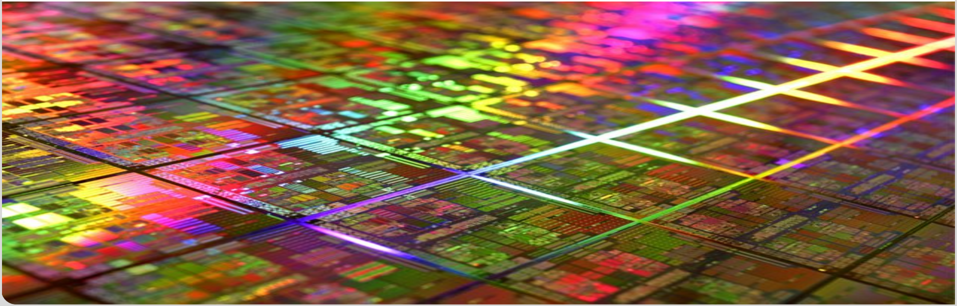
Towards Bringing Together Numerical Methods for Partial Differential Equation and Deep Neural Networks

Project discussion, Supervisor - Markus Hoffmann

Stanislav Arnaudov | January 8, 2020

CHAIR FOR COMPUTER ARCHITECTURE AND PARALLEL PROCESSING



Problem definition and motivation

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Partial differential equation (PDEs)

- used in simulations
- hard to solve numerically
- solutions have image representation

Idea: study non-classical ways for generating solutions of PDEs

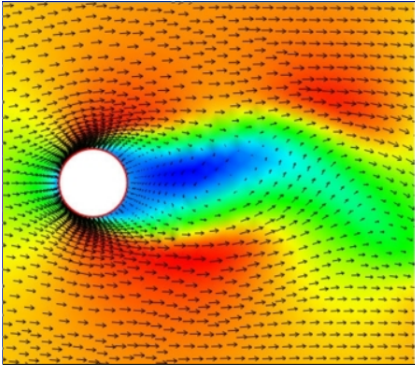

Figure: Flow Simulation[1]

[1] "Team for Advanced Flow Simulation and Modeling", Professor Tayfun E. Tezduyar, Sunil Sathe

Problem definition and motivation

Deep neural networks (DNNs)

- hot topic in recent years
- impressive results in image processing tasks

Idea: Use DNNs in order to solve PDEs

Research topic: The applicability of DNNs in generating solutions for PDEs.

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Problem definition and motivation

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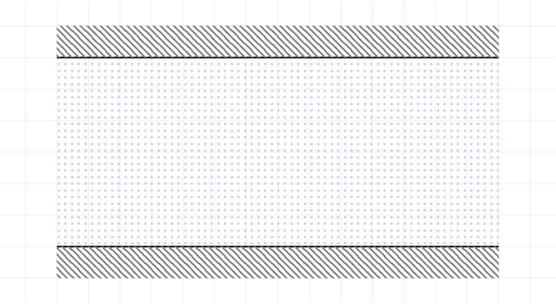
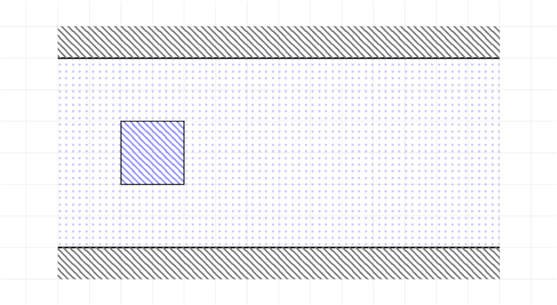


A channel with *incompressible* fluid in it.

Problem definition and motivation

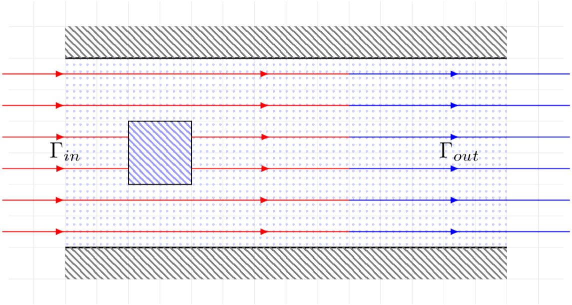
Concrete problem to study



An object placed inside of the channel.

Problem definition and motivation

Concrete problem to study



The fluid is flowing in from the one side and flowing out from the other one.

