14th Symposium of VKI PhD Research

8 March 2023

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An overview on the development and calibration of a 1D ejector model

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University supervisor	Pr. Yann Bartosiewicz

von KARMAN INSTITUTE FOR FLUID DYNAMICS

UCLouvain

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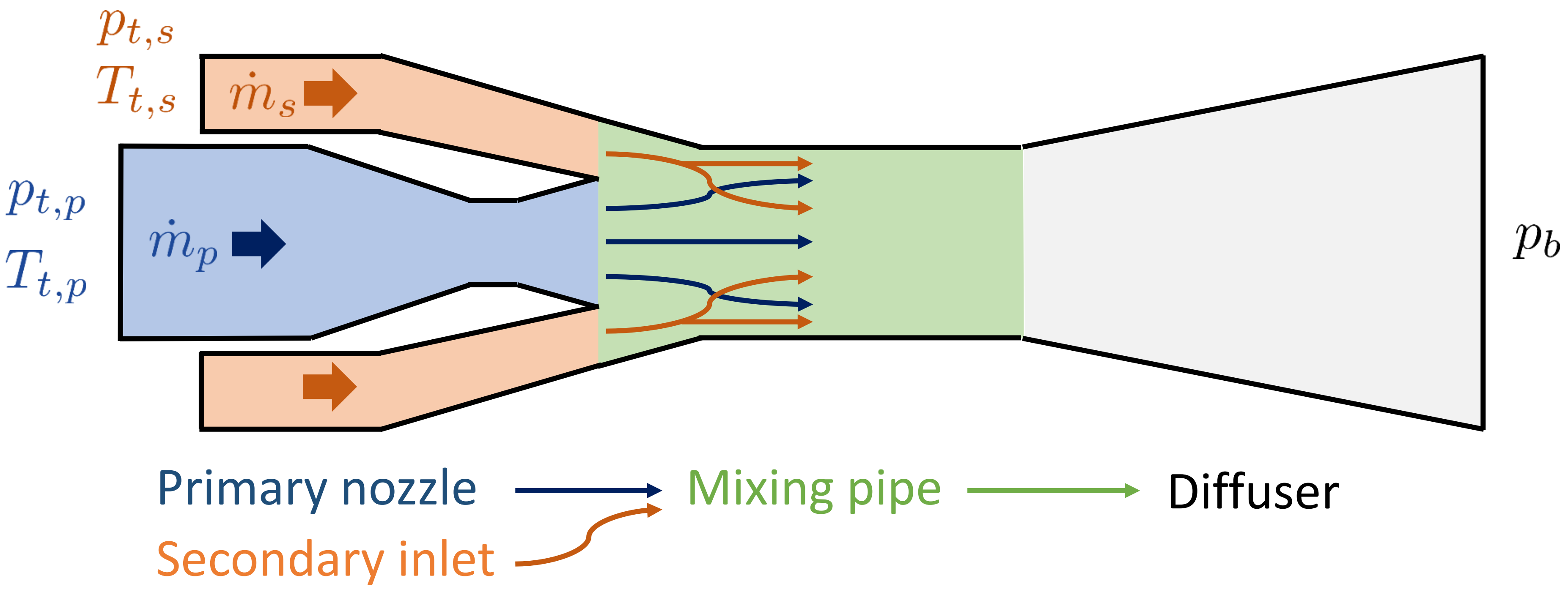
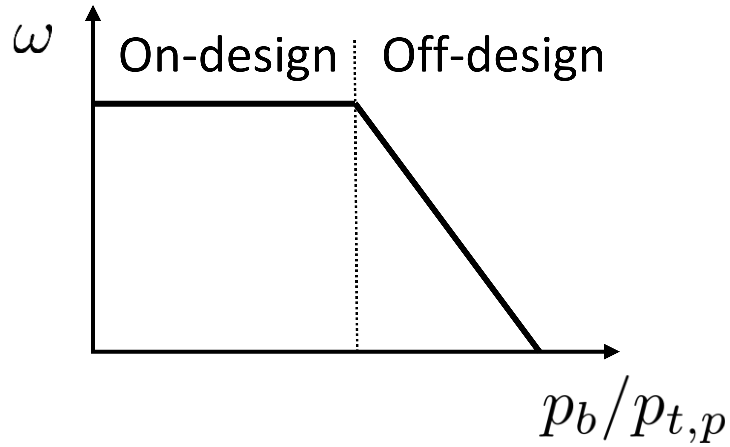
What is an ejector?

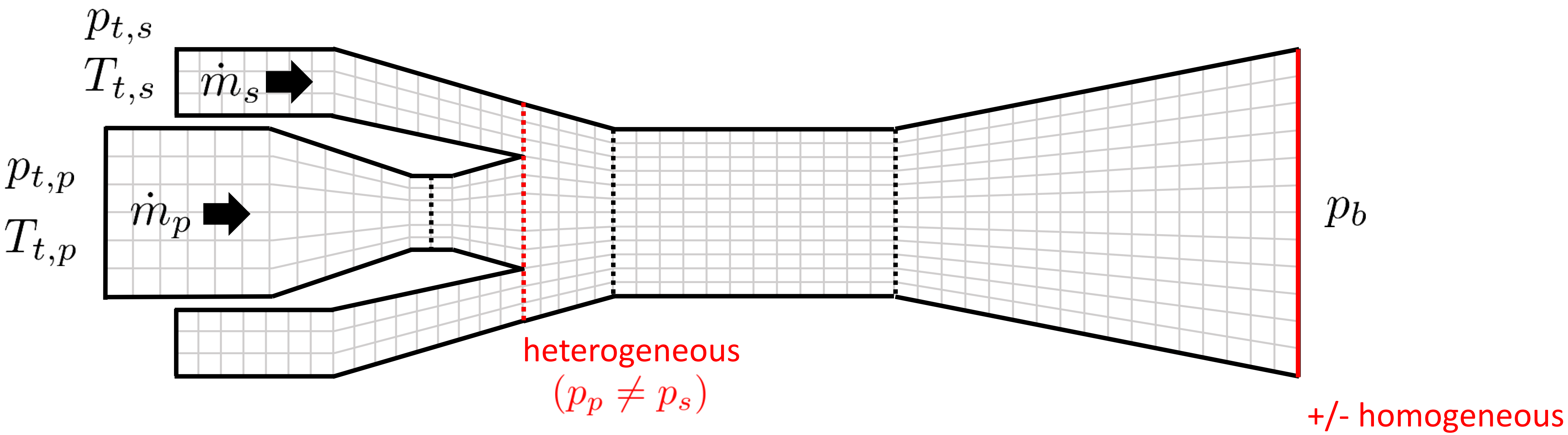


The back pressure p_b determines the entrainment ratio $\omega = \dot{m}_s/\dot{m}_p$

The mixed flow is choked in the on-design regime



What are the modelling options?



0D: global balances

- ✓ Fast
- ✗ Only global information
- ✗ Calibration

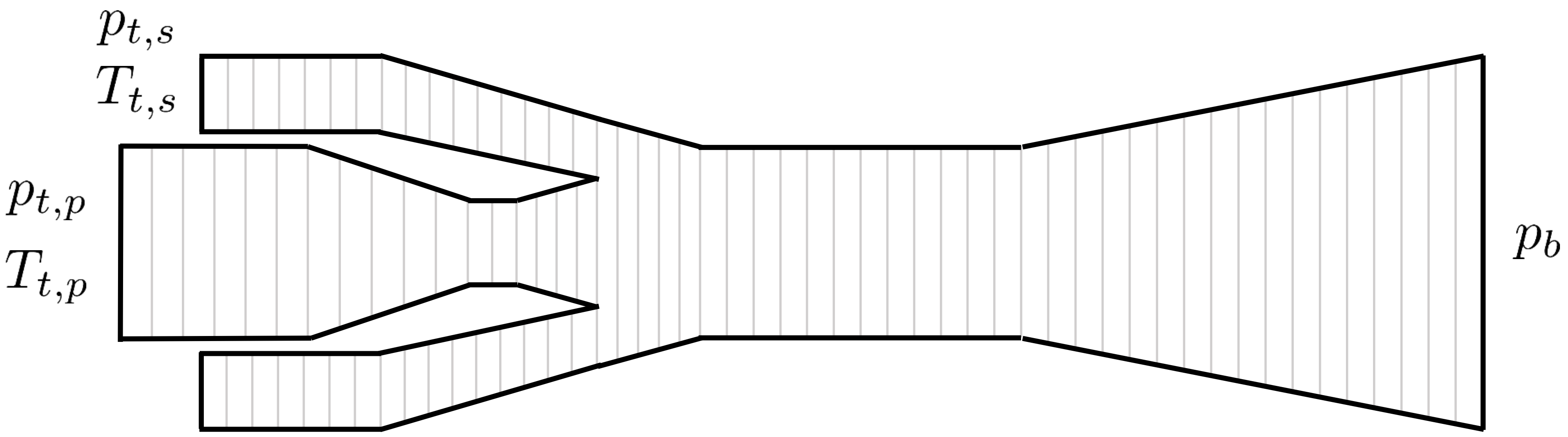
1D: a compromise

- ✓ Local information
- ✓ Fast
- ✗ Calibration (2D effects)
- ✗ Complex

2/3D: classic CFD

- ✓ Detailed flow field
- ✓ No calibration
- ✗ Computational cost
- ✗ Meshing and modelling

What do we want to develop?



