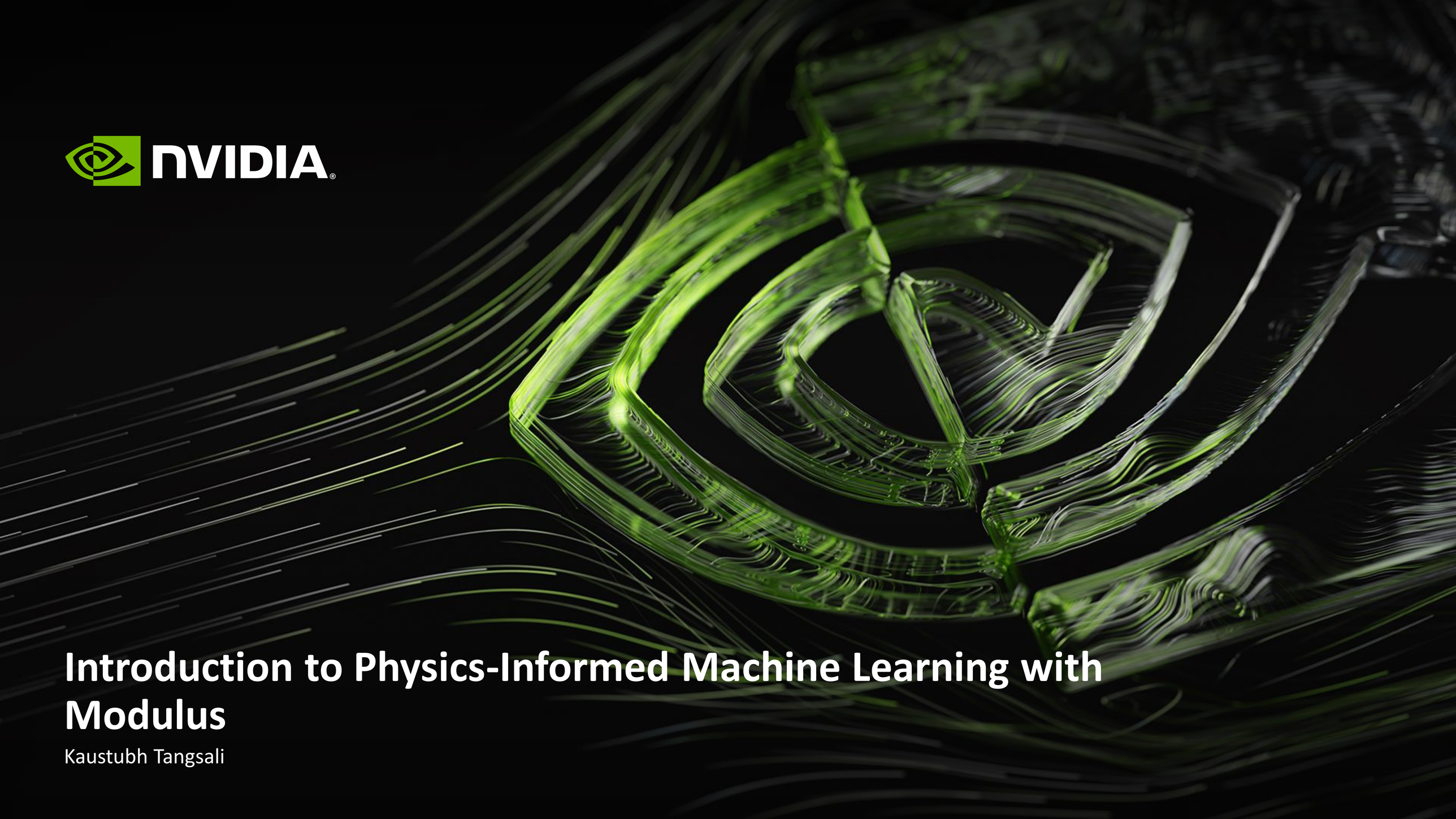


Introduction to Physics-Informed Machine Learning with Modulus

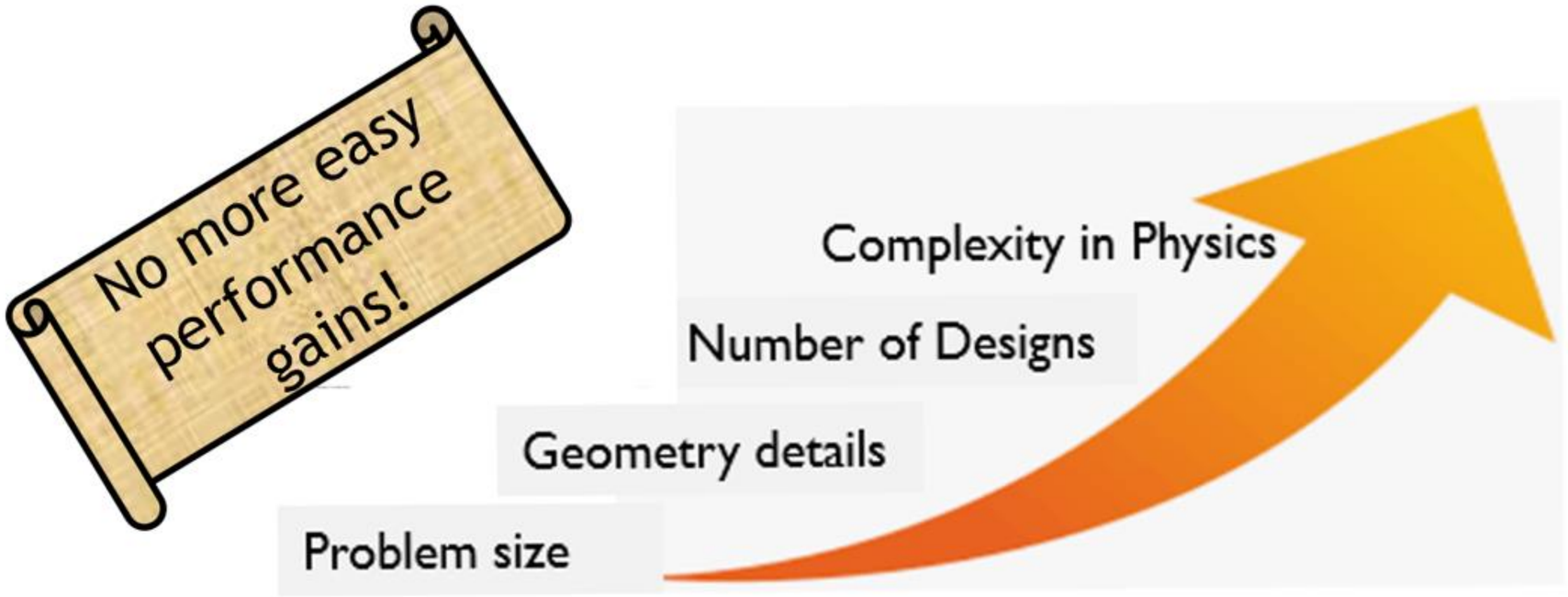
Kaustubh Tangsali

Saturating Performance in Traditional HPC

Simulations are getting larger and more complex

Traditional solution methods are:

- Computationally Expensive
- Plagued by Domain Discretization Techniques
- Not suitable for Data-assimilation or Inverse problems

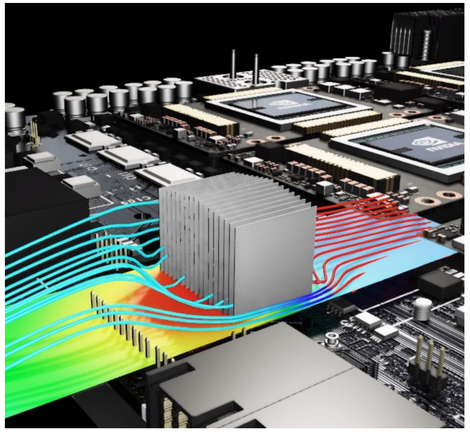


NVIDIA Modulus

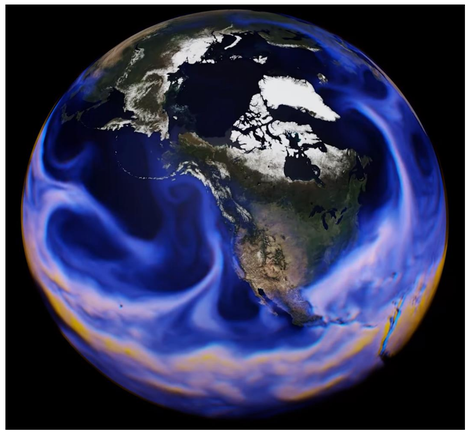
NVIDIA Modulus is a neural network framework that blends the power of physics in form of governing partial differential equations (PDEs) with data to build high-fidelity, parameterized surrogate models with near-real-time latency. It offers:

- **AI Toolkit**
  - Offers building blocks for developing physics-ML surrogate models
- **Scalable Performance**
  - Solves larger problems faster by scaling from single GPU to multi-node implementation
- **Near-Real-Time Inference**
  - Provides parameterized system representation that solves for multiple scenarios in near real time, trains once offline to infer in real time repeatedly
- **Easy Adoptability**
  - Includes APIs for domain experts to work at a higher level of abstraction. Extensible to new applications with reference applications serving as starting points

