IPP INSTITUTE OF PLASMA PHYSICS OF THE CZECH ACADEMY OF SCIENCES

Differentiable Numerical Simulations (Differentiable Physics)

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22.5.2023

MINISTRY OF EDUCATION, YOUTH AND SPORTS

Partial differential equations (PDEs)

1st era - analytical theory and analytical solutions (mid 18th century)

- partial differential equations (PDEs) become core of the physics
- focused on describing world by PDEs, on analytical theory and analytical solutions of PDEs

- 1746/7 - d'Alembert's solution to 1D wave equation followed by many others
- many solution methods: Fourier, Laplace transforms, Sturm-Liouville theory, Green's functions, …
- most focus on linear operators (tractable)

2nd era - computational approximations (mid 20th century)

- finite difference, finite element, spectral techniques, …
- rise of high-performance computing (HPC)
- but solutions to real-world strongly nonlinear, complex, high-dimensional PDE systems often still very demanding

⇩

3rd era - machine learning and optimization methods - starting now!

Examples of emerging techniques

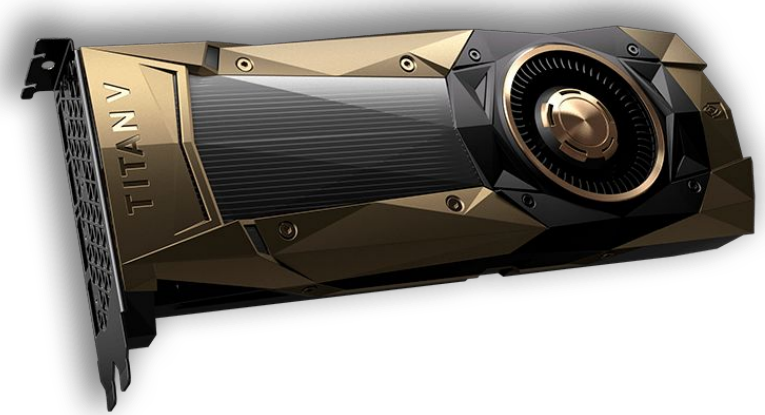
- **building surrogate models**
  - replace classical simulation or experiment that transforms f: $I_{nputs} \rightarrow O_{utput}$ with a fast surrogate model f': $I_{nputs} \rightarrow O_{utputs}$
- **solving inverse problems**
  - solve PDE with known data given elsewhere than at initial or boundary conditions, i.e. f^{-1}: $O_{utputs} \rightarrow I_{nputs}$
  - e.g. Physics Informed Neural Networks (PINNs) or differentiable physics
- **improving traditional numerical methods**
  - in terms of speed and/or accuracy
- **coarse-grained simulations**
  - fast/inaccurate coarse-grained simulation + correction by a model or real data
- **learning (simplified) governing equations from data or complex simulations**
  - e.g. SINDy, PDE-FIND
- **finding suitable coordinate systems** for non-linear PDEs and reduced representations
- **non-linear operator learning**
- …

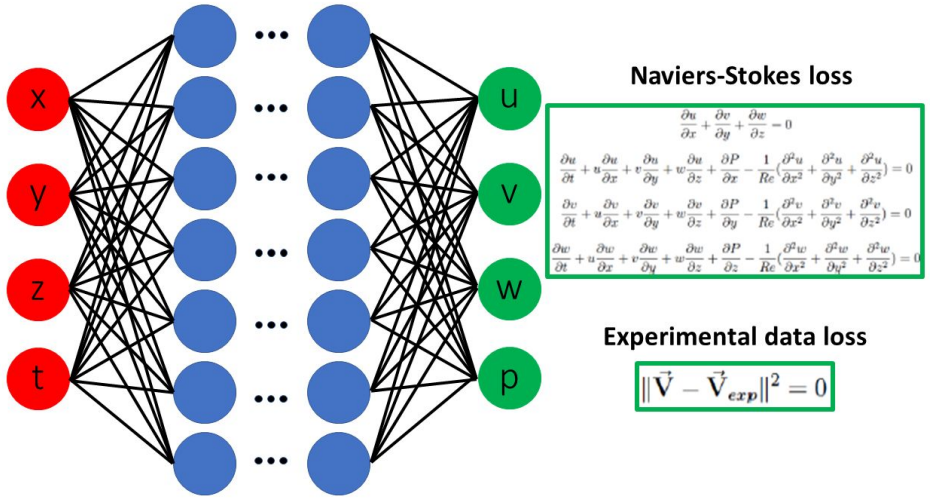
today we'll very briefly touch these parts

for references see e.g. reviews: [1] https://physicsbaseddeeplearning.org [2] Brunton, Kutz (2023), [3] Ramsundar (2021)

Today's topics

- Python for scientific computing and data science
- Speed up your simulations with GPU
- Automatic differentiation of computations
- What are Artificial Neural Networks (NN)
- Differentiable physics - solving inverse problems
- Implicit representation of functions with NN
- Physics Informed Neural Networks - solving PDEs using NN





Naviers-Stokes loss

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}-0$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}+\frac{\partial P}{\partial x}-\frac{1}{Re}\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)=0$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}+\frac{\partial P}{\partial y}-\frac{1}{Re}\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right)=0$$

$$\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}+\frac{\partial P}{\partial z}-\frac{1}{Re}\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right)=0$$

Experimental data loss

$$\|\vec{V}-\vec{V}_{exp}\|^2=0$$

Choosing programming language

Typical problem of scientific computing: solving (a system of) partial differential equations such as

$$\nabla \cdot \overline{u} = 0$$

$$\rho \frac{D\overline{u}}{Dt} = -\nabla p + \mu \nabla^2 \overline{u} + \rho \overline{F}$$

\+ some data "fixing" the solution

Steps:

- decide on the **methods** that will be used to solve the problem
- decide which **programming language** to use

Most of the high-performance codes in the fusion community are written in C/C++/Fortran, but **is it still the best way?**

C/C++/Fortran/…

- **:(** complex, steep learning curve, slow to develop
- **:)** realtime
- **:)** fast (if you know what you are doing)

high-level languages (e.g. Python)

- **:)** simple and rapid development, powerful feature-rich libraries
- **:(** not suitable for hard real time
- **:|** typically (but not always) somewhat slower

Cost of a simulation

(1) (2) (3)

$$\text{simulation cost} = \text{cost}_{\text{development}} + \text{cost}_{\text{run performance}} + \text{cost}_{\text{usage}}$$

complexity

often hidden / neglected
⇒ limits code usability, manpower costs, introduces mistakes & wrong results

often: performance cost < development & usability cost

C/C++/Fortran/…

- **:(** complex, steep learning curve, slow to develop
- **:)** realtime
- **:) faster** (if you know what you are doing)

we need this (2) …

high-level languages (Python)

- **:) simple and rapid development, powerful feature-rich libraries**
- **:(** not suitable for real time
- **:|** typically (but not always) somewhat slower

… and this (1), (3) at the same time

while it's not easy to simplify the low-level languages, the performance gap is gradually being closed by dedicated python libraries and new high-level languages like Julia or Mojo that are specifically designed for high-performance computations

Python techniques to speed-up the code

- vectorization (numpy, scipy, …)
- optimized algorithms and data structures (scipy, pandas, xarray, NetworkX, JAX, …)
- just-in-time (JIT) compilation (numba, JAX, …)
- parallelization (Dask, JAX, …)
- hardware acceleration with GPU/TPU (JAX, PyTorch, CuPy, …)
- distributed computations (Dask, JAX, Apache Spark, …)
- use Cython, Julia, Mojo, …
- write C/Fortran extension or use existing C/Fortran code under the hood

still high-level programming
+
large ecosystem - no need to DIY
(faster, safer)

different high-level language

use low-level language when you need it,
do the rest at high-level

Thanks to all this, Python is a language #1 for data science (incl. machine learning and AI) and its significance in technical computations steadily grows

Python techniques to speed-up the code

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see next slides

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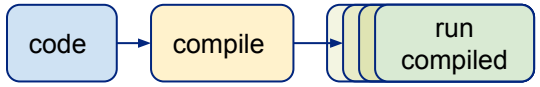
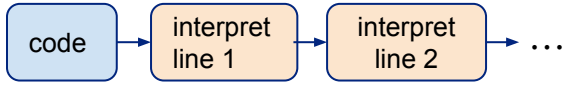
Just-in-time compilation

- C/C++/Fortran are **compiled languages**



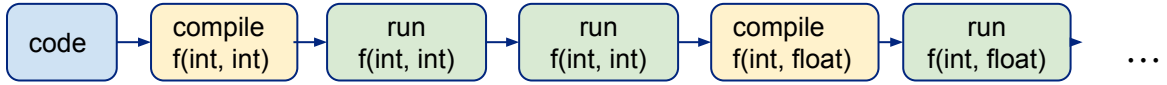
  - explicit compilation step to machine code run ahead of execution
  - compilation to machine code includes optimizations that boost performance in general + for a specific hardware target
  - statically typed → optimization ahead of time often possible

- Python is an **interpreted language**



  - code (converted to bytecode) executed by python interpreter at runtime using Python Virtual Machine; line by line - slow
  - dynamically typed → optimizations often not possible

- **Just-in-time (JIT) compilation** - a golden middle way



  - used by interpreted languages
  - block of code (e.g. function) is compiled to machine code at runtime at the time of first use
    - run-time overhead during the first execution of the code (x caching), but then performance on par with compiled languages
    - the input types and data shapes are known at runtime → performance optimization possible

JIT in Python (an example)

JAX

- developed by Google
- numpy-like interface + re-implementation of many numerical algorithms from scipy
- growing ecosystem of numerical and ML libraries
- based on TensorFlow's XLA (Accelerated Linear Algebra) compiler
- hardware acceleration (GPU/TPU) out of the box
- automatic differentiation capabilities