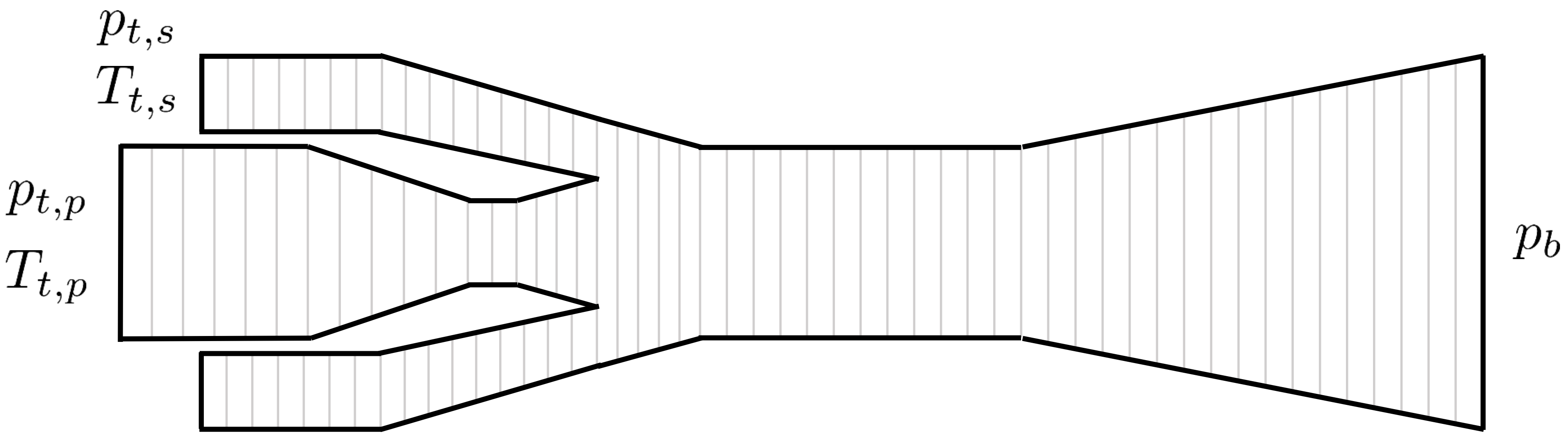
- A 1D ejector model
- A high-fidelity database for validation
- Machine learning-based calibration tools

An enhanced 1D ejector model, with closure relations learned from CFD and experiments

Goal of the thesis

Reconcile ejector models with CFD and experiments

What do we want to develop?



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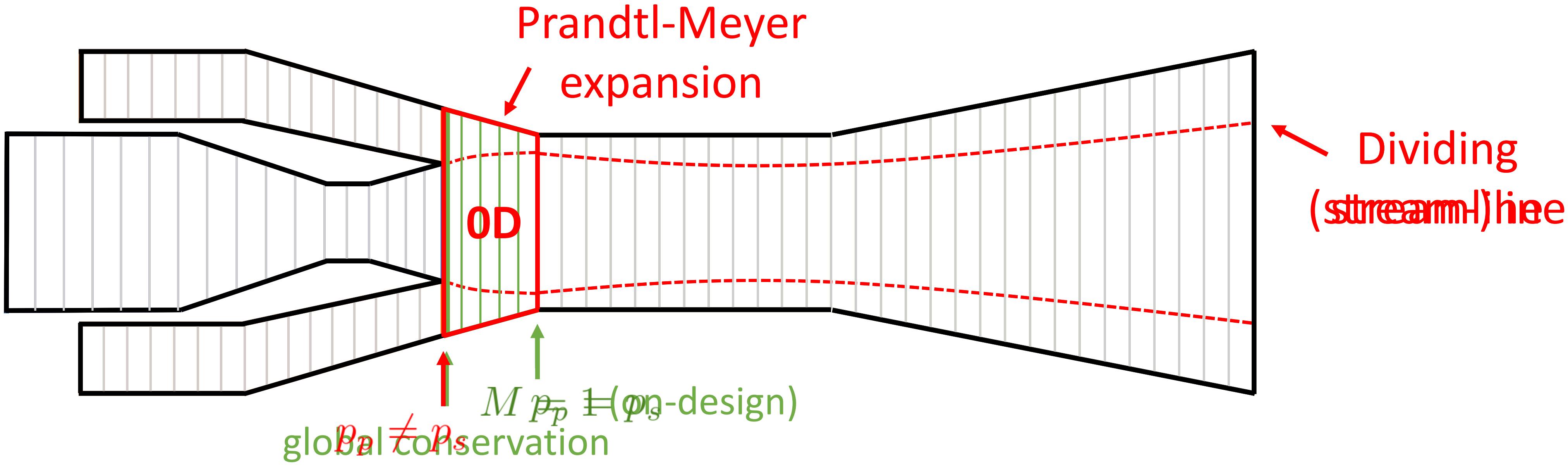
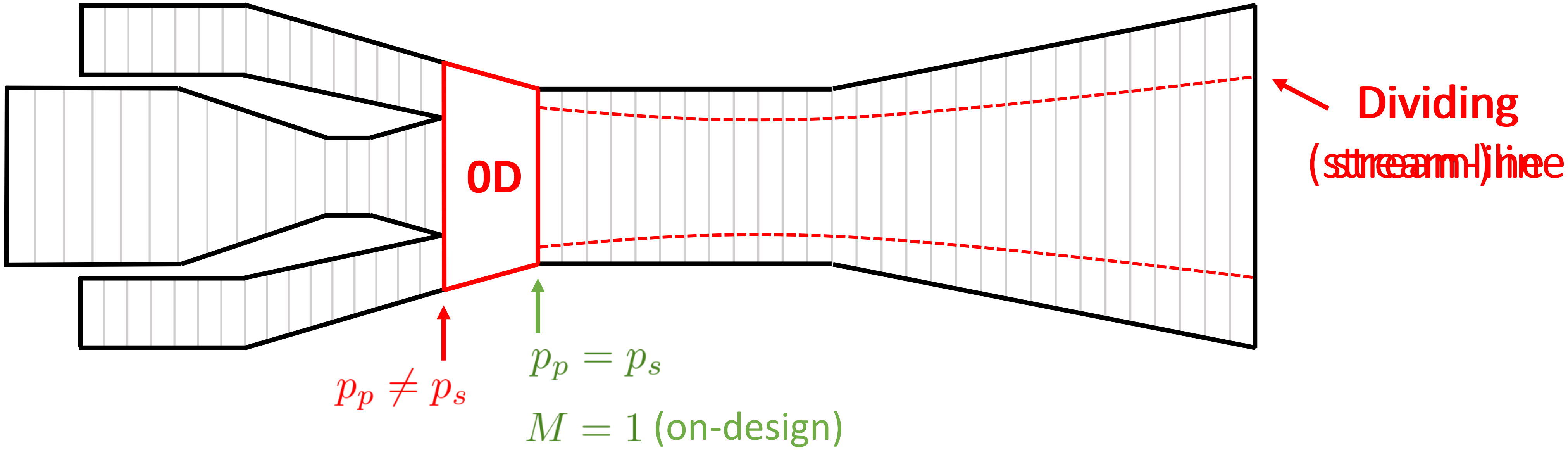
Existing 1D models



Single stream [1]	Double stream [2]	Double stream + 0D [3]
✓ On-design	✓ On-design	✗ On-design
✓ Off-design	✗ Off-design	✓ Off-design
✗ Shear	✗ Shear	✓ Shear
✗ Pressure equalization	✓ Pressure equalization	✗ Pressure equalization

Current state of the proposed model



Euler equations in the mixing p

Double stream + 0D + choking

$$
\begin{cases}
d_x(\rho_p A_p V_p) & = 0 \\
d_x(\rho_p A_p V_p^2) & = -A_p d_x p_p + F_p \\
d_x(\rho_p A_p V_p h_{t,p}) & = 0 \\
d_x(\rho_s A_s V_s) & = 0 \\
d_x(\rho_s A_s V_s^2) & = -A_s d_x p_s + F_s \\
d_x(\rho_s A_s V_s h_{t,s}) & = 0
\end{cases}
$$

- ✗✓ On-design
- ✓ Off-design
- ✓ Shear
- ✗ Pressure equalization

Shear and friction: $\begin{cases} F_p = -\tau_{ps} l_{ps} \\ F_s = \tau_{ps} l_{ps} - \tau_w l_w \end{cases}$

Constraints: $\begin{cases} p_p(x) = p_s(x) & = p(x) \\ A_p + A_s & = A \end{cases}$

How does a double stream choke?

Compound choking of a double stream

Single stream

$$\frac{d_x p}{p} = \frac{d_x A}{A\frac{(1-M^2)}{\gamma M^2}}$$

Singular if $M = 1$, possible if $d_x A = 0$.

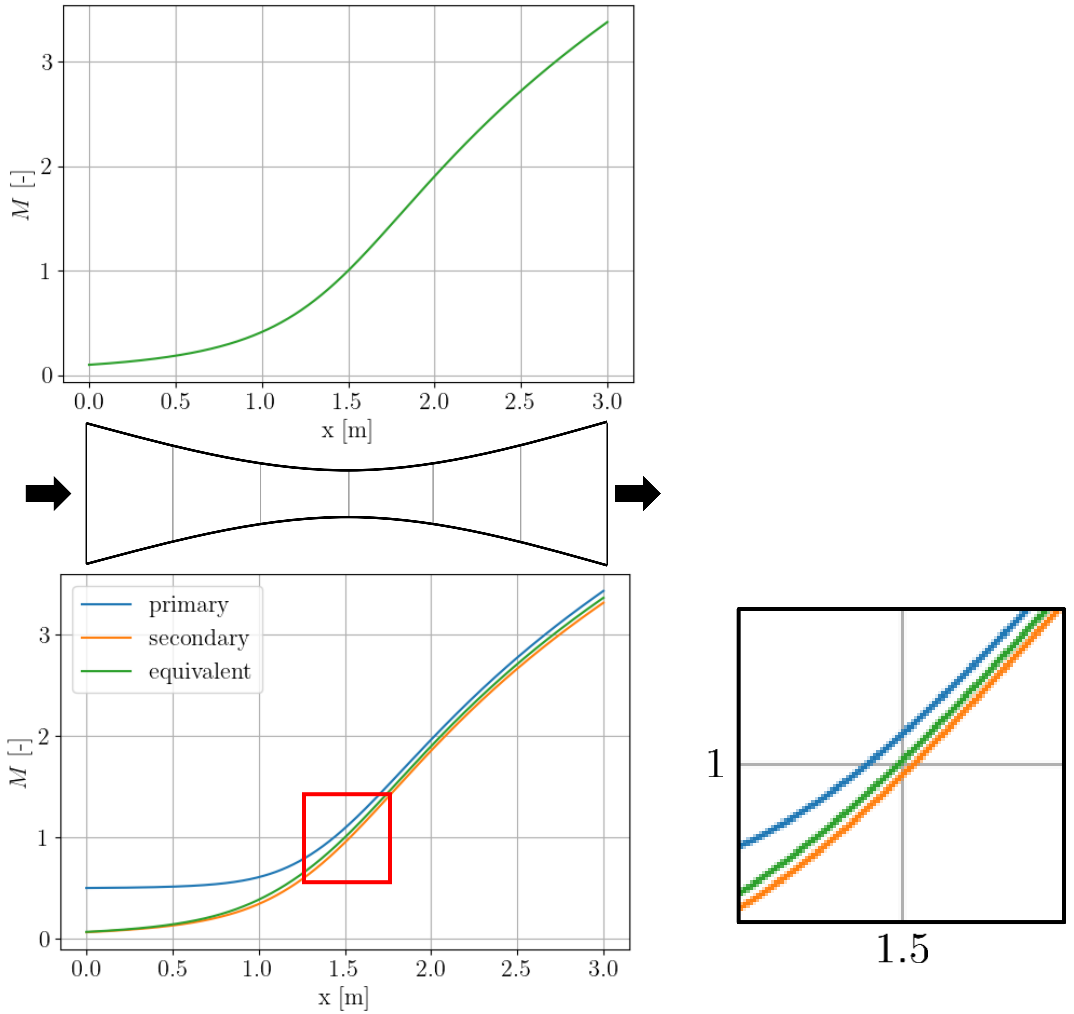
Double “compound” stream [4]