Problem definition and motivation

Incompressible Navier-Stokes Equation

$$
\begin{aligned}
-\nu\Delta u + (u\cdot\nabla)u + \frac{1}{\rho}\nabla p &= 0, \quad \text{in } \Omega \\
\nabla\cdot u &= 0, \quad \text{in } \Omega \\
u &= g, \quad \text{on } \Gamma_{in} \\
(-\mathcal{I}p + \nu\nabla u)\cdot n &= 0, \quad \text{on } \Gamma_{out} \\
u &= 0, \quad \text{on } \partial\Omega/(\overline{\Gamma_{in}\cup\Gamma_{out}})
\end{aligned}
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Parameters:

- fluid viscosity and density – ρ and n
- inflow speed – g

Problem definition and motivation

Incompressible Navier-Stokes Equation

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Solutions:

- velocity field – u
- pressure field – p

Problem definition and motivation

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DNNs in the context of the described problem

- The solutions of the PDE can be visualized as images
- DNNs perform well on image processing tasks

$\Longrightarrow$ use DNNs to generate solutions of the simulation in image form

Problem definition and motivation

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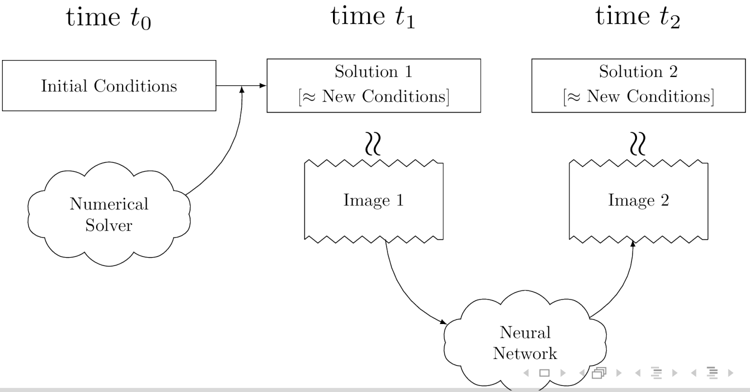

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- Why use images as input for the network?
- Why are images useful as network output?

Problem definition and motivation

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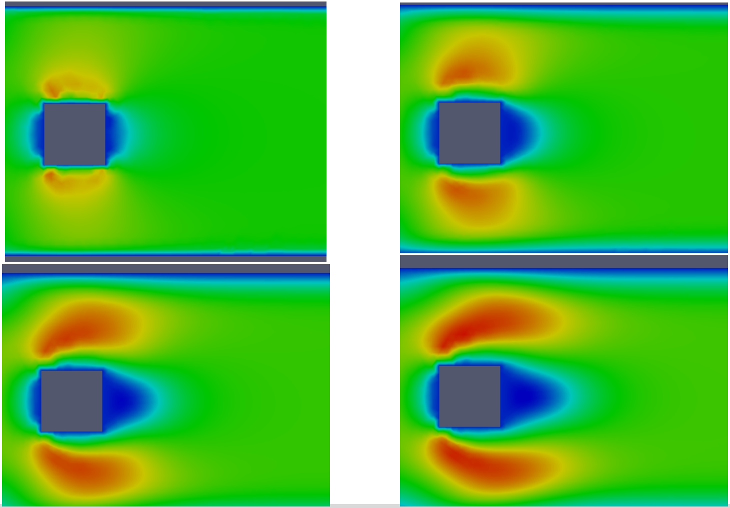
Images of simulations



Definition

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Research topic

The applicability of DNNs in generating solutions for PDEs in numerical simulation context.

Research question

To what extend can DNNs generalize the parameters of a simulation of an incompressible fluid flow inside a channel according to the Navier-Stokes equation? The parameters of interest are:

- Fluid viscosity and density
- Inflow speed

To be studied is a DNN-based model that processes the image representations of the solutions of the simulation.

Related Work & State-of-the-Art

Related Work & State-of-the-Art

DNNs in Image processing

(with focus on image-to-image mapping)

- Used in wide variety of tasks
  - Image Segmentation
  - Semantic Image Synthesis
- We build upon the work of *pix2pixHD*[2]
  - “general-purpose solution to image-to-image translation problems”
  - has not yet been applied to generation of simulation images

[2] Ting-Chun Wang, Ming-Yu Liu, Jun-Yan Zhu, Andrew Tao, Jan Kautz, and Bryan Catanzaro. “High-resolution image synthesis and semantic manipulation with conditional gans.”