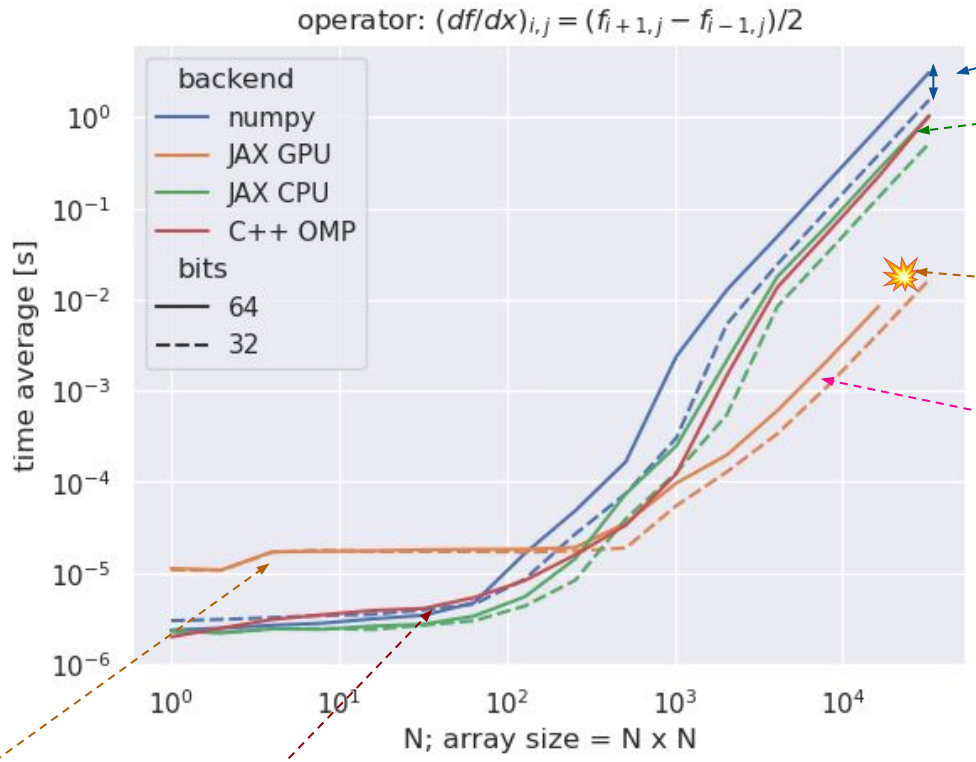
- JAX has some specifics (e.g. specific treatment of conditions and loops), but in general as simple as:

```
# numpy


def central_difference(f):
    return  (f[2:, :] - f[:-2, :]) / 2
```

optimize and run at GPU/TPU (if available)

```
# JAX
import jax

@jax.jit
def central_difference(f):
    return (f[2:, :] - f[:-2, :]) / 2
```

JIT speed-up



would 32-bit precision be sufficient for your application?

JIT can be comparable to C++ code

GPUs can easily run out of memory for large arrays 😦

100x speed-up w/ GPU at the cost of a single line of code! 😍

current WIP project at IPP (J. Seidl, P. Macha):
porting fluid plasma turbulence models to GPU w/ JAX

inefficient number of OMP threads in C++

GPU may have overhead ⇒ pays-off only for larger arrays

Note: this is a simple example, different problems may scale somewhat differently

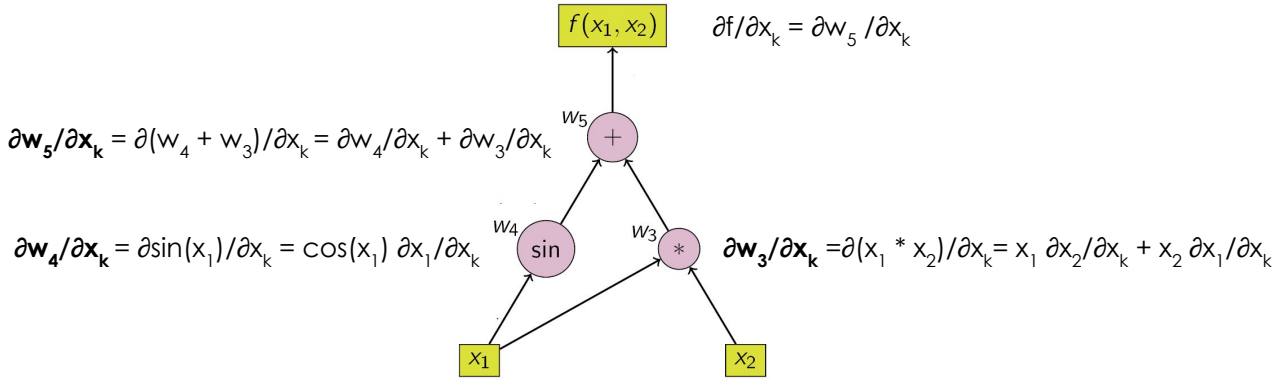
Automatic differentiation (AD)

AD is a technique for computing function derivatives **efficiently** and **accurately** (no discretization) by applying

the chain rule: $\partial(g \circ f)/\partial x|_x = \partial g / \partial f|_{f(x)} * \partial f / \partial x|_x$ (or its generalisation for multivariate functions)

AD works on functions that are (arbitrarily deep) composition of functions with known derivatives, e.g.:

$\mathbf{sin(x_1) + x_1 * x_2}$



AD represents function as a call-graph of elementary functions whose derivatives (Jacobians) are analytically known

equation images taken from stackexchange

AD modes

$$\mathbf{y} = h(g(f(\mathbf{x})))$$

$$\mathbf{a} = f(\mathbf{x}), \quad \mathbf{b} = g(\mathbf{a}), \quad \mathbf{y} = h(\mathbf{b})$$

multiplication of Jacobians

$$\underbrace{\frac{\partial \mathbf{y}}{\partial \mathbf{x}}}_{|\mathbf{y}|\times|\mathbf{x}|} = \underbrace{\frac{\partial h(\mathbf{b})}{\partial \mathbf{b}}}_{|\mathbf{y}|\times|\mathbf{b}|} \underbrace{\frac{\partial g(\mathbf{a})}{\partial \mathbf{a}}}_{|\mathbf{b}|\times|\mathbf{a}|} \underbrace{\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}}_{|\mathbf{a}|\times|\mathbf{x}|}$$

Jacobian matrix sizes:

forward mode

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial h(\mathbf{b})}{\partial \mathbf{b}} \left(\frac{\partial g(\mathbf{a})}{\partial \mathbf{a}} \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right)$$

- # multiplications: |x|·|a|· |b| + |x|·|b|·|y|
- **forward mode better when |y| > |x|** **(# outputs > # inputs)**
- single forward pass evaluating function values & gradients
- Ex: sensitivity analysis of a simulation
  - few simulation input parameters, many outputs on large grid

reverse mode

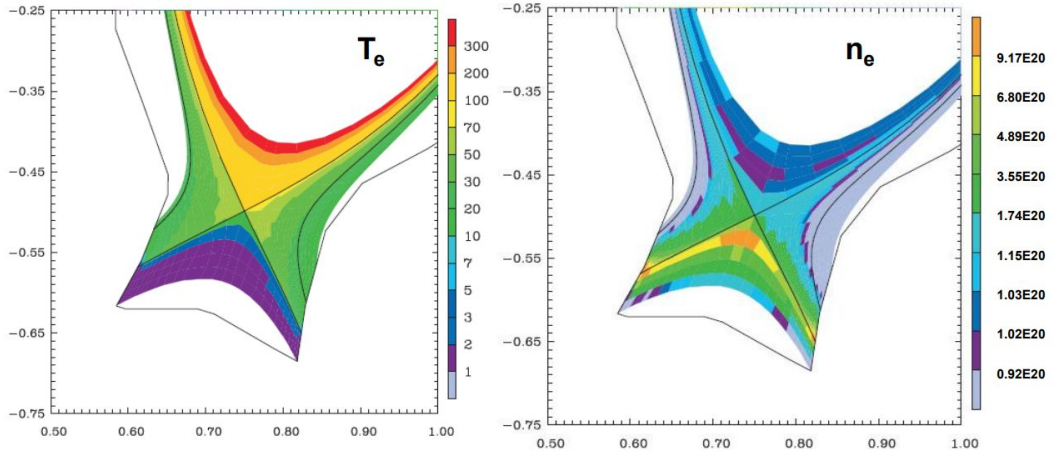
$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \left(\frac{\partial h(\mathbf{b})}{\partial \mathbf{b}} \frac{\partial g(\mathbf{a})}{\partial \mathbf{a}} \right) \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}$$

- # multiplications: |y|·|a|·|b| + |y|·|b|·|x|
- **backward mode better when |x| > |y|** **(# inputs > # outputs)**
- 2 passes: forward (function values) & backward (gradients)
  ⇒ memory intensive

Ex: optimization; neural networks
- many features on input (e.g. image pixels; x > 1) and only scalar loss (y=1) at output

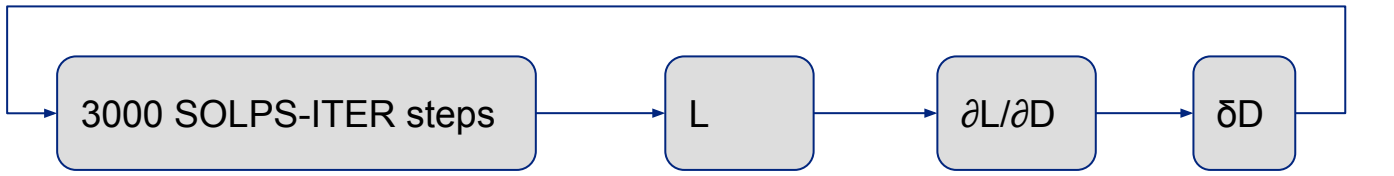
Automatic differentiation in SOLPS-ITER

- SOLPS = workhorse of tokamak edge transport modelling
  - complicated long-running code (days-weeks)
  - lots of free input parameters
  - radial transport described by diffusion coefficients (free par.)
- AD: optimization of diffusion coefficients
  to match exp. profiles or simplified turbulent model