$$\frac{d_x p}{p} = \frac{d_x A_p + d_x A_s + \text{force terms}}{A_p \frac{1-M_p^2}{\gamma M_p^2} + A_s \frac{1-M_s^2}{\gamma M_s^2}} \longrightarrow \beta$$

Singular if $\beta = 0$, possible if $d_x A = 0$.

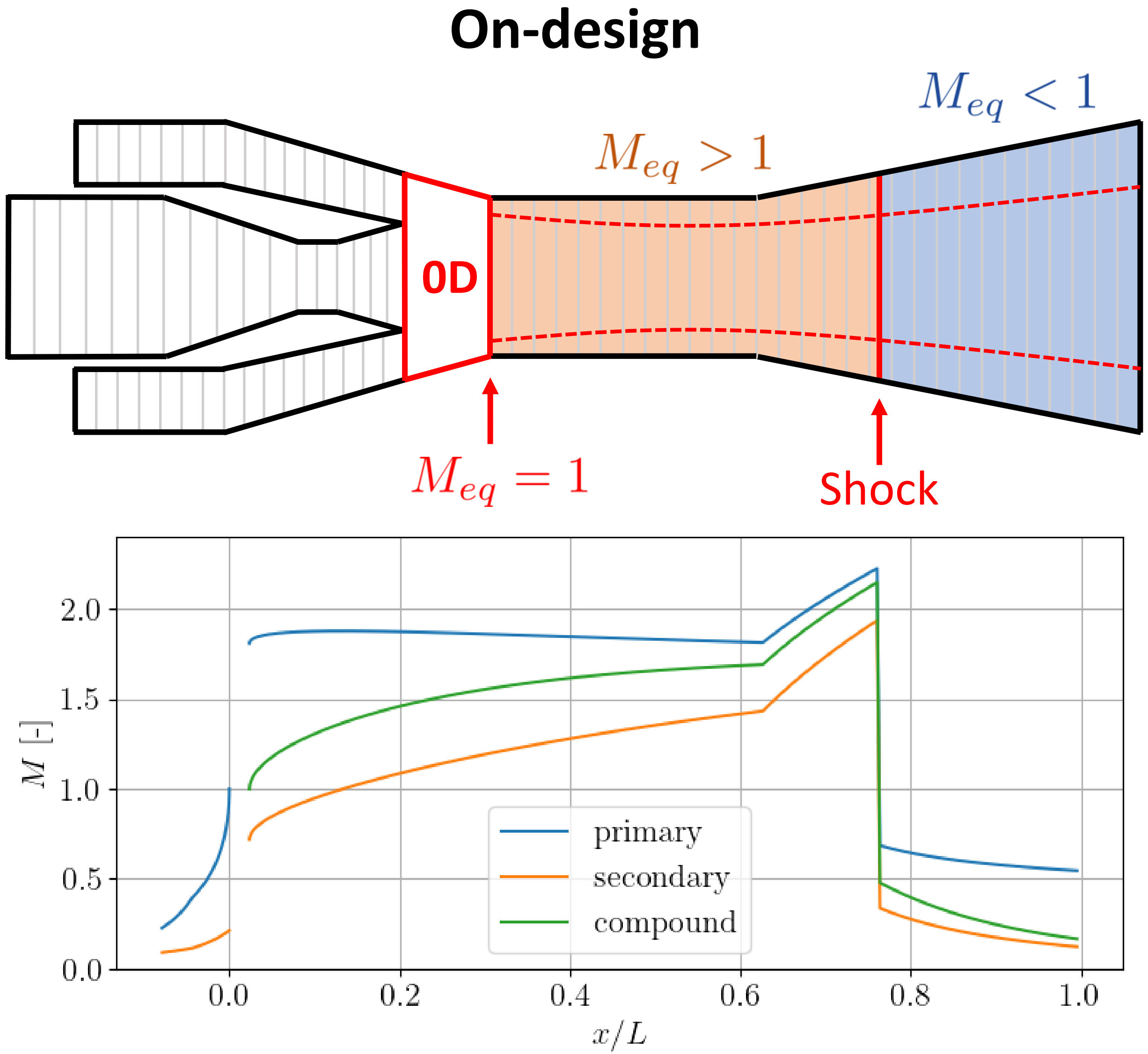
$$\begin{cases} M_p = 1, \;\; M_s = 1 \\ M_p > 1, \;\; M_s < 1 \end{cases}$$ ➡ Multiple options!

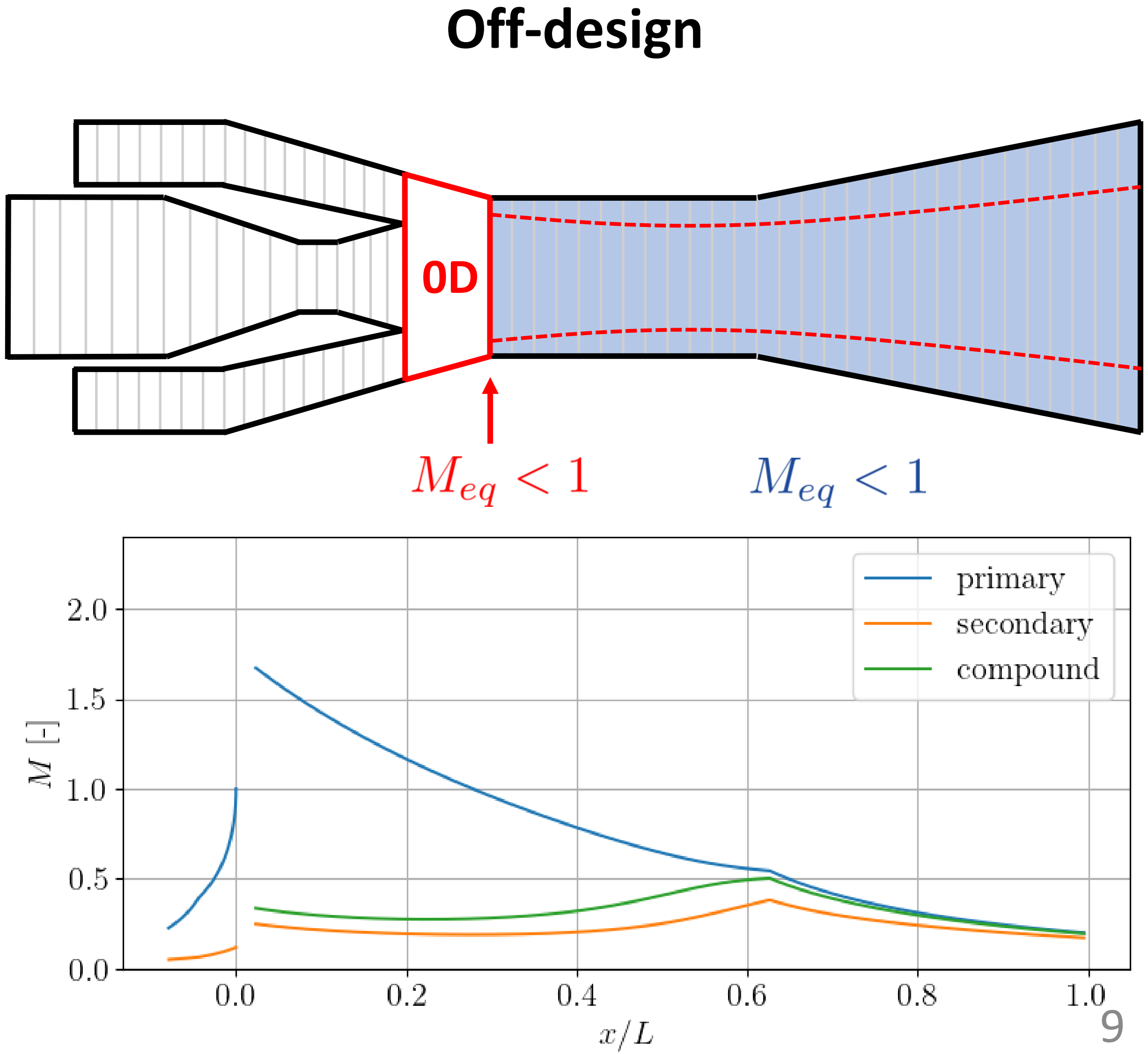
$$\beta \approx A\frac{1 - M^2}{\gamma M^2} \quad ➡ \quad M_{eq}^2 = \left(\gamma\frac{\beta}{A} + 1\right)^{-1}$$