Related Work & State-of-the-Art

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Neural Networks in numerical simulations

(with focus on Navier-Stoke problems)

- Study of Deep Learning Methods for Reynolds-Averaged Navier-Stokes Simulations of Airfoil Flows[3]
  - considers the Reynolds-Averaged Navier-Stokes equations
  - maps boundary conditions to velocity and pressure fields

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[3] Nils Thuerey, Konstantin Weissenow, Harshit Mehrotra, Nischal Mainali, Lukas Prantl. (2018). "....". 481-490. 1810.08217.

Methodology

Methodology

Standard machine learning project

Methodology

Standard machine learning project.

$\Longrightarrow$

1) Generate training data
2) Build and train model
3) Evaluate model

Methodology

1) Generate training data
2) Build and train model
3) Evaluate model

- Use *HiFlow* to run simulations
- Use *ParaView* to generate images based on the simulation results

Methodology

1) Generate training data
2) Build and train model
3) Evaluate model

- Implement a model in *PyTorch*
  - following the framework of *pix2pix*
  - *GAN* (Generative Adversarial Network) based approach
- Train with the generated data

Methodology

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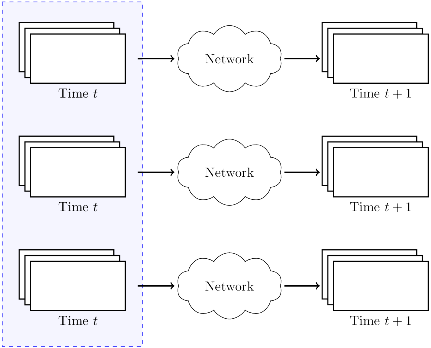
1) Generate training data
2) Build and train model
3) Evaluate model

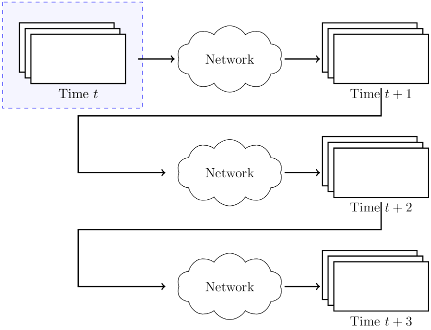
- Deviation from the true solution-image as an error measurement
- Two evaluation cases to consider:
  - Error when applying the model on individual data points
  - Error when applying the model recursively

Methodology

Individual Images



Recursive Application



Definition

...

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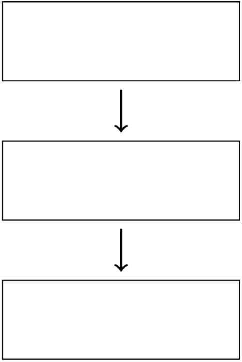
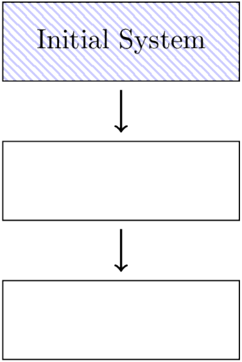
Methodology\Workplan

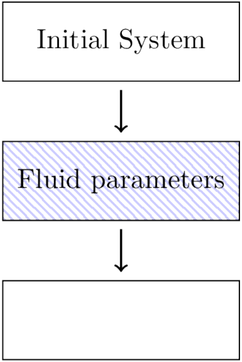


Methodology\Workplan



- Data generation
- Implementation of core components
  - Data loader
  - Model architecture
  - Training infrastructure
  - Evaluation infrastructure
- Training and evaluating a baseline model
  - works only with image data
  - thought of as the basis for further development

Methodology\Workplan



- Model modifications
    - fluid viscosity and density as input
- Training and evaluating

Methodology\Workplan

Initial System

↓

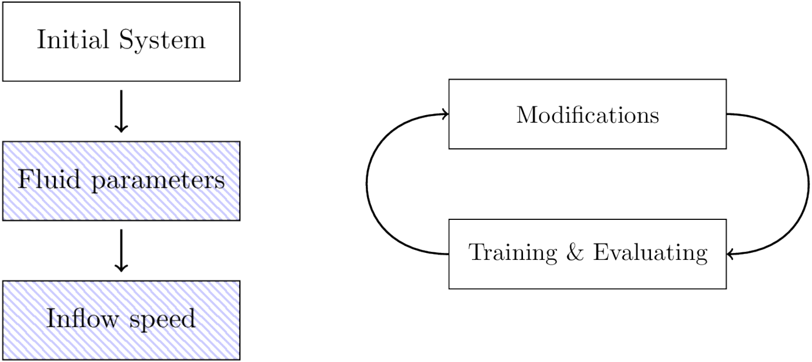
Fluid parameters

↓

Inflow speed

- Model modifications
  - inflow speed as input
- Training and evaluating

Methodology\Workplan



Project Development

Project Development

Data Generation

Project Development

Data Generation

- The simulation has several adjustable parameters
  - inflow speed
  - fluid viscosity
  - fluid density

Project Development

Data Generation

- The simulation has several adjustable parameters
  - What is a good choice for the parameters.