[Carli (2022)]

loss L: weighted MSE of discrepancy from exp data



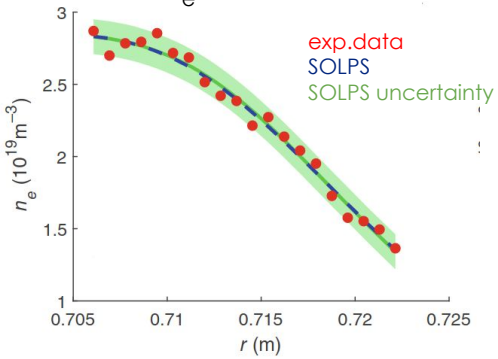
let the simulation converge

model-exp discrepancy

AD through SOLPS-ITER

update value of D

fit to exp n_e profile at midplane



Differentiable Numerical Simulations (Differentiable Physics)

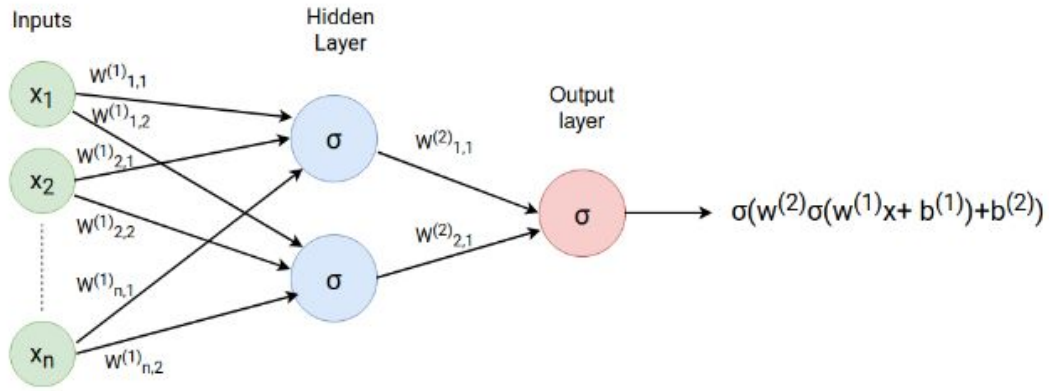
differentiable physics: differentiable phys. models and methods that can compute gradients of outputs wrt inputs and parameters

Neural networks (NN)

Feedforward (FF) Neural Network: $\mathbf{y} = \sigma_i(\mathbf{W_i} \cdot \sigma_{i-1} (\mathbf{W_{i-1}} \cdot \sigma_{i-2} (\dots \cdot \sigma_1(\mathbf{W_1} \cdot \mathbf{x} + \mathbf{b_1})\dots)))$

x … input feature vector
y … network output
$\mathbf{W_i}$ … weight matrix (learnable parameters!)
σ_i … nonlinear activation function

- e.g. ReLU(x) = (x if x > 0 else 0)
  tanh(x)
  …



Universal approximation theorem:
any continuous function can be approximated arbitrarily well by a neural network with at least 1 hidden layer and finite number of weights

Automatic differentiation can be used to compute $\partial y/\partial W_i$ and $\partial y/\partial x$

Gradient Descent

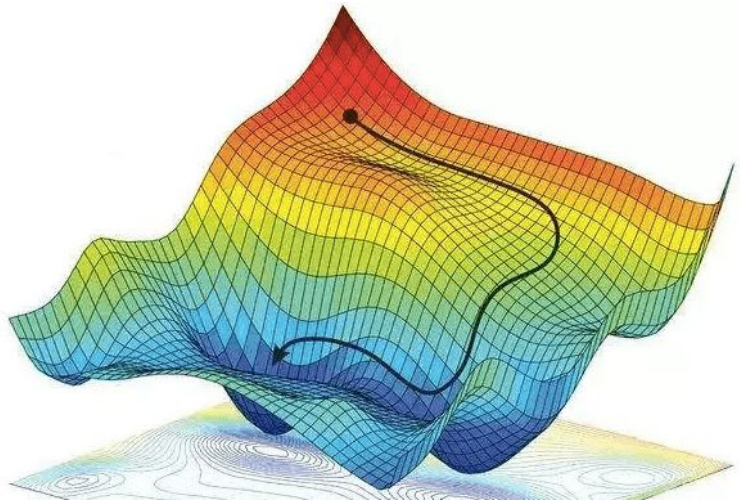
Feedforward (FF) Neural Network $f_{NN}(\mathbf{x}, \mathbf{W})$: $\mathbf{y} = \sigma_i(\mathbf{W_i} \cdot \sigma_{i-1} (\mathbf{W_{i-1}} \cdot \sigma_{i-1} (\dots \cdot \sigma_1(\mathbf{W_1} \cdot \mathbf{x})\dots)))$

Data $\{(\mathbf{x_k}, \mathbf{y_k})\}$: values of an unknown function **f(x)** sampled at points $\mathbf{x_k}$

Task: Find values of the weights $\mathbf{W_i}$ such that $f_{NN}(\mathbf{x}; \mathbf{W})$ will represent the unknown function f(x) as good as possible
as good as possible ⟷ value of a scalar loss function $\mathbf{L(f_{NN}(x_k; W), y_k)}$ is minimal

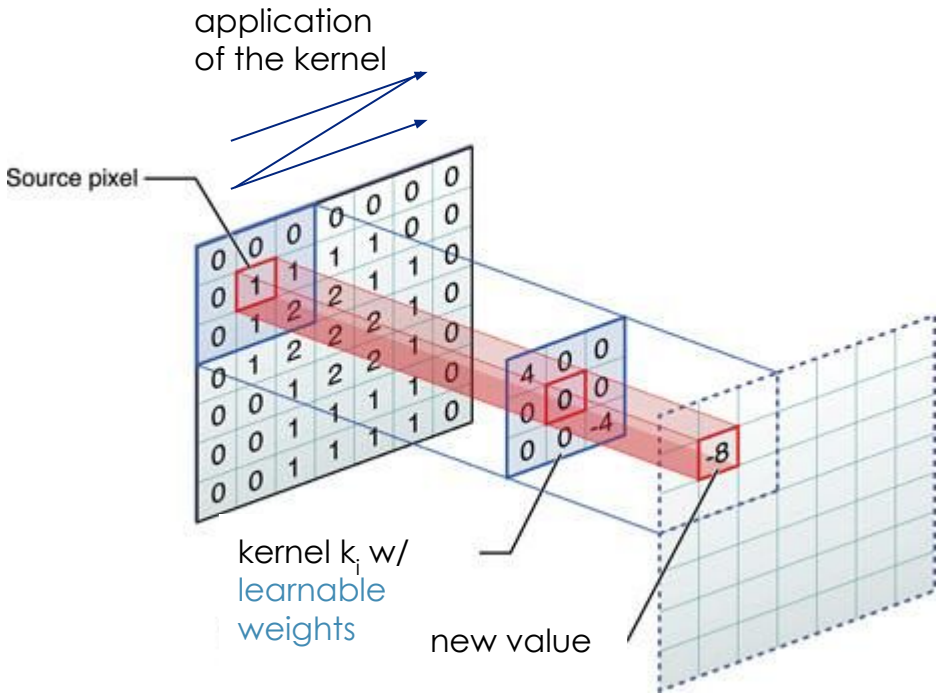
Method: (Stochastic) Gradient Descent

1. Evaluate $y_k = f_{NN}(x_k)$ at some or all $\mathbf{x_k}$
2. Compute $\partial L / \partial w_{ij}$ using reverse mode of AD (backpropagation)
3. Update values of w_{ij} in the direction of best improvement
   $w_{ij} \rightarrow w_{ij}$ - learning_rate $\cdot \partial L / \partial w_{ij}$
4. Repeat until L is sufficiently small or stops decreasing



Convolutional NN (CNN)

Replace matrix multiplication in FF NN by discrete convolution (applied on n-dimensional data)



$$\mathbf{y} = \sigma_i(\, \mathbf{k_i} * \sigma_{i-1}\, (\mathbf{k_{i-1}} * \sigma_{i-1}\, (\, \ldots * \sigma_1(\mathbf{k_1} * \mathbf{x})\ldots)))$$

variant of NN suitable for gridded data with correlated neighbors
- images, simulation grids, …

convolution easily parallelizable ⇒ fast at GPU

Example 1 - hybrid method for solving Poisson equation

$$\Delta\varphi = \omega$$

Poisson equation is a key equation in most high-temperature plasma turbulence simulations.

Poisson equation - classical approach

Poisson equation: $\Delta\varphi = \omega$ (to be computed; ω known)

Laplace stencil:

$\partial^2/\partial y^2$

	1	
1	-4	1
	1	

$\partial^2/\partial x^2$

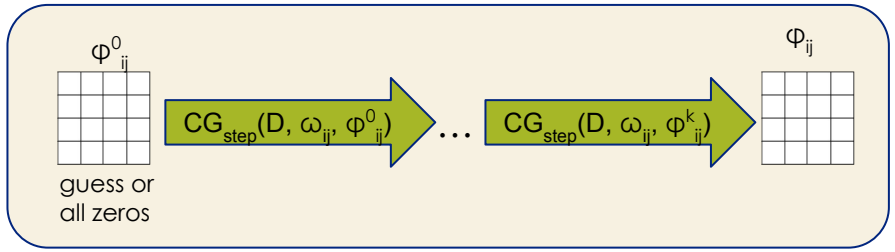
classical approach:

invert $-D =$

$$\begin{bmatrix}
4 & -1 & 0 & 0 & \dots & -1 & 0 & 0 & \dots & & & 0 \\
-1 & 4 & -1 & 0 & 0 & \dots & -1 & 0 & 0 & \dots & & 0 \\
0 & -1 & 4 & -1 & 0 & 0 & \dots & -1 & 0 & 0 & \dots & 0 \\
 & & & \ddots & & & & & \ddots & & & \\
-1 & & & -1 & 4 & -1 & & & & -1 & & \\
0 & -1 & & & -1 & 4 & -1 & & & & -1 & \\
0 & 0 & -1 & & & -1 & 4 & -1 & & & & -1 \\
0 & 0 & 0 & \ddots & & & \ddots & \ddots & \ddots & & & \ddots
\end{bmatrix}
\begin{matrix}
\dots \varphi_{11} \\
\dots \varphi_{12} \\
\dots \varphi_{13} \\
\dots \\
\dots \\
\dots \varphi_{nn-2} \\
\dots \varphi_{nn-1} \\
\dots \varphi_{nn}
\end{matrix}$$

and $\varphi = D^{-1}\omega$

or use iterative solver:



direct inversion typically done for small D, iterative methods for large D

- LU decomposition, Cholesky decomposition, conjugate gradient (CG), ...