Note: shear and friction forces can be included

Results


On-design
$M_{eq} < 1$
$M_{eq} > 1$
0D
$M_{eq} = 1$
Shock
M [-]
x/L
primary
secondary
compound


Off-design
0D
$M_{eq} < 1$
$M_{eq} < 1$
M [-]
x/L
primary
secondary
compound

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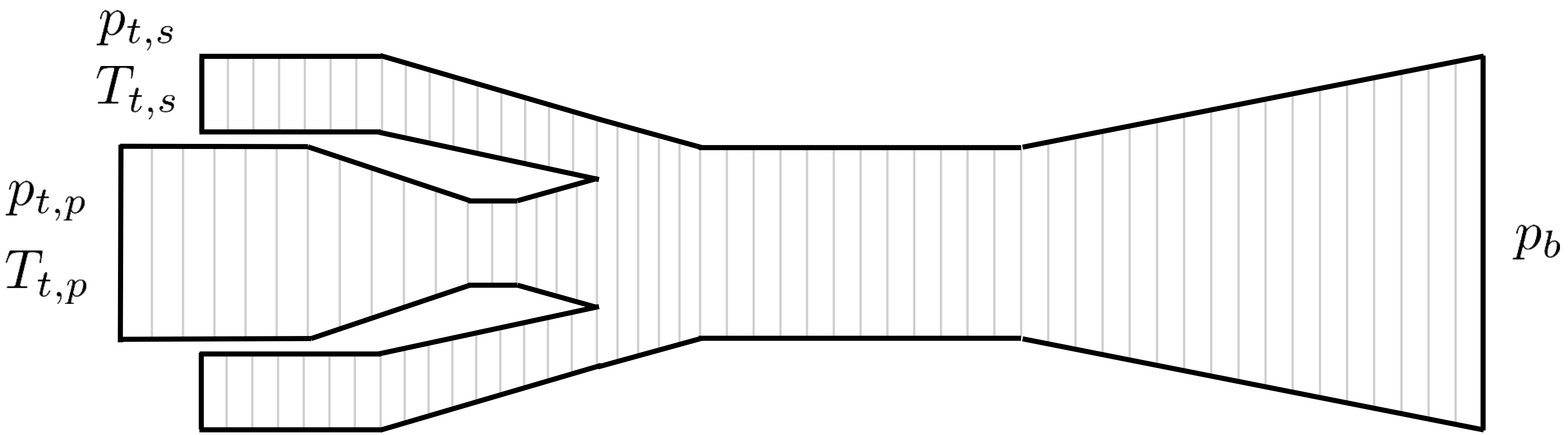

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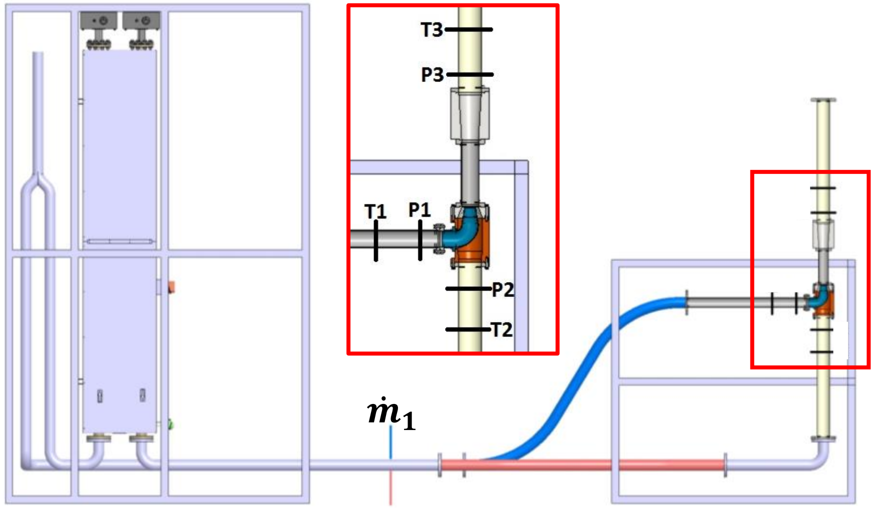
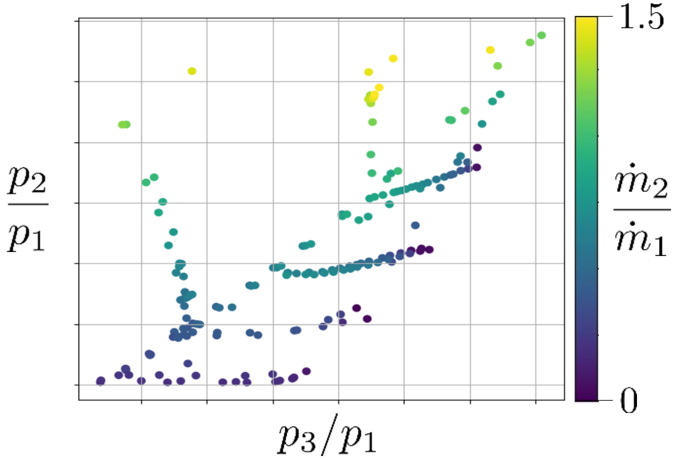
Reconcile ejector models with CFD and experiments

Available tools for experiments and CFD

Experimental facility at VKI

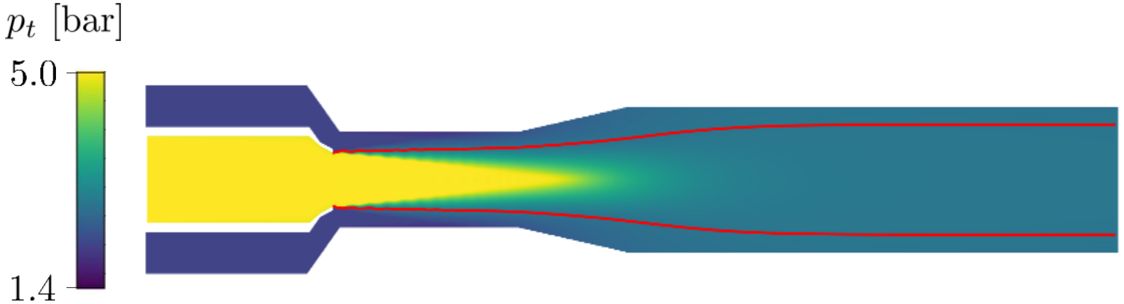


Pressure and temperature regulation

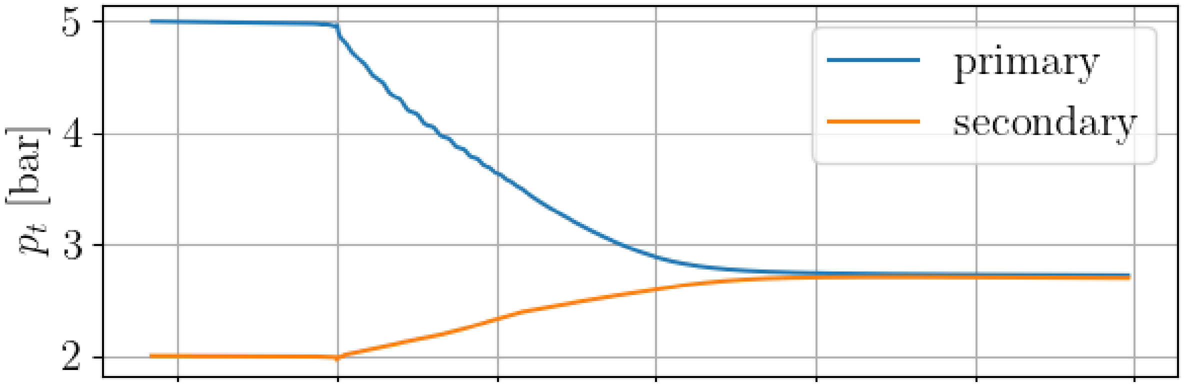


Global validation data
+
Local pressure taps

Feature extraction from CFD at UCL



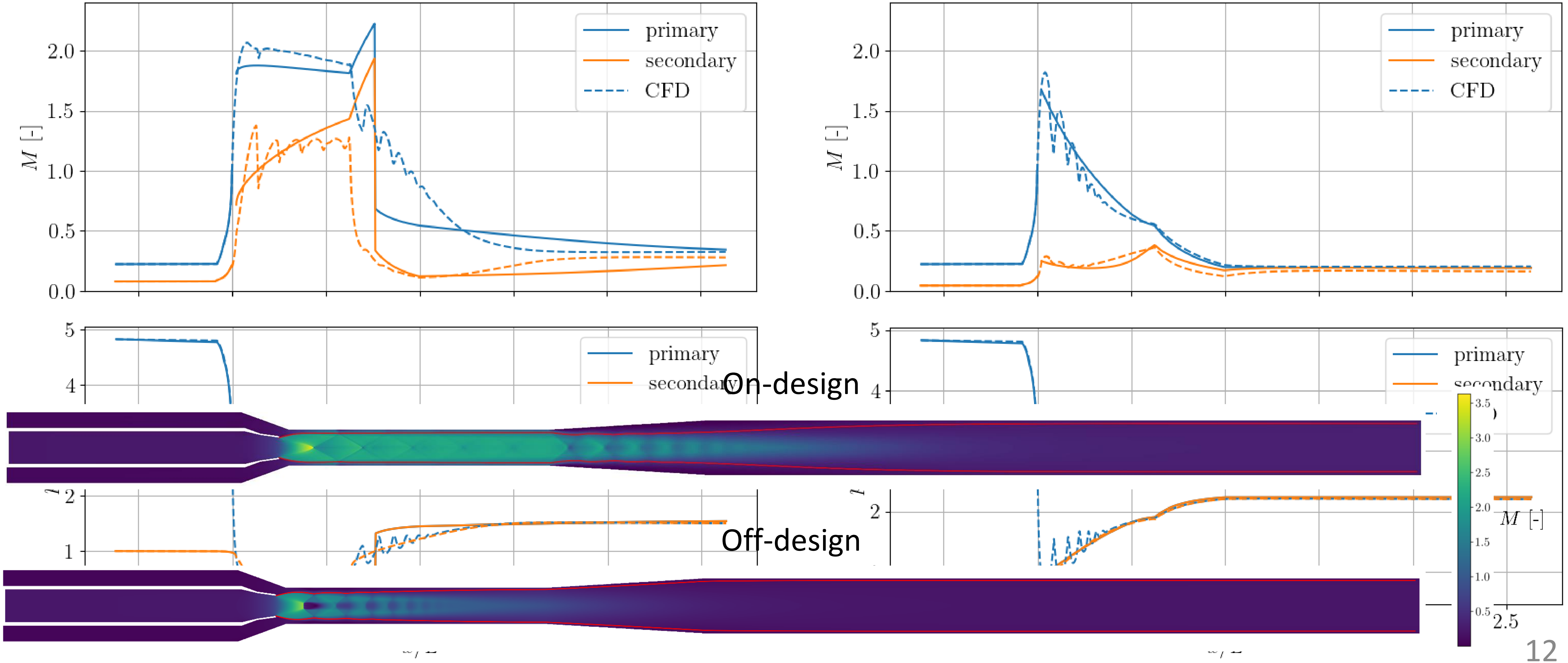
1. Calculate the dividing streamline
2. Average over the 2 sections



