} = \mathcal{F}_\theta(u)$: encoder

$u = \mathcal{G}_\theta(\bar{u})$: decoder

Learning:

$$\hat{\theta} = \text{argmin} \sum_{i=1}^{N_d} ||u_i - \mathcal{G}_\theta(\mathcal{F}_\theta(u_i))||^2$$

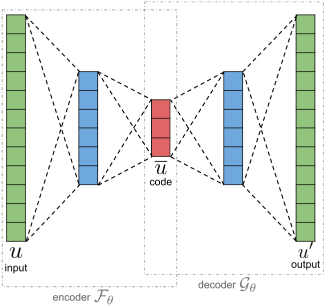
→ (u_i): extracted from numerical simulations at different times

→ $\mathcal{G}_\theta \circ \mathcal{F}_\theta \approx$ Id on the data

Architecture:

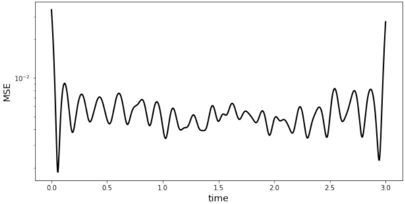
→ pooling/unpooling

→ light architecture to reduce the number of parameters



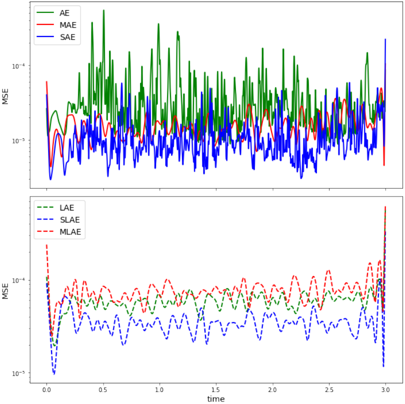
Test-case: one numerical simulation with $N = 1000$ particles

PSD reduction $K = 20$



$\rightarrow$ error $\approx 10^{-2}$

Auto-encoder reduction $K = 7$



$\rightarrow$ error $\approx 10^{-4}$

2. Determine the dynamics of the reduced variables:

$$\forall j \in \{1, \dots, K\}, \qquad \begin{aligned} \frac{d\bar{X}_k}{dt} &= \nabla_{V_k} \bar{H}_\theta(\bar{X}, \bar{V}) \\ \frac{d\bar{V}_k}{dt} &= -\nabla_{X_k} \bar{H}_\theta(\bar{X}, \bar{V}) \end{aligned}$$

Neural network Hamiltonian function: $H_\theta(\bar{X}, \bar{V})$

→ assumption: separable Hamiltonian

→ take implicitly into account the electric force

→ ensure large time stability of the reduced dynamics

Learning

$$\hat{\theta} = \underset{\theta\in\Theta}{\text{argmin}} \sum_{i=1}^{N_d} \left\| \frac{\bar{X}_i^{+\Delta t} - \bar{X}_i}{\Delta t} - \nabla_{\bar{V}} \bar{H}_\theta(\bar{X}_i, \bar{V}_i) \right\| + \left\| \frac{\bar{V}_i^{+\Delta t} - \bar{V}_i}{\Delta t} + \nabla_{\bar{X}} \bar{H}_\theta(\bar{X}_i, \bar{V}_i) \right\|$$

data: numerical simulations at different times $(\bar{X}, \bar{V}, \bar{X}^{+\Delta t}, \bar{V}^{+\Delta t})_i$

Architecture fully connected

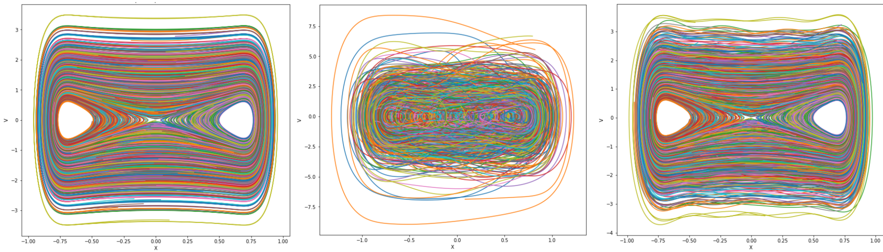
Initial condition:

$$f(x, v, t) = 1_{[-0.5,0.5]}(x)\exp(-v^2/2)$$

Numerical method:

1. compression
2. simulation of the reduced model
3. decompression

Phase portrait



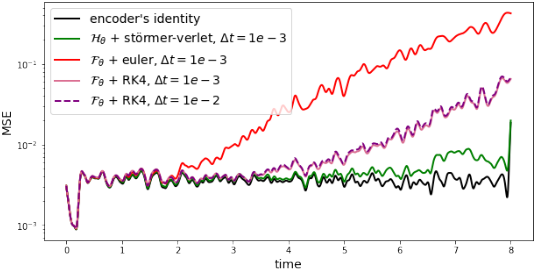
Reference (PIC) PSD reduction (K=35) Neural Network reduction (K=8)

Initial condition:

$$f(x, v, t) = 1_{[-0.5,0.5]}(x) \exp(-v^2/2)$$

Numerical method:

1. compression
2. simulation of the reduced model
3. decompression



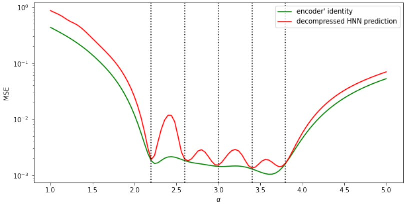
→ Hamiltonian reduced dynamics: better control of the numerical error

Initial conditions:

$$f(x,v,t) = C\,x^{\alpha}(1-x)^{3/2}\exp(-v^2/2)$$

Goal: learn the dynamics for $\alpha \in [2.2, 3.6]$

Data: dynamics of $N = 10^4$ particles with $\alpha \in \{2.2, 2.6, 3, 3.4, 3.6\}$



Error for the whole strategy

→ reduced method: 25 times faster

Plan

Construction of reduced models

- Fluid closure based on a V-net architecture supervised learning
- Particle reduced dynamics based on auto-encoder architecture semi-supervised learning
- stability properties observed/ensured

Perpectives:

- Extension to dimension 2 or 3
- Add a magnetic field
- Use in real applications

Ongoing ANR project with Max-Planck Institut für Plasma Physics (Garching).