Poisson equation as an optimization problem

Poisson equation: $\Delta\varphi = \omega$

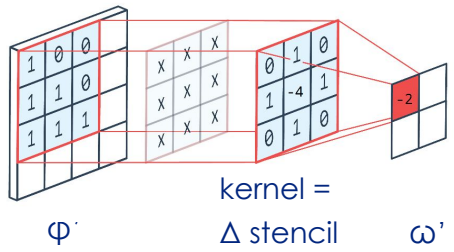
Laplace stencil:

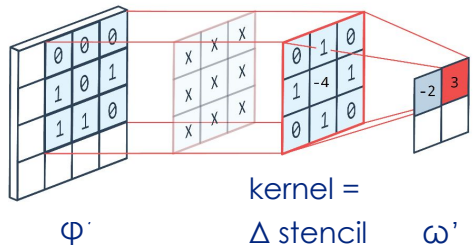
	1	
1	-4	1
	1	

$\partial^2/\partial y^2$ (vertical), $\partial^2/\partial x^2$ (horizontal)

Reformulate as an optimization problem (in this form inefficient!)

1. randomly initialize solution φ
2. apply convolution with Laplace stencil on φ
   → find ω to which the current φ corresponds





3. compute scalar loss: $L = \sum_{ij}(\omega'_{ij} - \omega_{ij})^2 + \alpha \sum_{BC}(\varphi'_{BC} - \varphi_{BC})^2$
4. compute gradients $\partial L/\partial \varphi'_{ij}$
5. optimize the values of φ'_{ij}, e.g by gradient descent, to find φ'_{ij} that will minimize L: $\varphi'_{ij} \rightarrow \varphi'_{ij} - \text{learning\_rate} \cdot \partial L/\partial \varphi'_{ij}$
6. go to (2) and repeat

Poisson equation as an optimization problem

Poisson equation: $\Delta\varphi = \omega$

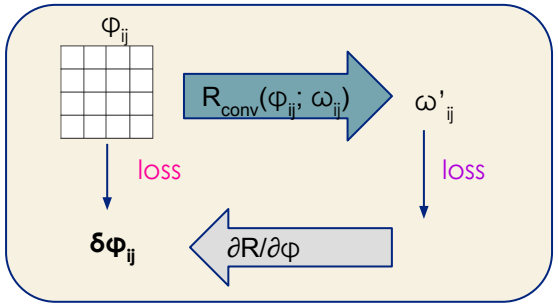
Laplace stencil:

$\partial^2/\partial y^2$

	1	
1	-4	1
	1	

$\partial^2/\partial x^2$

Reformulate as an optimization problem (in this form inefficient!)



$$L = \sum_{ij}(\omega'_{ij} - \omega_{ij})^2 + a \sum_{BC}(\varphi'_{BC} - \varphi_{BC})$$

reconstruction **boundary/initial conditions on φ**

finds only single solution to single ω at a time; GD optimization inefficient

Poisson equation - CNN model of D^{-1}

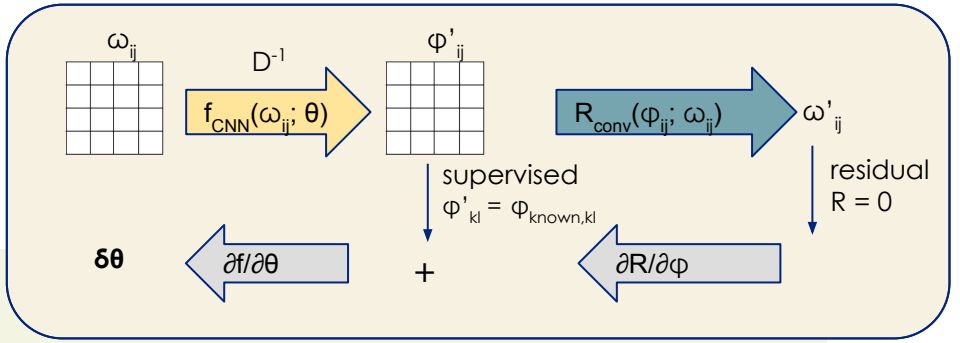
Poisson equation: $\Delta\varphi = \omega$

Laplace stencil:

$\partial^2/\partial y^2$

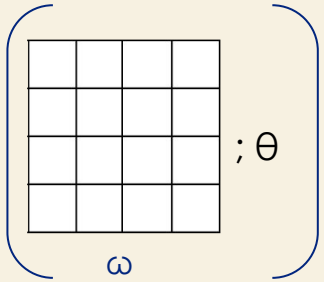
	1	
1	-4	1
	1	

$\partial^2/\partial x^2$



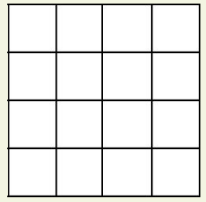
Find a CNN model of D^{-1}:

new step (D^{-1})

f_{CNN}  ; θ

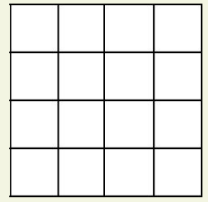
ω

compute gradients as before…



φ'

convolution w/ Laplace stencil



ω'

; $L = \sum_{ij}(\omega'_{ij} - \omega_{ij})^2 + \alpha \sum_{BC}(\varphi'_{BC} - \varphi_{BC})$

⟹ now optimization of parameters θ of the model f_{CNN} using backpropagation (AD)

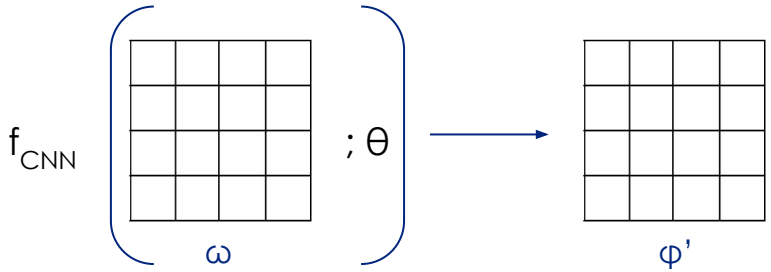
finds a transformation $f_{CNN}(\omega, \theta)$, representing Δ^{-1}, i.e. the whole **class of solutions**

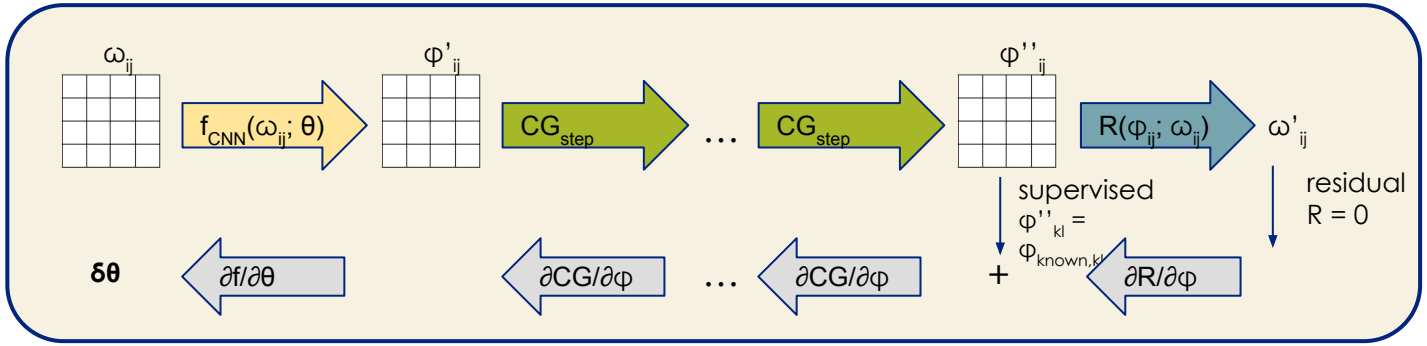
Poisson equation - CNN model of D^{-1} + iterative solver

Poisson equation: $\Delta\varphi = \omega$

Initialize classical solver with CNN model of D^{-1}

1. train f_{CNN} as a proxy of D^{-1} (see prev. slide)





hybrid method combining NN and classical solver

2. use φ' as an initial state for a CG iterative solver computing $\omega = D^{-1}\varphi$
   - good initial guess speeds up convergence of the solver

why to use the method: performance increase

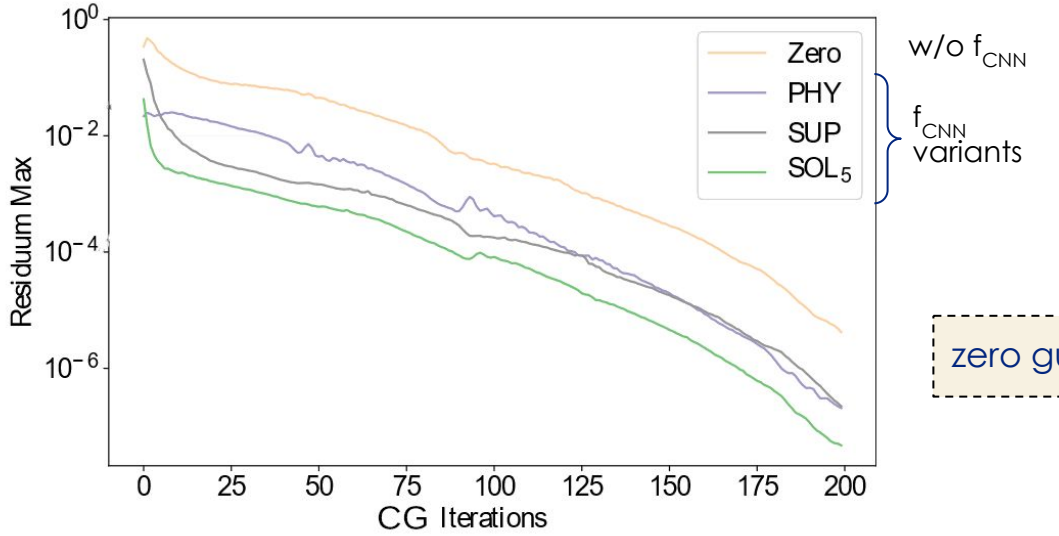
Note: f_{CNN} can be trained separately or together with the attached solver