Local data for verification

Results with manual calibration

On-design | **Off-design**



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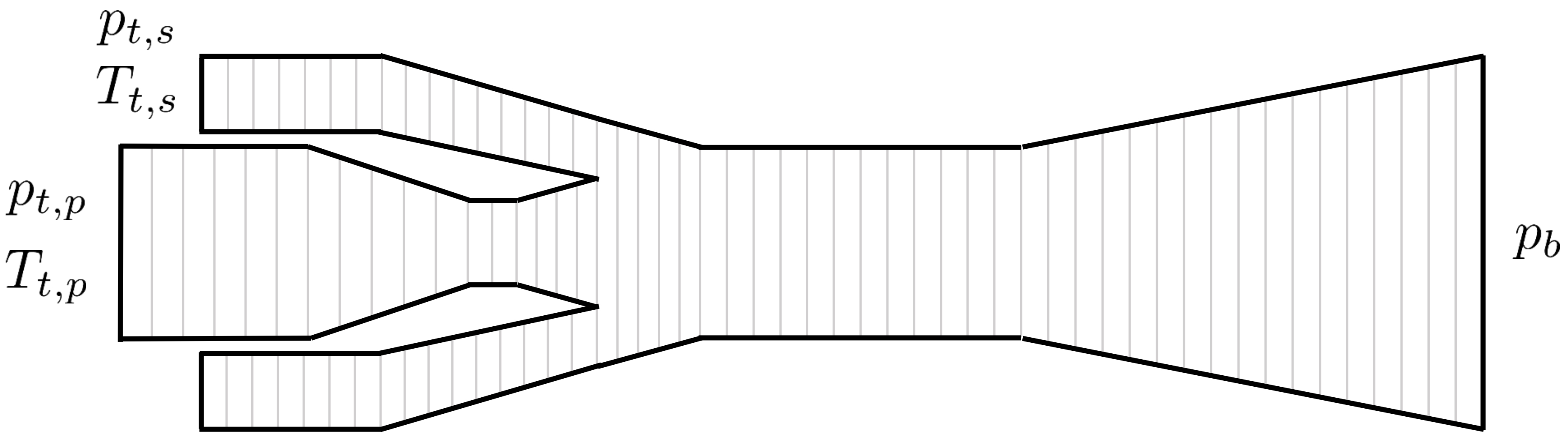

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Calibration of a system of ODEs

General framework

A system of ODEs:

$$\frac{d\boldsymbol{u}}{dx} = f(\boldsymbol{u}, x, \boldsymbol{p})$$

Question: which parameters $\boldsymbol{p}$ lead to a close match to observations $\tilde{\boldsymbol{u}}$?

Solution: define a cost function and calculate its gradient:

$$J(\boldsymbol{p}) = \int_0^L (\boldsymbol{u} - \tilde{\boldsymbol{u}})^2 \, dx$$

$$d_{\boldsymbol{p}} J = 2 \int_0^L (\boldsymbol{u} - \tilde{\boldsymbol{u}}) \boxed{d_{\boldsymbol{p}} \boldsymbol{u}} \, dx$$

Tricky to calculate!

➡ Adjoint

Question: how to find a closure relation between the parameters $\boldsymbol{p}$ and the state $\boldsymbol{u}$?

Solution: machine learning with a parametric function!

$$\boldsymbol{p} = g(\boldsymbol{u}, x; \boldsymbol{w})$$

Adjoint Directly from g

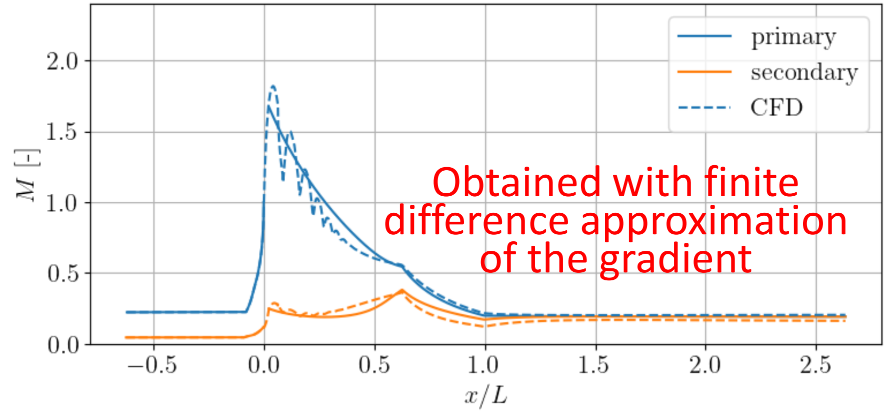
$$d_{\boldsymbol{w}} J = 2 \int_0^L (\boldsymbol{u} - \tilde{\boldsymbol{u}}) \boxed{d_{\boldsymbol{p}} \boldsymbol{u}} \boxed{d_{\boldsymbol{w}} \boldsymbol{p}} \, dx$$

Application on the ejector model

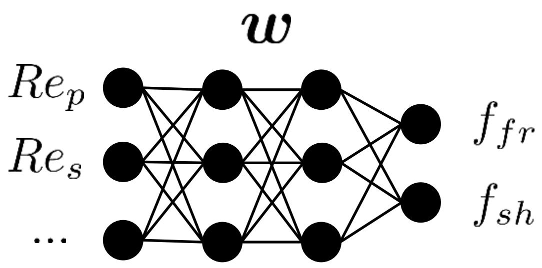
$$\boldsymbol{u} = [p, p_{t,p}, p_{t,s}, T_{t,p}, T_{t,s}, A_p, A_s]$$

$$\frac{d\boldsymbol{u}}{dx} = \text{Conservation equations + shear + friction}$$

$$\boldsymbol{p} = [f_{sh}, f_{fr}] \quad \text{Shear and friction coefficient}$$



$$[f_{sh}, f_{fr}] = g(Re_p, Re_s, M_p, M_s, \ldots)$$



A first test case: non-linear advection of a scalar

General framework

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Test case

A scalar PDE:

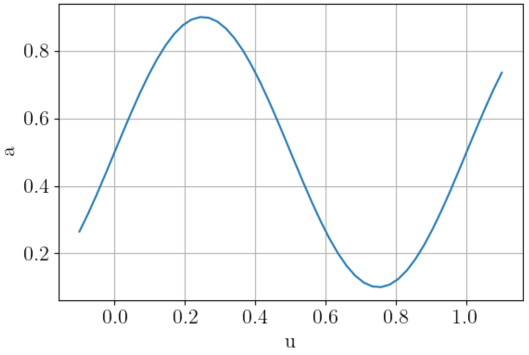
$$\frac{du}{dt} = a \frac{du}{dx}$$
$$a = g(u)$$

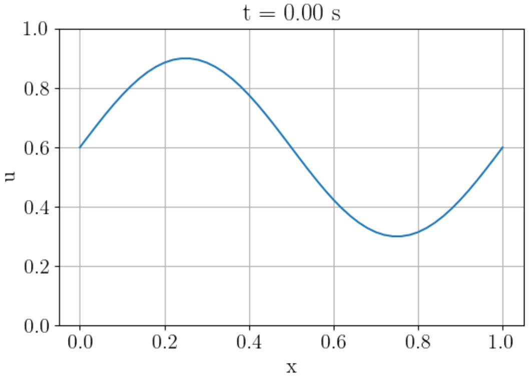
Semi-discretization

A system of ODEs:

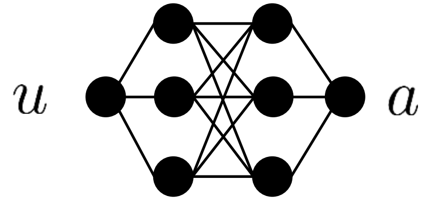
$$\frac{d\boldsymbol{u}}{dt} = a \left(\boldsymbol{A} \boldsymbol{u} \right)$$
$$\boldsymbol{a} = g(\boldsymbol{u})$$