Project Development

Data Generation

- The simulation has several adjustable parameters
  - Reynold's number in the range of [90, 350]

Project Development

Data Generation

- The simulation has several adjustable parameters
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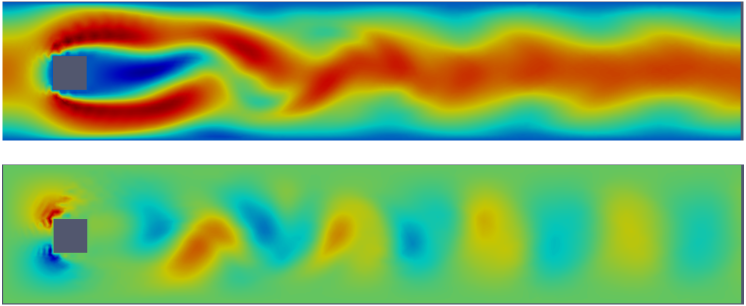

Figure: Karman vortex street

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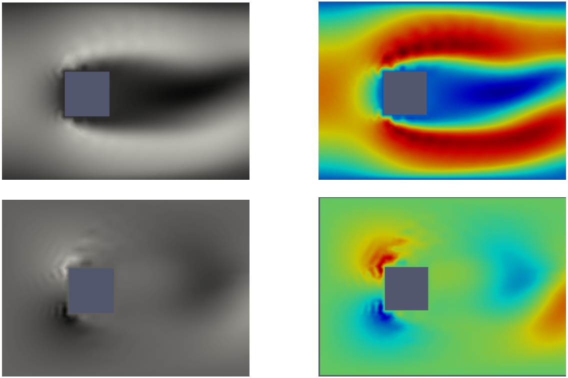
Data Generation

- Choosing appropriate color space
  - Grayscale
  - RGB



Project Development

Models

Project Development

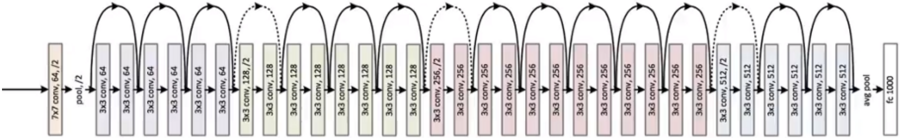
Models

- Two types of architectures based on our preliminary research:

Project Development

Models

- Two types of architectures based on our preliminary research:
  - ResNet



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- Two types of architectures based on our preliminary research:
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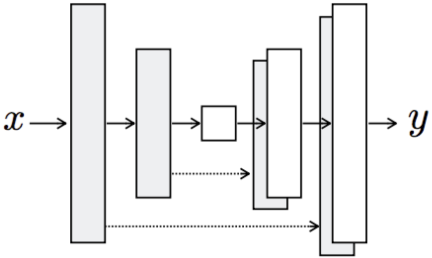

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Data Use

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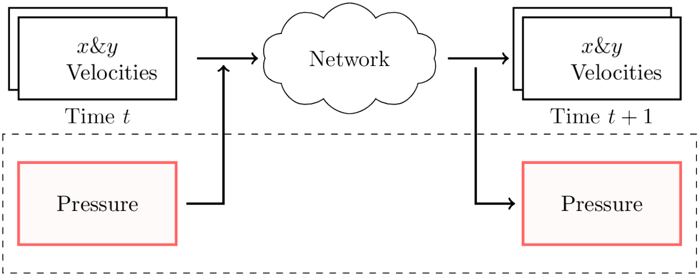
Data Use