Poisson equation - model of D^{-1} + iterative solver

Poisson equation: $\Delta\varphi = \omega$

Initialize classical solver with CNN model of D^{-1}

$\Delta\varphi = \nabla p$; $f_{CNN} \rightarrow$ CG solver



zero guess → f_{CNN}: **~60 iterations (30%) less** to reach given precision

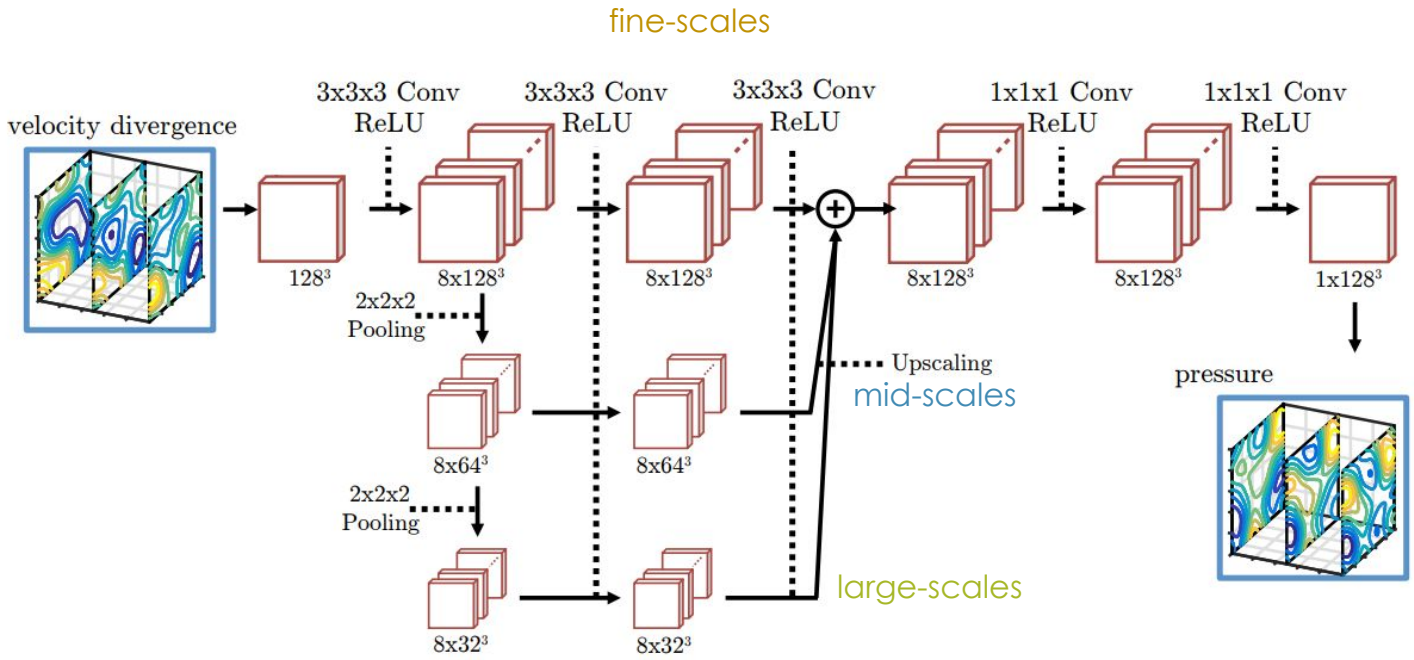
why to use the method: performance increase

[https://github.com/tum-pbs/CG-Solver-in-the-Loop]

Poisson equation - CNN model of D^{-1}

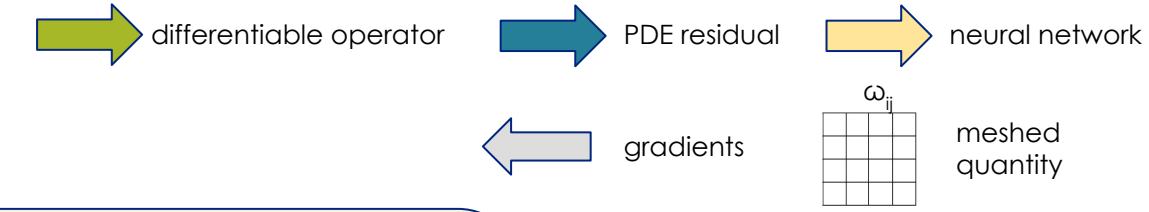
Example f_{CNN} architecture for $\Delta p = \nabla u$ in 3D:

[Tompson 2017]

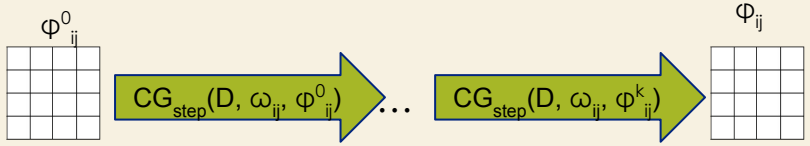


U-net architecture allows long-distance interactions

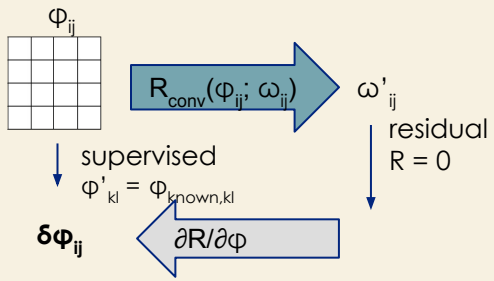
Graphical representation



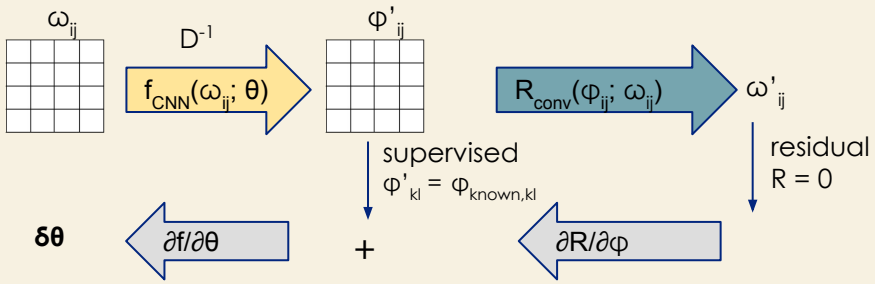
1. classical iterative solver:



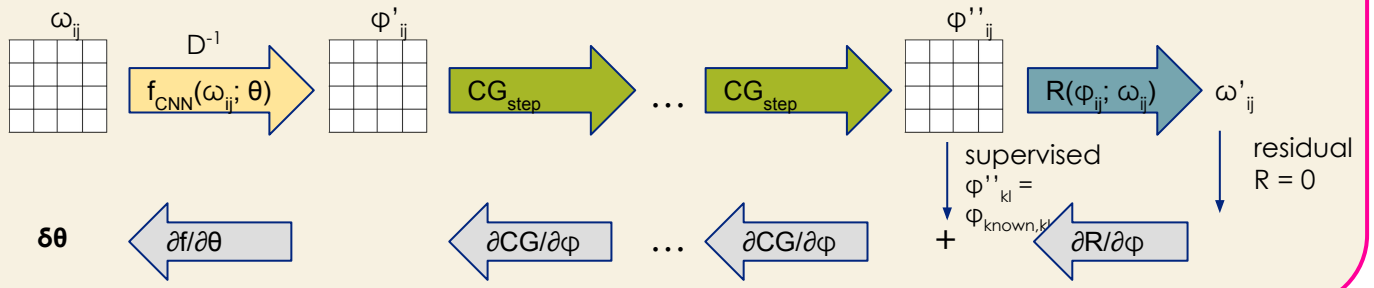
2. direct optimization:



3. NN model of D^{-1}



4. hybrid method - NN model of D^{-1} + iterative optimizer



Example 2 - flexible method for solving Poisson equation

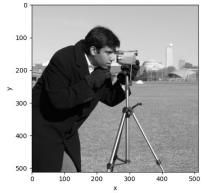
$$\Delta\varphi = \omega$$

Poisson equation is a key equation in most high-temperature plasma turbulence simulations.