Reference solution for observations: $a = \sin(u)$

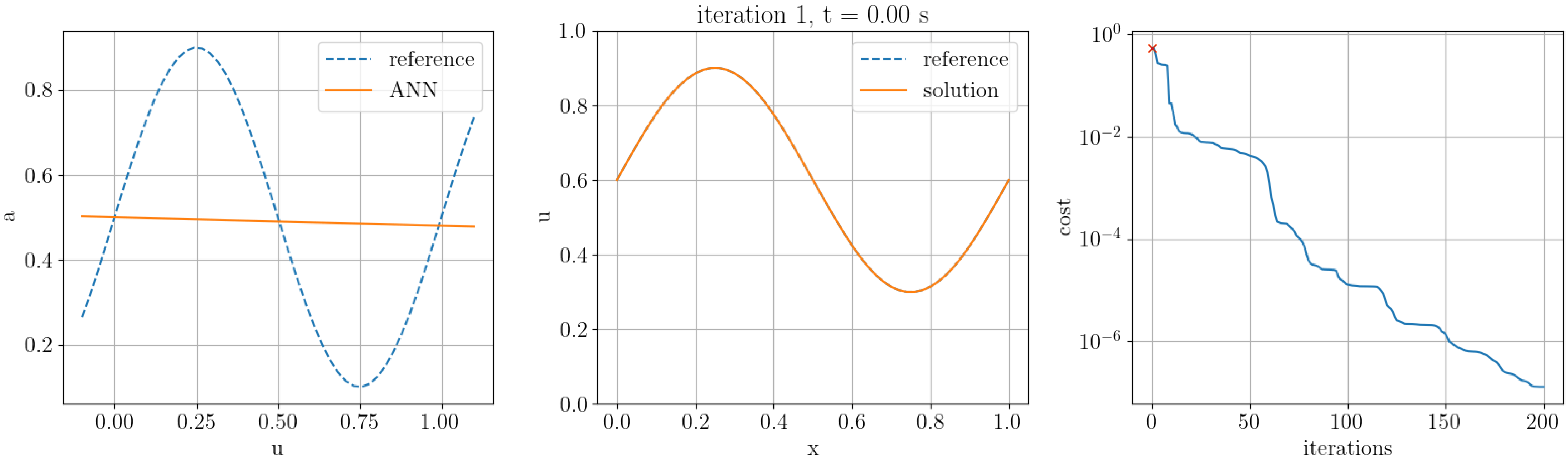




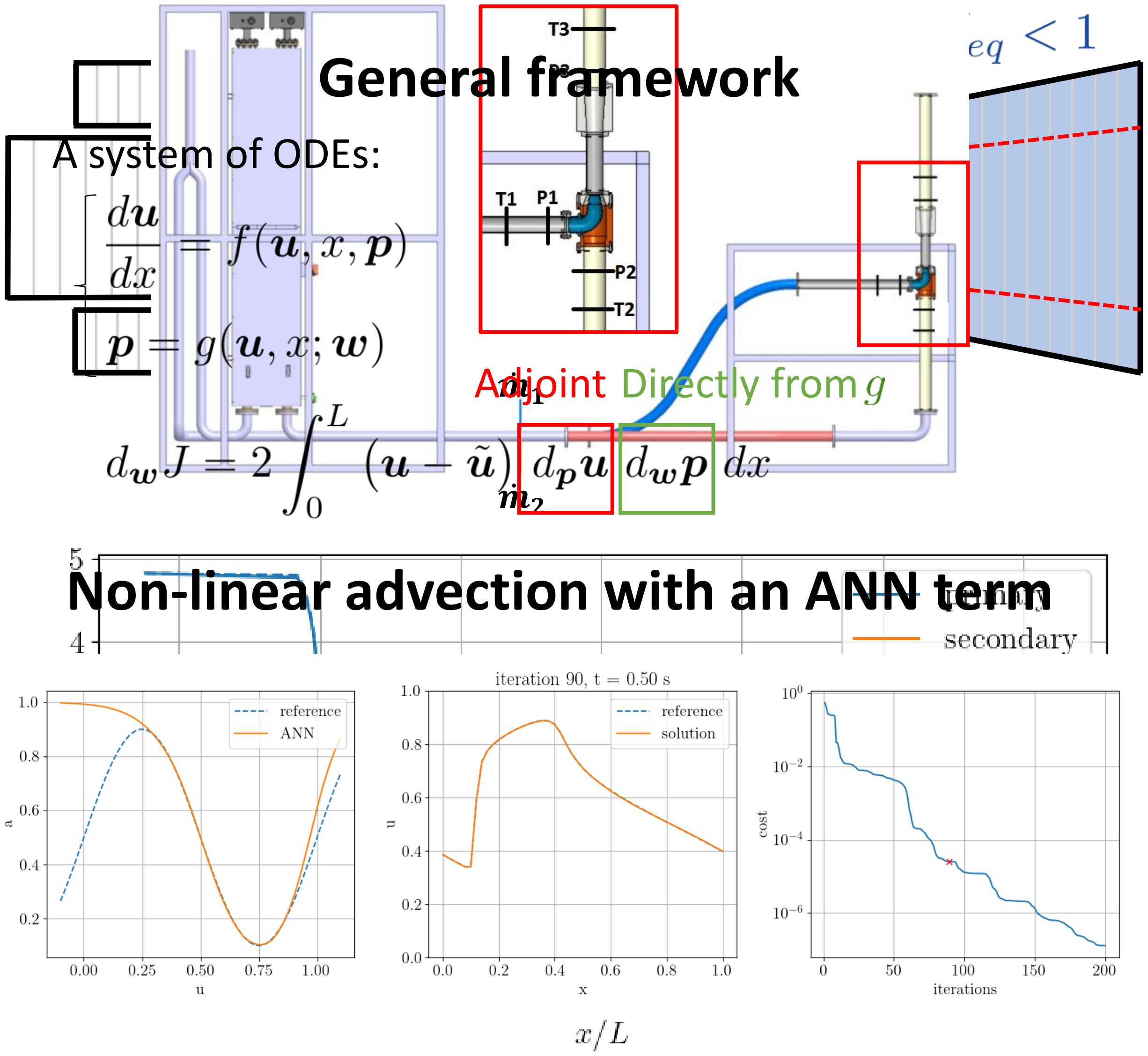
Can a neural network learn this function through observations of u ?



A first test case: results



Conclusion



- **A 1D ejector model**
  - A robust and coherent framework
  - Extension of the compound flow theory

Include a pressure equalization mechanism (full 1D)

- **A high-fidelity database for validation**
  - Experimental mass flow rates – more local pressure taps underway
  - A first calibration on post-processed CFD

CFD on ejectors with a supersonic primary nozzle

- **Machine learning-based calibration tools**
  - A general framework
  - A first scalar test case

Increase the complexity of the test cases up to the ejector model

References

1. J. Van den Berghe, B. R. Dias, Y. Bartosiewicz, M. A. Mendez. “A 1D model for the unsteady gas dynamics of ejectors”, Energy 267, 2023.
2. J. G. del Valle, J. M. S. Jabardo, F. C. Ruiz, J. S. J. Alonso. “A one dimensional model for the determination of an ejector entrainment ratio”, International Journal of Refrigeration, 35(4), 2012.
3. K. Banasiak and A. Hafner. “1d computational model of a two-phase r744 ejector for expansion work recovery”, International Journal of Thermal Sciences, 50(11): 2235–2247, 2011.
4. A. Bernstein, W. Heiser, and C. Hevenor. “Compound-compressible nozzle flow”, 1967.

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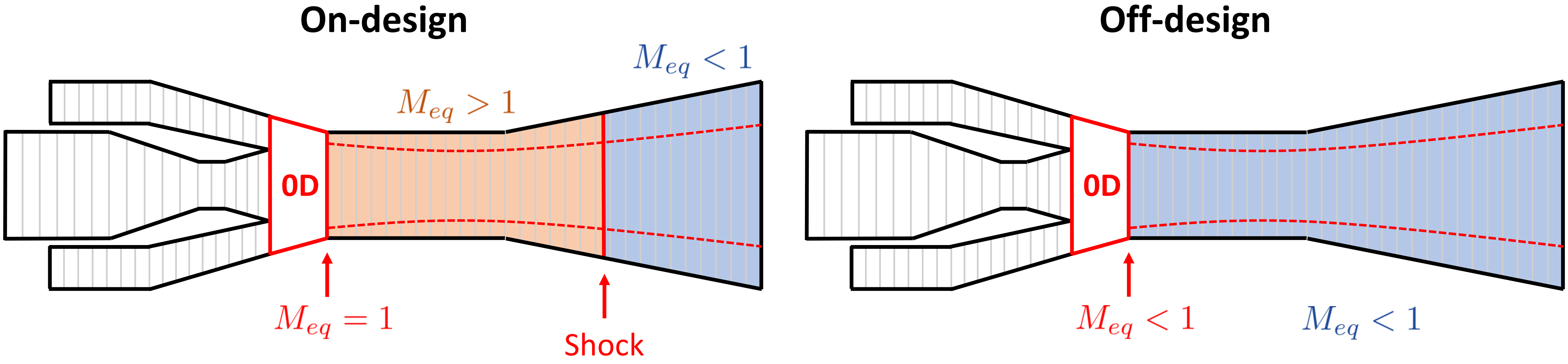
Back-up slides

Calculation procedure



1. Primary nozzle (assumed choked)
2. 0D junction (impose M_{eq})
3. Secondary inlet
4. Mixing pipe

Shooting method to match the back pressure:
- Iterate on the position of the shock (on-design)
- Iterate on M_{eq} at the exit of the 0D junction

Compound equations

Compound flow equations with shear

Euler equations in the primary and the secondary domain:

$$\begin{cases} d_x(\rho_p A_p V_p) & = 0 \\ d_x(\rho_p A_p V_p^2) & = -A_p d_x p_p + F_p \\ d_x(\rho_p A_p V_p h_{t,p}) & = 0 \\ d_x(\rho_s A_s V_s) & = 0 \\ d_x(\rho_s A_s V_s^2) & = -A_s d_x p_s + F_s \\ d_x(\rho_s A_s V_s h_{t,s}) & = 0 \end{cases}$$

constrained by:

$$\begin{cases} p_p(x) = p_s(x) & = p(x) \\ A_p + A_s & = A \end{cases}$$

Equivalently:

$$\frac{d_x p}{p} = \left[\frac{1 + (\gamma - 1) M_i^2}{1 - M_i^2}\right] \frac{F_i}{A_i p} + \left[\frac{\gamma M_i^2}{1 - M_i^2}\right] \frac{d_x A_i}{A_i}$$

$$\frac{d_x p_{t,i}}{p_{t,i}} = \frac{F_i}{A_i p} \qquad i \in [p, s]$$

$$\frac{d_x T_{t,i}}{T_{t,i}} = 0$$

Compound flow equations with shear

Let’s reformulate the pressure equation:

$$\frac{d_x p}{p} = \left[\frac{1+(\gamma-1)\,M_i^2}{1-M_i^2}\right]\frac{F_i}{A_i p} + \left[\frac{\gamma M_i^2}{1-M_i^2}\right]\frac{d_x A_i}{A_i} \quad \Rightarrow \quad d_x A_i = \left[A_i\frac{1-M_i^2}{\gamma M_i^2}\right]\frac{d_x p}{p} - \left[\frac{1+(\gamma-1)\,M_i^2}{\gamma M_i^2}\right]\frac{F_i}{p}$$