- Usage of pressure field



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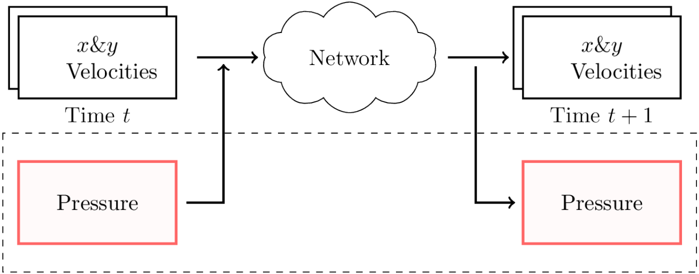
Data Use

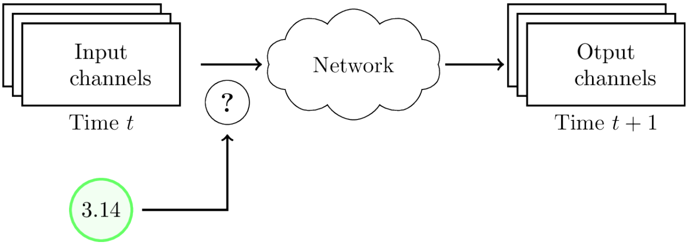
- Usage of pressure field $\rightarrow$ the pressure field turned out to be useful



Project Development

Data Use

- Processing of real values



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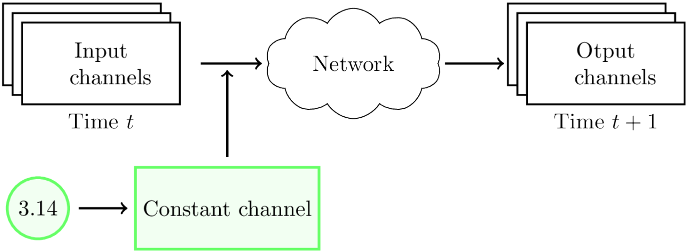
Data Use

- Processing of real values → extra image channel filled with the value



Project Development

Results consideration

Image processing

Numerical Simulation

Project Development

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Image processing

- Perceived qualities of the image results
- Metrics:
  - Peak signal-to-noise ratio - PSNR
  - Correlation

Numerical Simulation

Project Development

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Results consideration

Image processing

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- Metrics:
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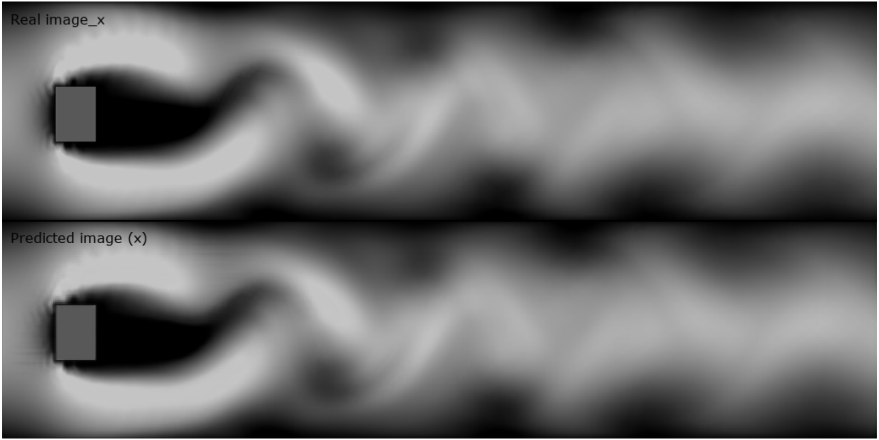
Numerical Simulation

- Real differences between the predicted and the actual values
- Metrics:
  - Average percentage difference
  - Max percentage difference

Results

Individual Images

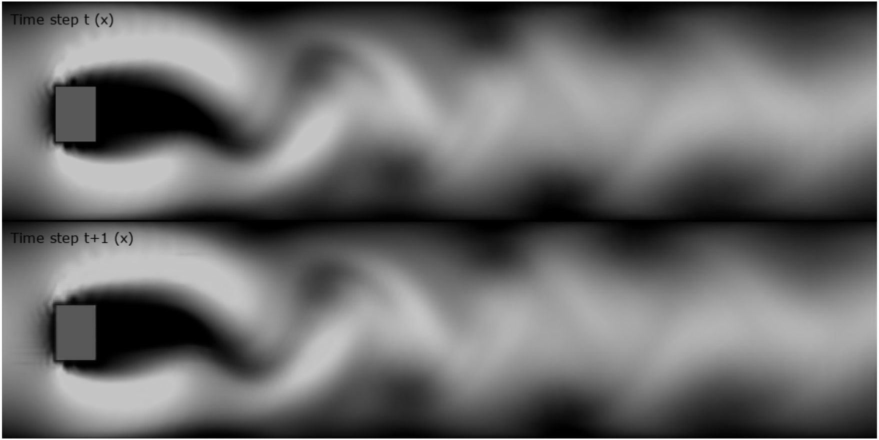
Prediction image:



Results

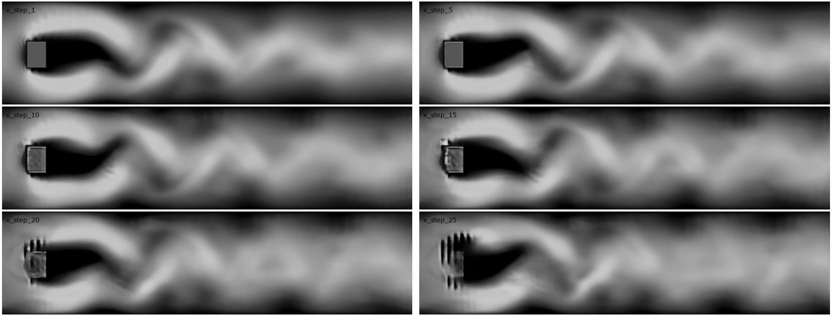
Individual Images

Timestep image:



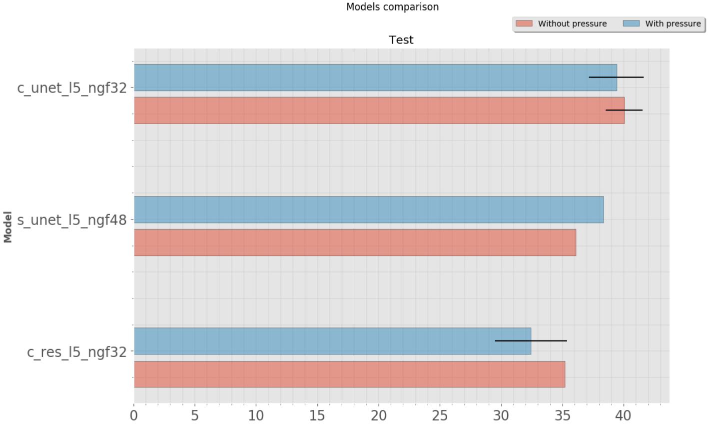
Results

Recursive application – constant model



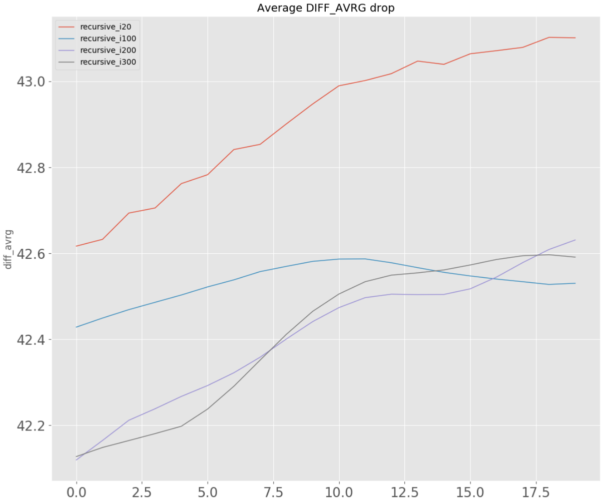
Results

PSNR Comparison

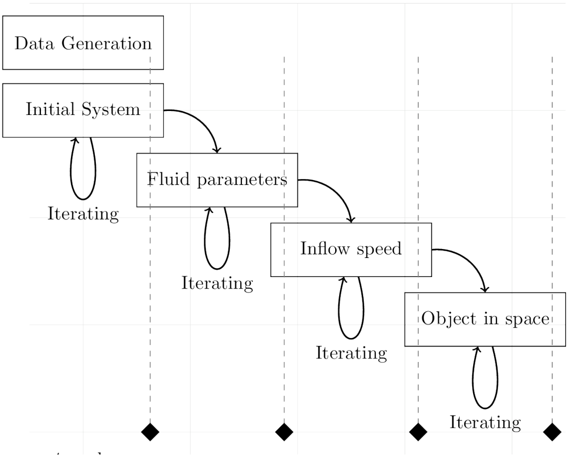


Results

Recursive application — percentual difference change



Further development



Thank you for your attention.

Questions?