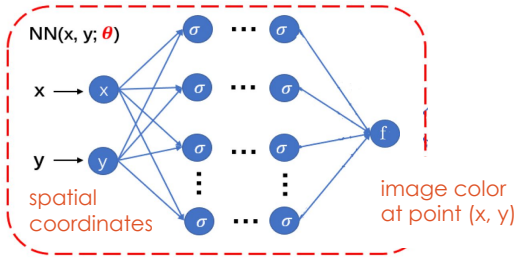
Implicit representation of data by NN

- NNs are typically used as models of data transforming functions
- but NN can be used also as a model of the data itselves / data generating func (implicit representation of the data)
  - implicit = representation of data structure and relations is hidden in the parameters of the NN
  - simplest case: no PDE, just known data

known data



(check e.g. this notebook or [Sitzman 2020])



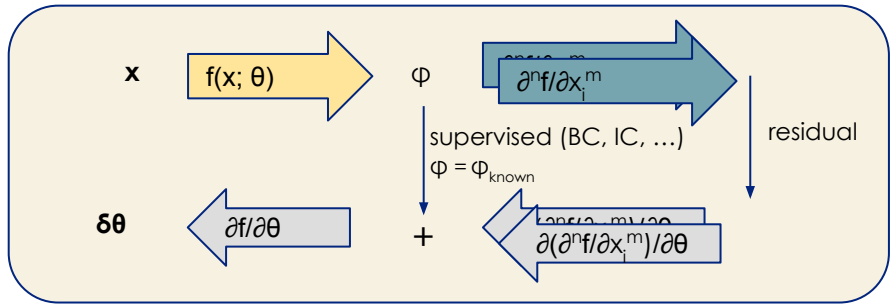
  - PINN: similar principle, but the NN output is also constrained by the PDE

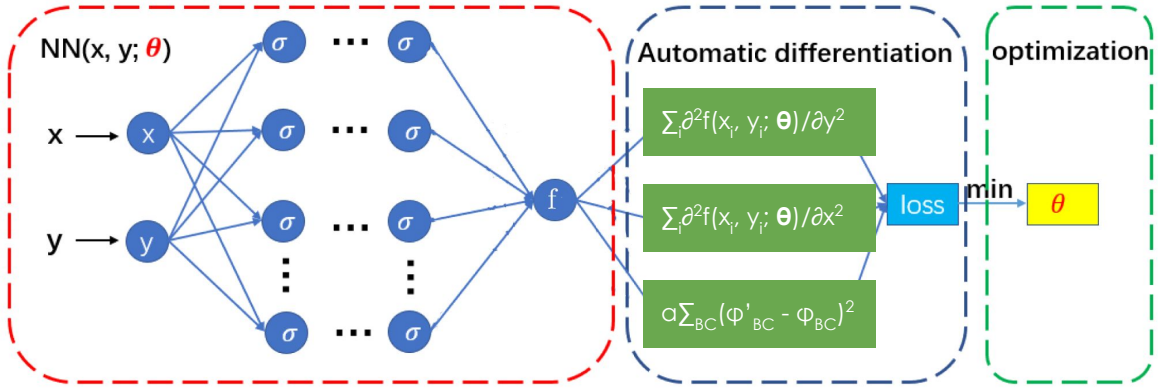
Poisson equation - Physics Informed Neural Network (PINN)

Poisson equation: $\Delta\varphi = \omega$

Find a NN for φ that solves the Poisson equation:

similar to fitting the image (known values of φ at BC), but now adding constraints on the output, given by PDE





now exact derivatives — mesh-free ⇒ anywhere

Loss = residual of PDE + α · distance from data

Q: think what happens when the data are not consistent with the PDE and what is the role of factor α

mesh-free C^{inf} solution with exact derivatives to single ω at a time; simple use, but often **slow/poor convergence**

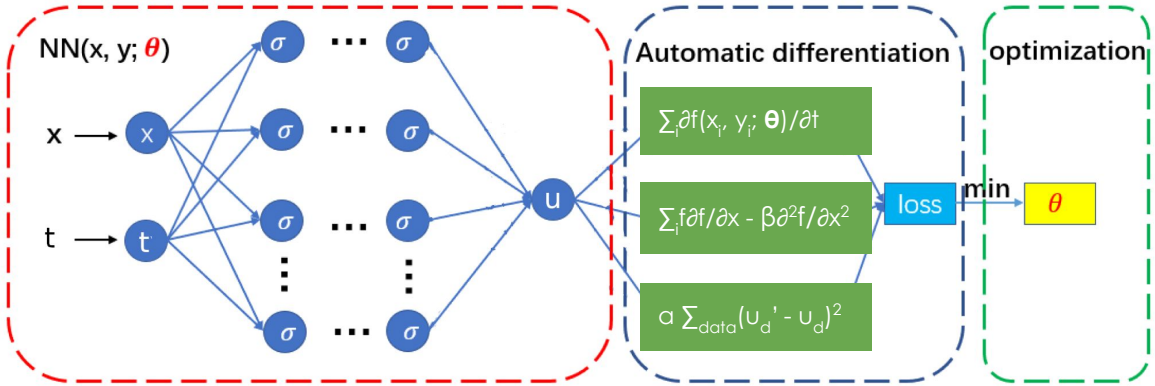
[Raissi 2019]

Example 3 - flexible method for solving time-dependent problem

Time-dependent PDE - PINN

Burgers equation: $u_t + uu_x - \beta u_{xx} = 0$

Full PDE solution implicitly represented by a differentiable NN

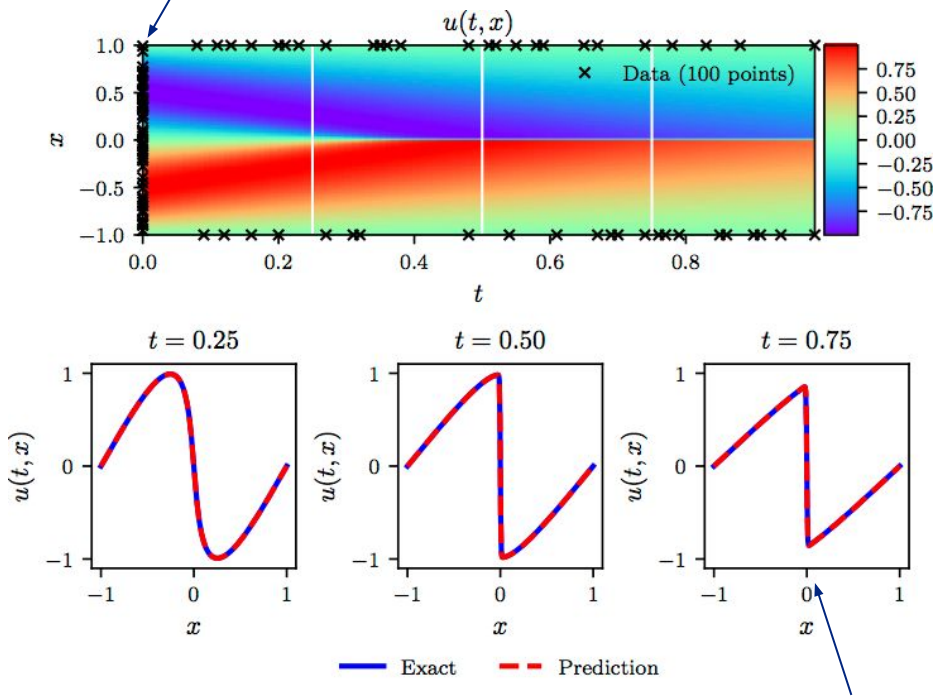


with a good library, basically all you need to do is just to define the PDE to solve:

```
def loss(x, u, params):
    pde = diff(u, 't') + u * diff(u, 'x') - params['beta'] * diff(u, ('x', 'x'))
    return pde(x) ** 2
```

[Raissi (2019)]

this is a forward problem, but the known points can be anywhere (inverse problem)



handles shocks out of the box

why to use the method: easy to use, flexible

combining or extending PDEs is simple

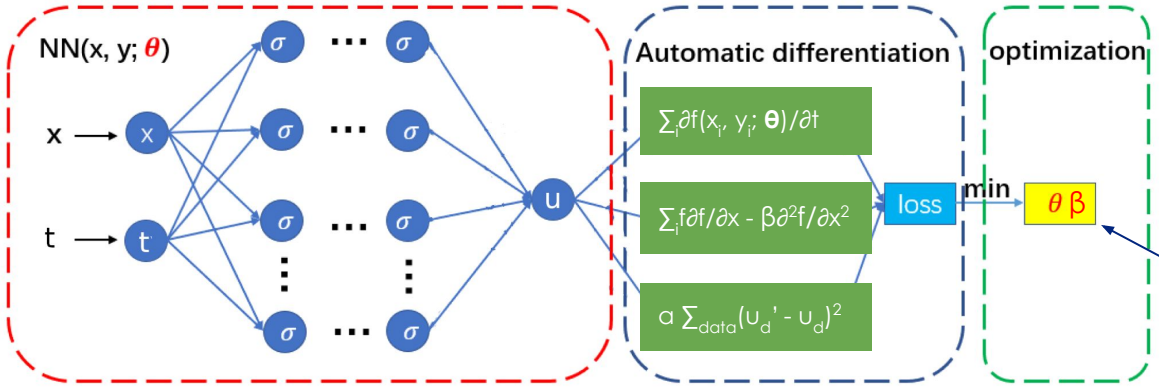
[Raissi (2019)]

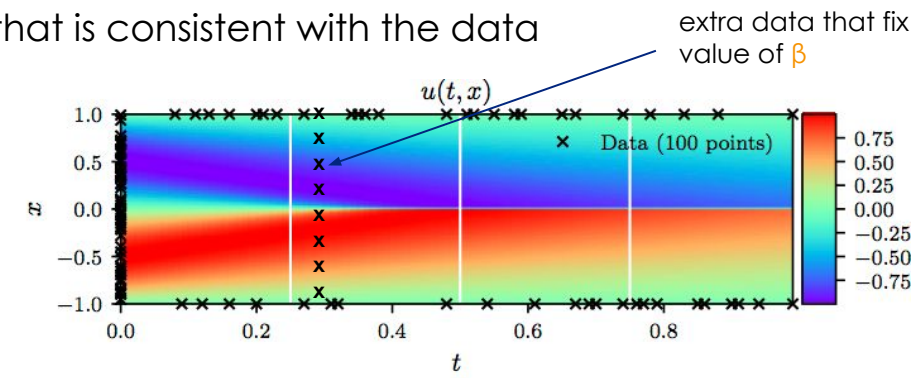
Time-dependent PDE - PINN

Burgers equation: $u_t + uu_x - \beta u_{xx} = 0$

modification: identification of parameter β from data

Assume the data are measured at different times → looking for value of β that is consistent with the data





just treat β as an optimized parameter, i.e. compute $\partial L/\partial \beta$ and optimize jointly with Θ

why to use the method: easy to use, flexible

Example 4 - hybrid method for solving time-dependent problem

[Raissi (2019)]