The total cross-section comes forward after summing the equations for both domains:

$$\sum_i d_x A_i = d_x A = \left[A_p\frac{1-M_p^2}{\gamma M_p^2} + A_s\frac{1-M_s^2}{\gamma M_s^2}\right]\frac{d_x p}{p} - \left[\frac{1+(\gamma-1)\,M_p^2}{\gamma M_p^2}\right]\frac{F_p}{p} - \left[\frac{1+(\gamma-1)\,M_s^2}{\gamma M_s^2}\right]\frac{F_s}{p}$$

Reformulating:

$$\frac{d_x p}{p} = \frac{1}{\beta}\left(d_x A + \left[\frac{1+(\gamma-1)\,M_p^2}{\gamma M_p^2}\right]\frac{F_p}{p} + \left[\frac{1+(\gamma-1)\,M_s^2}{\gamma M_s^2}\right]\frac{F_s}{p}\right) \quad \text{with} \quad \beta = A_p\frac{1-M_p^2}{\gamma M_p^2} + A_s\frac{1-M_s^2}{\gamma M_s^2}$$

Comparison to the single stream equations

Single stream:

$$\frac{d_x p}{p} = \left[\frac{1+(\gamma-1)\,M^2}{1-M^2}\right]\frac{F}{Ap} + \left[\frac{\gamma M^2}{1-M^2}\right]\frac{d_x A}{A}$$

Equivalently:

$$\frac{d_x p}{p} = \frac{\gamma M^2}{A\,(1-M^2)}\left(d_x A + \left[\frac{1+(\gamma-1)\,M^2}{\gamma M^2}\right]\frac{F}{p}\right)$$

Compound equation:

$$\frac{d_x p}{p} = \frac{1}{\beta}\left(d_x A + \left[\frac{1+(\gamma-1)\,M_p^2}{\gamma M_p^2}\right]\frac{F_p}{p} + \left[\frac{1+(\gamma-1)\,M_s^2}{\gamma M_s^2}\right]\frac{F_s}{p}\right) \quad \text{with} \quad \beta = A_p\frac{1-M_p^2}{\gamma M_p^2} + A_s\frac{1-M_s^2}{\gamma M_s^2}$$

These equations are equivalent if $M_p = M_s$!

Choking occurs if these equations become singular:

- $M = 1$ for the single stream
- $\beta = 0$ for the compound flow

Physically only possible if the numerator is also zero (no infinite pressure gradient).
The pressure gradient follows from a (considerably more complicated) quadratic equation.

A note on choking

The pressure equation is singular if $M = 1$:

$$\frac{d_x p}{p} = \left[\frac{1 + (\gamma - 1) M^2}{1 - M^2}\right] \frac{F}{Ap} + \left[\frac{\gamma M^2}{1 - M^2}\right] \frac{d_x A}{A}$$

Equivalently:

$$\frac{d_x p}{p} = \frac{1}{1 - M^2} \left(\left[\gamma M^2\right] \frac{d_x A}{A} + \left[1 + (\gamma - 1) M^2\right] \frac{F}{Ap} \right)$$

The gradient is only finite (and thus physical) if the numerator is also zero.
In case $F = 0$: $d_x A = 0$ (so at the throat)
In case of friction: $F < 0$, so $d_x A > 0$.
Friction moves the choked section downstream!

The pressure gradient follows from de l'Hôpital's rule:

$$\frac{d_x p}{p} = \frac{0}{0} = \frac{1}{-d_x \left(M^2\right)} d_x \left(\left[\gamma M^2\right] \frac{d_x A}{A} + \left[1 + (\gamma - 1) M^2\right] \frac{F}{Ap} \right)$$

Which results in a quadratic equation for the pressure gradient (a subsonic and a supersonic solution).

Choked conditions

We obtained the following equation:

$$\frac{d_x p}{p} = \frac{1}{\beta}\left(d_x A + \left[\frac{1+(\gamma-1)M_p^2}{\gamma M_p^2}\right]\frac{F_p}{p} + \left[\frac{1+(\gamma-1)M_s^2}{\gamma M_s^2}\right]\frac{F_s}{p}\right) \quad \text{with} \quad \beta = A_p\frac{1-M_p^2}{\gamma M_p^2} + A_s\frac{1-M_s^2}{\gamma M_s^2}$$

In choked conditions, both the numerator and the denominator are equal to zero. Through de l'Hôpital's rule:

$$a_{dxp}\left(\frac{d_x p}{p}\right)^2 + b_{dxp}\frac{d_x p}{p} + c_{dxp} = 0 \;\Rightarrow\; \frac{d_x p}{p} = -\frac{b_{dxp}}{2a_{dxp}} \pm \frac{1}{2a_{dxp}}\sqrt{b_{dxp}^2 - 4a_{dxp}c_{dxp}}$$

Sub- and supersonic solution

$a_{dxp} = \sum_{i=p,s}\left[A_i\frac{\left(1-M_i^2\right)^2 + 2\left(1+\frac{\gamma-1}{2}M_i^2\right)}{\gamma^2 M_i^4}\right]$	$c_{dxp} = -\,d_{xx}A + \alpha_{axi}\frac{f_{sh}l_{sh}}{2}\frac{\left(M_p^2-M_s^2\right)^2}{M_p^2M_s^2}\left(\frac{1+(\gamma-1)M_p^2}{\gamma M_p^2}\right)\frac{F_p}{pA_p}$ $- 2f_{sh}l_{sh}\frac{M_p^4-M_s^4}{M_p^2M_s^2}\left[\frac{1+\frac{\gamma-1}{2}M_p^2}{\gamma M_p^2}\frac{F_p}{A_p p} - \frac{1+\frac{\gamma-1}{2}M_s^2}{\gamma M_s^2}\frac{F_s}{A_s p}\right]$ $- \alpha_{axi}\frac{f_{wall}l_{wall}}{2}\left(\frac{1+(\gamma-1)M_s^2}{2}\right)\frac{d_x A}{A}$ $- f_{wall}l_{wall}\frac{\gamma-1}{\gamma}\left[1+\frac{\gamma-1}{2}M_s^2\right]\frac{F_s}{A_s p}$
$b_{dxp} = \sum_{i=p,s}\left[-\frac{\left(1-M_i^2\right)^2 + 2\left(1+\frac{\gamma-1}{2}M_i^2\right)}{\gamma^2 M_i^4} - \frac{1-M_i^2}{\gamma M_i^2}\right]\frac{F_i}{p}$ $- \alpha_{axi}\frac{f_{sh}l_{sh}}{2}\frac{\left(M_p^2-M_s^2\right)^2}{M_p^2M_s^2}\left(\frac{1-M_p^2}{\gamma M_p^2}\right) - 2f_{sh}l_{sh}\left(M_p^2-M_s^2\right)\frac{M_p^4-M_s^4}{\gamma M_p^4 M_s^4}$ $+ f_{wall}l_{wall}\frac{\gamma-1}{\gamma}\left[1+\frac{\gamma-1}{2}M_s^2\right]$	

Choked conditions without additional forces

The pressure equation simplifies:

$$\frac{d_x p}{p} = \frac{1}{\beta}\left(d_x A\right) \qquad \text{with} \quad \beta = A_p \frac{1 - M_p^2}{\gamma M_p^2} + A_s \frac{1 - M_s^2}{\gamma M_s^2}$$

In choked conditions, both the numerator and the denominator are equal to zero. Through de l'Hôpital's rule:

$$a_{dxp}\left(\frac{d_x p}{p}\right)^2 + b_{dxp}\frac{d_x p}{p} + c_{dxp} = 0 \;\Rightarrow\; \frac{d_x p}{p} = -\frac{b_{dxp}}{2a_{dxp}} \pm \frac{1}{2a_{dxp}}\sqrt{b_{dxp}^2 - 4a_{dxp}c_{dxp}}$$

Sub- and supersonic solution

$a_{dxp} = \sum_{i=p,s}\left[A_i \frac{\left(1 - M_i^2\right)^2 + 2\left(1 + \frac{\gamma-1}{2}M_i^2\right)}{\gamma^2 M_i^4}\right]$	$c_{dxp} = -d_{xx}A$
$b_{dxp} = 0$	

1. Since a > 0, c must be < 0. The nozzle must form a throat! ($d_{xx}A > 0$)
2. This expression matches with the original paper proposing compound choking [1]

Compound flow equations with shear and friction

We obtained the following equation:

$$\frac{d_x p}{p} = \frac{1}{\beta}\left(d_x A + \left[\frac{1+(\gamma-1)\,M_p^2}{\gamma M_p^2}\right]\frac{F_p}{p} + \left[\frac{1+(\gamma-1)\,M_s^2}{\gamma M_s^2}\right]\frac{F_s}{p}\right) \quad \text{with} \quad \beta = A_p\frac{1-M_p^2}{\gamma M_p^2} + A_s\frac{1-M_s^2}{\gamma M_s^2}$$

Let's fill in the shear force and the friction force:

$$F_p = -\tau_{sh} l_{sh} = -f_{sh}\left(\rho_p v_p^2 - \rho_s v_s^2\right) l_{sh} = -f_{sh}\gamma p\left(M_p^2 - M_s^2\right) l_{sh}$$

$$F_s = \tau_{sh} l_{sh} + \tau_{wall} l_{wall} = f_{sh}\gamma p\left(M_p^2 - M_s^2\right) l_{sh} - \frac{1}{2} f_{wall}\gamma p M_s^2 l_{wall}$$

After some manipulations:

$$\frac{d_x p}{p} = \frac{1}{\beta}\left(d_x A + f_{sh} l_{sh}\frac{\left(M_p^2 - M_s^2\right)^2}{M_p^2 M_s^2} - \frac{1}{2} f_{wall} l_{wall}\left(1 + (\gamma-1)\,M_s^2\right)\right)$$

The two last terms are always positive but have a different sign in front.