Time-dependent PDE - standard numerical schemes

PDE: $u(t, x) = N[u(t, x); \boldsymbol{\theta}_{PDE}]$

Standard forward solve: iterative application of an operator P that moves the solution in time $u(t, x) \rightarrow u(t + dt, x)$

$$u(t, x) = P \circ P \circ P \circ P \circ P \circ P \ldots . \circ P(u_0(x); \boldsymbol{\theta}_{PDE})$$

E.g.: Euler scheme: $P: u(t, \mathbf{x}; \boldsymbol{\theta}_{PDE}) \rightarrow u(t+dt, \mathbf{x}; \boldsymbol{\theta}_{PDE}) = u(t, \mathbf{x}; \boldsymbol{\theta}_{PDE}) + dt \cdot N[u(t, \mathbf{x}); \boldsymbol{\theta}_{PDE}]$

With AD, the time-shift operator can be made differentiable to (back) propagate gradients through temporal evolution

- $\partial(u(t_1) - u_{data}(t_1))^2 / \partial\, u(t_2)$ allows finding solution $u(t_2)$ in any time t_2
- $\partial(u(t_1) - u_{data}(t_1))^2 / \partial\, \boldsymbol{\theta}_{PDE}$ allows identification of the value of unknown PDE parameters $\boldsymbol{\theta}_{PDE}$ from the measured data

[Raissi (2019)]

Time-dependent PDE - inverse problem

Burgers equation: $u_t + uu_x - \beta u_{xx} = 0$

Task: from known data at arbitrary time $u_{known}(t_1, x)$ infer initial conditions in time t_0 that generated them:

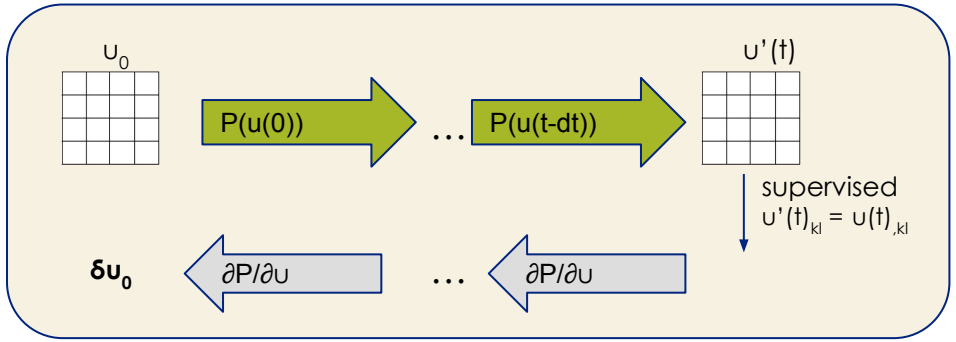
random $\rightarrow u_0$

while L large:

$u_t = P \circ P \circ \ldots \circ P(u_0)$

$L = \sum(u_t - u_{known})^2$

$u_0 \rightarrow u_0 - lr \cdot \partial L / \partial u_0$



Note: the larger the $|t_1 - t_0|$, the harder the optimization (vanishing gradients)

[Raissi (2019)]

Time-dependent PDE - mesh free

Burgers equation: $u_t + uu_x - \beta u_{xx} = 0$ **modification:** generate u_0 by mesh-free NN

Task: from known data $u_{known}(t_1, x)$ infer initial conditions in time t_0 that generated them:

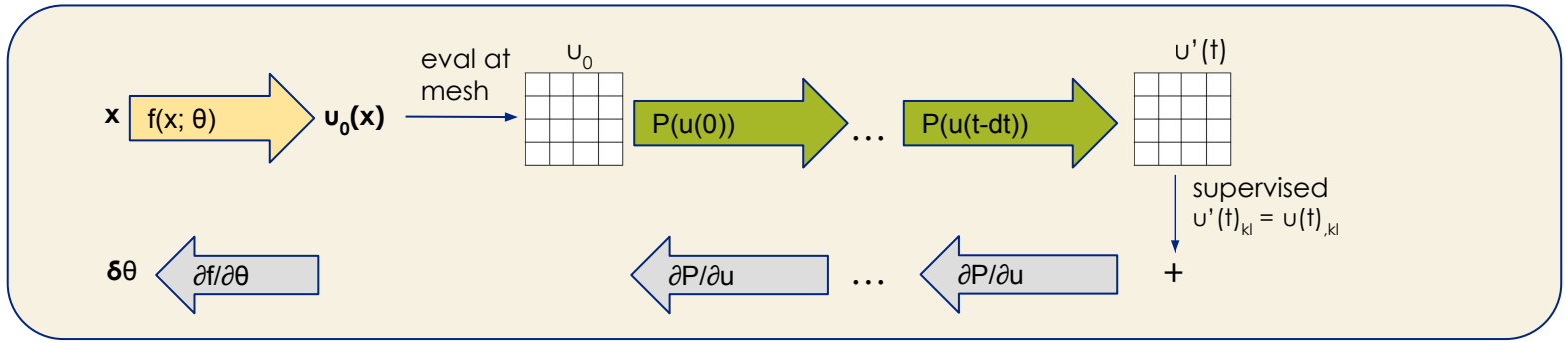
~~random → u_θ~~
random → θ

while L large:

$u_t = P \circ P \circ \ldots \circ P(f_{NN}(x; \theta))$

$L = \sum(u_t - u_{known})^2$

~~$u_\theta \rightarrow u_\theta - lr \cdot \partial L / \partial u_\theta$~~
$\theta \rightarrow \theta - lr \cdot \partial L / \partial \theta$



Note: the larger the $|t_1 - t_0|$, the harder the optimization (vanishing gradients)

[Raissi (2019)]

Time-dependent PDE

Burgers equation: $u_t + uu_x - \beta u_{xx} = 0$ **modification:** find dependence of u_0 on β

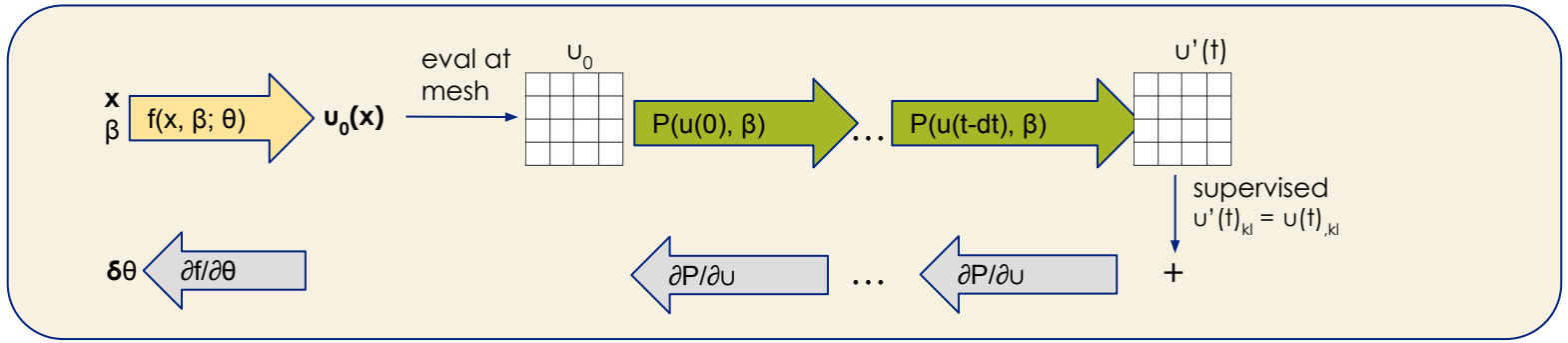
Task: from known data $u_{known}(t_1, x)$ infer initial conditions in time t_0 that generated them for any plausible value of β:

~~random → u_0~~
random → θ

while L large:
random → β
$u_t = P \circ P \circ \ldots \circ P(f_{NN}(x, \beta; \theta))$

$L = \sum(u_t - u_{known})^2$

~~$u_0 \rightarrow u_0 - lr \cdot \partial L / \partial u_0$~~
$\theta \rightarrow \theta - lr \cdot \partial L / \partial \theta$



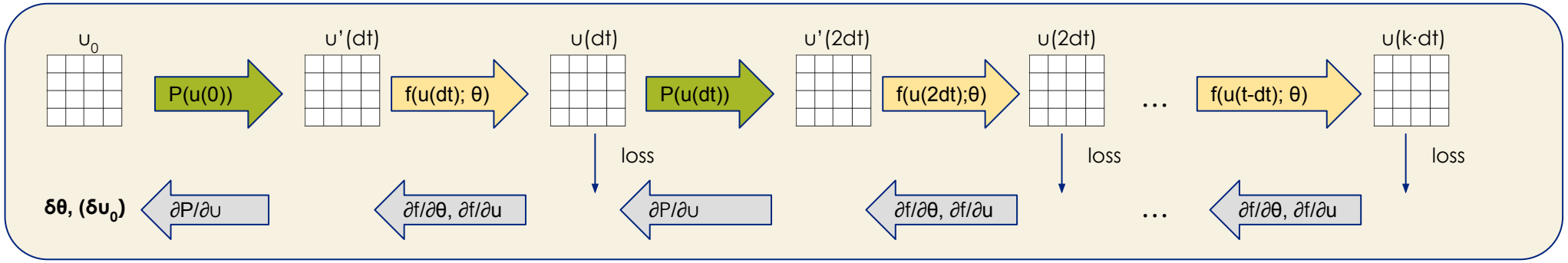
Note: the larger the $|t_1 - t_0|$, the harder the optimization (vanishing gradients)