- Shear 'pushes' the choked section to a convergent section
- Friction 'pushes' it to a divergent section

The position of the choked section depends on the flow!

Adjoint computations

The continuous adjoint method

General dynamical system of ODEs:

$$\dot{\boldsymbol{u}} = f(\boldsymbol{u}, t, \boldsymbol{p})$$

Question: which parameters $\boldsymbol{p}$ lead to a close match to observations $\tilde{\boldsymbol{u}}$?

Solution: define a cost function and calculate its gradient:

$$J(\boldsymbol{p}) = \int_0^T (\boldsymbol{u} - \tilde{\boldsymbol{u}})^2 \; dt$$

$$d_{\boldsymbol{p}} J = 2 \int_0^T (\boldsymbol{u} - \tilde{\boldsymbol{u}}) \boxed{d_{\boldsymbol{p}} \boldsymbol{u}} dt$$

Tricky to calculate!

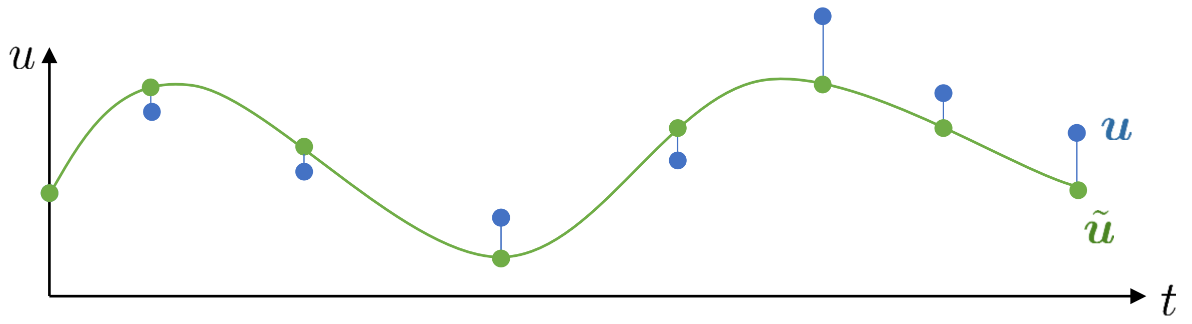
$\boldsymbol{u}$ follows from integration of f :

$$\boldsymbol{u} = \boldsymbol{u}^0 + \int_0^{t_n} \dot{\boldsymbol{u}} \; dt = \boldsymbol{u}^0 + \int_0^{t_n} f(\boldsymbol{u}, t, \boldsymbol{p}) \; dt$$

$\boldsymbol{u}$ is thus directly affected by $\boldsymbol{p}$ through the integration, but also indirectly through $\boldsymbol{u}$ at all previous times!

Notation

$\boldsymbol{u}$	state vector
$\tilde{\boldsymbol{u}}$	observed state vector
t	time
$\boldsymbol{p}$	vector of closure parameters
f	function for the time derivative of $\boldsymbol{u}$
J	cost function
$\boldsymbol{\lambda}$	adjoint state vector



The continuous adjoint method

We consider a constrained optimization problem:

Minimize $J(\boldsymbol{p}) = \int_0^T (\boldsymbol{u} - \tilde{\boldsymbol{u}})^2 \, dt$ s.t. $\dot{\boldsymbol{u}} = f(\boldsymbol{u}, t, \boldsymbol{p})$

Using a Lagrange multiplier:

Minimize $\mathcal{L}(\boldsymbol{p}) = \int_0^T (\boldsymbol{u} - \tilde{\boldsymbol{u}})^2 + \int_0^T \lambda(t) \underbrace{\big(\dot{\boldsymbol{u}} - f(\boldsymbol{u}, t, \boldsymbol{p})\big)}_{=0} \, dt$

We compute the gradient:

$$d_{\boldsymbol{p}}\mathcal{L} = \int_0^T 2\big(\boldsymbol{u} - \tilde{\boldsymbol{u}}\big) \, d_{\boldsymbol{p}}\boldsymbol{u} \, dt + \int_0^T \lambda\big(d_{\boldsymbol{p}}\dot{\boldsymbol{u}} - d_{\boldsymbol{p}} f\big) \, dt$$

f depends directly AND indirectly on $\boldsymbol{p}$: $d_{\boldsymbol{p}} f = \partial_{\boldsymbol{p}} f + \partial_{\boldsymbol{u}} f \, d_{\boldsymbol{p}}\boldsymbol{u}$

$$d_{\boldsymbol{p}}\mathcal{L} = \int_0^T 2\big(\boldsymbol{u} - \tilde{\boldsymbol{u}}\big) \, d_{\boldsymbol{p}}\boldsymbol{u} \, dt + \int_0^T \lambda\big(d_{\boldsymbol{p}}\dot{\boldsymbol{u}} - \partial_{\boldsymbol{p}} f - \partial_{\boldsymbol{u}} f \, d_{\boldsymbol{p}}\boldsymbol{u}\big) \, dt$$

$$d_{\boldsymbol{p}}\mathcal{L} = \int_0^T 2\big(\boldsymbol{u} - \tilde{\boldsymbol{u}}\big) \, d_{\boldsymbol{p}}\boldsymbol{u} \, dt + \boxed{\int_0^T \lambda d_{\boldsymbol{p}}\dot{\boldsymbol{u}} \, dt} - \int_0^T \lambda \partial_{\boldsymbol{p}} f \, dt - \int_0^T \lambda \partial_{\boldsymbol{u}} f \, d_{\boldsymbol{p}}\boldsymbol{u} \, dt$$

The continuous adjoint method

$$d_{\boldsymbol{p}}\mathcal{L} = \int_0^T 2(\boldsymbol{u}-\tilde{\boldsymbol{u}})\ d_{\boldsymbol{p}}\boldsymbol{u}\ dt + \boxed{\int_0^T \lambda d_{\boldsymbol{p}}\dot{\boldsymbol{u}}\ dt} - \int_0^T \lambda\partial_{\boldsymbol{p}}f\ dt - \int_0^T \lambda\partial_{\boldsymbol{u}}f\ d_{\boldsymbol{p}}\boldsymbol{u}\ dt$$

We integrate by parts:

$$d_{\boldsymbol{p}}\mathcal{L} = \int_0^T 2(\boldsymbol{u}-\tilde{\boldsymbol{u}})\ d_{\boldsymbol{p}}\boldsymbol{u}\ dt + \boxed{\Big[\lambda d_{\boldsymbol{p}}\boldsymbol{u}\Big]_0^T - \int_0^T \dot{\lambda} d_{\boldsymbol{p}}\boldsymbol{u}\ dt} - \int_0^T \lambda\partial_{\boldsymbol{p}}f\ dt - \int_0^T \lambda\partial_{\boldsymbol{u}}f\ d_{\boldsymbol{p}}\boldsymbol{u}\ dt$$

Regrouping:

$$d_{\boldsymbol{p}}\mathcal{L} = \int_0^T \Big[2(\boldsymbol{u}-\tilde{\boldsymbol{u}}) - \dot{\lambda} - \lambda\partial_{\boldsymbol{u}}f\Big]\ d_{\boldsymbol{p}}\boldsymbol{u}\ dt + \Big[\lambda d_{\boldsymbol{p}}\boldsymbol{u}\Big]_0^T - \int_0^T \lambda\partial_{\boldsymbol{p}}f\ dt$$

The expression for the gradient becomes very easy if the terms between the brackets would be zero. Therefore we impose:

$$\begin{cases} \dot{\lambda} = 2(\boldsymbol{u}-\tilde{\boldsymbol{u}}) - \lambda\partial_{\boldsymbol{u}}f \\ \lambda(T) = 0 \end{cases}$$

($d_{\boldsymbol{p}}\boldsymbol{u}(0) = 0$ because the IC is fixed)

$$d_{\boldsymbol{p}}\mathcal{L} = d_{\boldsymbol{p}}J = -\int_0^T \lambda\partial_{\boldsymbol{p}}f\ dt$$

By constructing an **adjoint** system and solving it **backwards** in time, we compute how the parameters have acted over time.

The gradient is obtained by 1 forward and 1 backward solution, independently of the number of parameters.

ODEs with a neural network term

The dynamical system of ODEs now contains a neural network term to predict the parameters $\boldsymbol{p}$:

$$\dot{\boldsymbol{u}} = f(\boldsymbol{u}, t, \boldsymbol{p})$$

$$\boldsymbol{p} = g(\boldsymbol{u}, t; \boldsymbol{w})$$

We're now interested in the gradient with respect to the weights $\boldsymbol{w}$ (could be thousands) of the network

$$J(\boldsymbol{w}) = \int_0^T (\boldsymbol{u} - \tilde{\boldsymbol{u}})^2 \, dt$$

The adjoint system becomes slightly more complicated:

$$\begin{cases} \dot{\boldsymbol{\lambda}} = 2(\boldsymbol{u} - \tilde{\boldsymbol{u}}) - \boldsymbol{\lambda}\big(\partial_{\boldsymbol{u}} f + \partial_{\boldsymbol{p}} f \; \partial_{\boldsymbol{u}} \boldsymbol{p}\big) \\ \boldsymbol{\lambda}(T) = 0 \end{cases}$$

$$d_{\boldsymbol{w}} \mathcal{L} = d_{\boldsymbol{w}} J = -\int_0^T \lambda \partial_{\boldsymbol{p}} f \partial_{\boldsymbol{w}} \boldsymbol{p} \, dt$$

All the rest remains the same!

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All the rest remains the same!