Hybrid forward solver

PDE: $u(t, x) = N[u(t, x); \boldsymbol{\theta}]$

modification: alternate time shift operator and solution correction by NN

Task: improve accuracy of a standard integration scheme



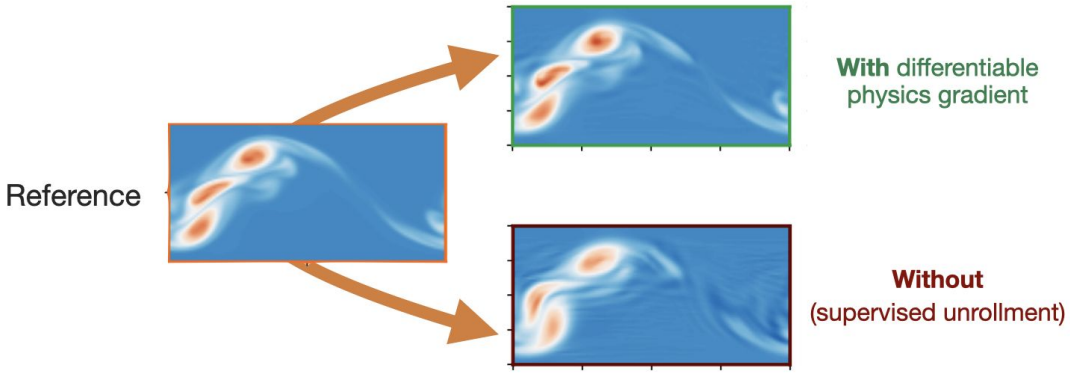
- Each time step is **predicted** by classical method and **corrected** (e.g. conservation laws) by NN
- Since NN acts as a correction of u', often better: $u = u' + f_{NN}(u', \theta)$
- f is a single NN receiving feedback from multiple time steps

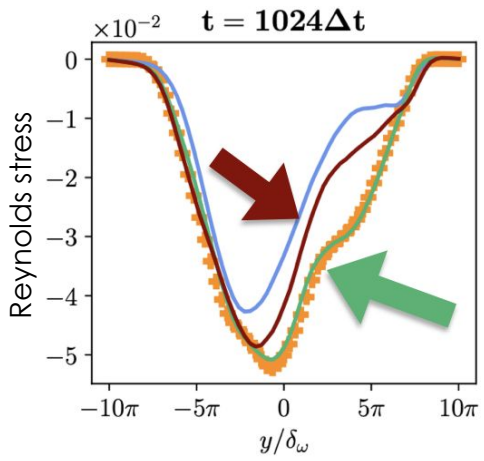
why to use the method: improved precision

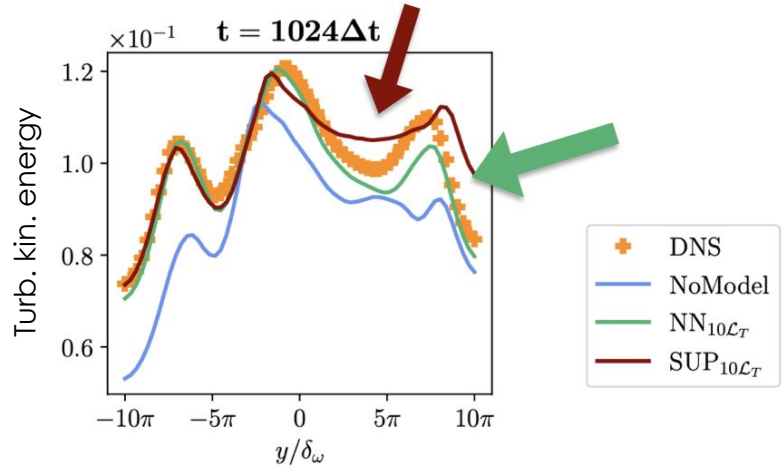
Coarse-grained simulations

- f_{CNN} correction step can learn to implicitly up-sample the solution
  ⇒ the main simulation can run spatially or temporarily under-resolved ⇒ **speedup**

- **how:** perform high-resolution simulation (DNS) + train hybrid solver on a coarse-grained grid / approximate equations
  - use supervised L2 loss against the high-resolution ground truth
    + additional losses capturing differences in important quantities (energy spectrum, strain, mean flow, …)



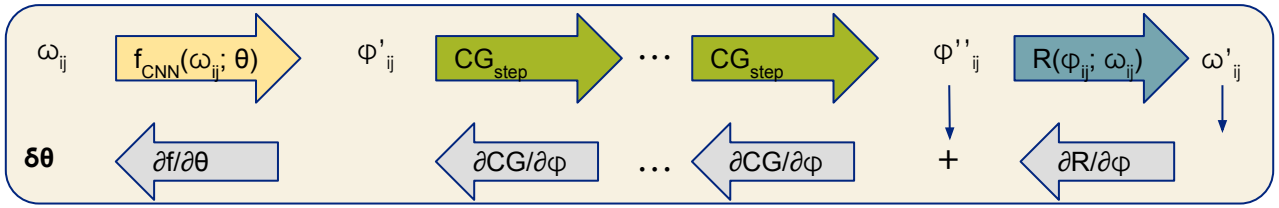




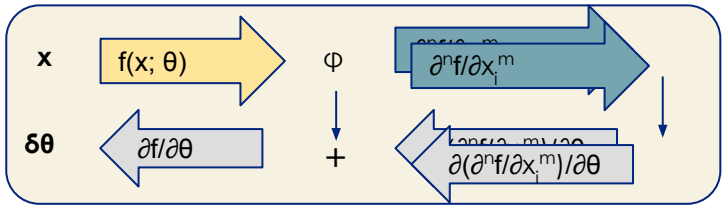
[Bjoern (2022)]

Summary

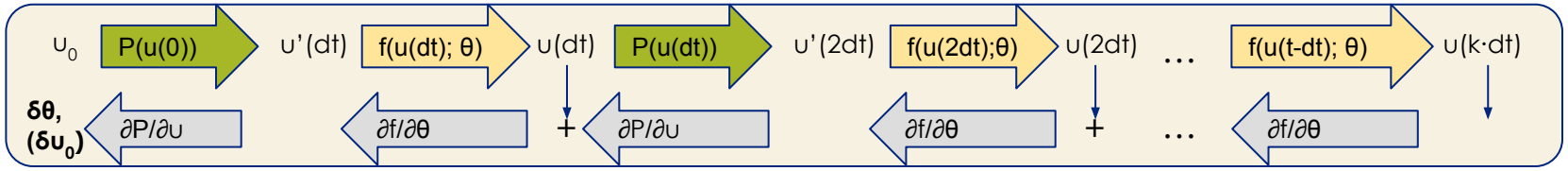
- Differentiable physics can improve standard methods of solving PDEs in terms of accuracy, speed and flexibility
  - slowly penetrating into high-temperature fusion plasma simulations
  - many schemes and applications how to combine NN and classical methods are possible, we touched just a few:

- 

NN model of D^{-1} + iterative optimizer for speed-up

- 

PINN for simplicity, flexibility and getting mesh-free, but typically slow

- 

hybrid solver for precision and speed-up (coarse-graining)

Hybrid operators

Pros:

- **leverages and improves existing efficient numerical solvers and discretizations**
  - efficient
  - good control of solution precision

Cons:

- more complicated implementation
- needs discretization
- needs deeper understanding of the solved problem

Physics Informed Neural Networks

Pros:

- **simple flexible formulation, ease of use**
  - simple to combine multiple PDEs (e.g. grad-shafranov equilibrium + braginskii transport in SOL)
- exact analytical derivatives via AD
- mesh-free

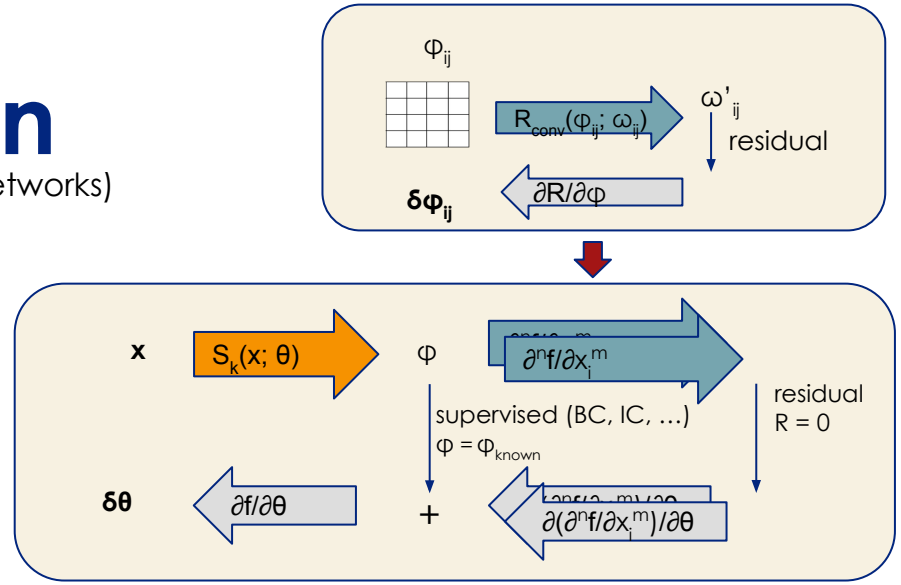
Cons:

- expensive evaluation
- incompatible with existing numerical methods
- poor control of solution precision
  - depends on the capacity of NN to represent it and proper convergence

Backup slides

Poisson equation - spline solution

(typically not used but may help with understanding the principle of Physics Informed Neural Networks)



Poisson equation: $\Delta\varphi = \omega$

Find a spline representation of φ that solves the Poisson equation:

spline $S_k(x; \theta)$: piecewise n-D polynomial with parametric continuity C^{k-1}

AD can compute exact spline derivatives

1. randomly initialize spline parameters **θ**

$$\varphi = S_k(x, y; \boldsymbol{\theta}_{random})$$

2. AD: 2nd derivatives at random points

exact derivatives: $\partial^2 S_k(x, y; \boldsymbol{\theta})/\partial x^2$; $\partial^2 S_k(x, y; \boldsymbol{\theta})/\partial y^2$

3. Exact residual loss

$$L(x, y, \boldsymbol{\theta}) = \sum[\partial^2 S_k(x, y; \boldsymbol{\theta})/\partial x^2 + \partial^2 S_k(x, y; \boldsymbol{\theta})/\partial y^2 - \omega(x, y)] + \alpha \sum_{BC}(\varphi'_{BC} - \varphi_{BC})$$

4. optimize, e.g by gradient descent, to find **θ** that will minimize L, i.e. fit the spline to the PDE

finds single C^{k-1} **continuous solution with exact derivatives** to single ω at a time