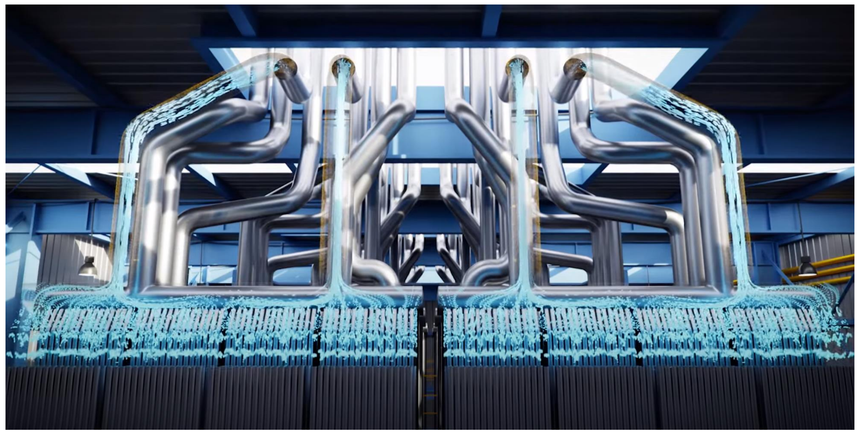
Wind Farm Super Resolution



FPGA Heatsink Design Optimization



Extreme Weather Prediction

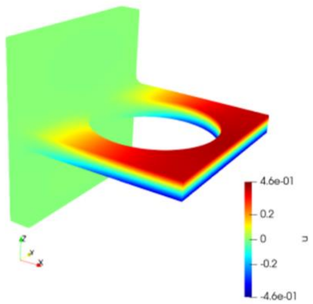


Industrial Digital Twin

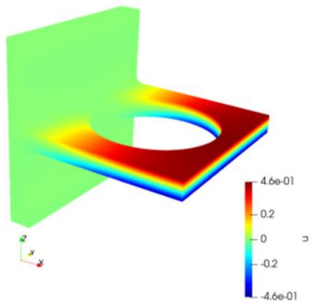
What is Modulus?

Modulus is a PDE solver

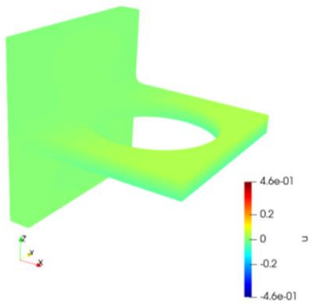
- Like traditional solvers such as Finite Element, Finite Difference, Finite Volume, and Spectral solvers, Modulus can solve PDEs



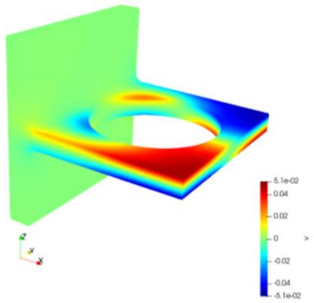
(a) u (Modulus)



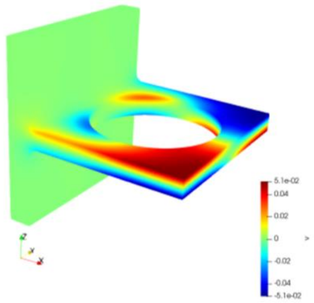
(b) u (Commercial solver)



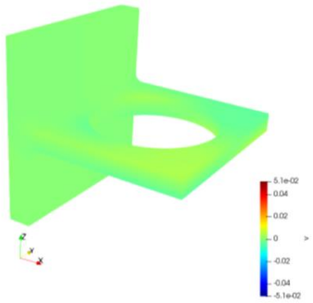
(c) u (Difference)



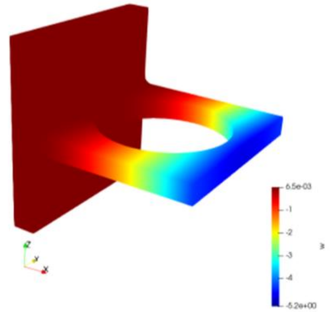
(d) v (Modulus)



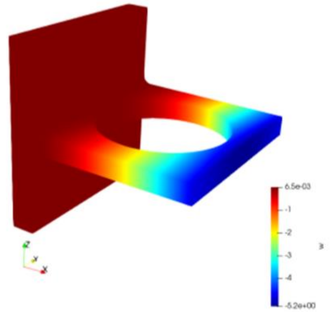
(e) v (Commercial solver)



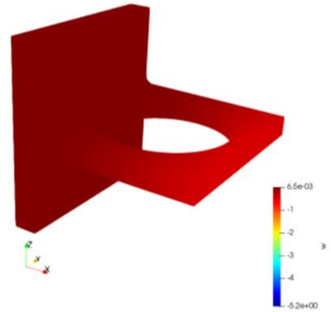
(f) v (Difference)



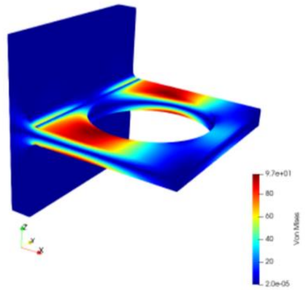
(g) w (Modulus)



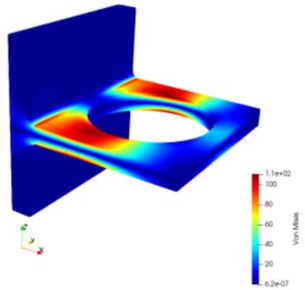
(h) w (Commercial Solver)



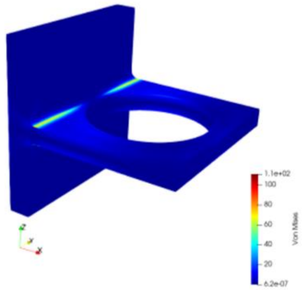
(i) w (Difference)



(j) σ_{VM} (Modulus)



(k) σ_{VM} (Commercial Solver)



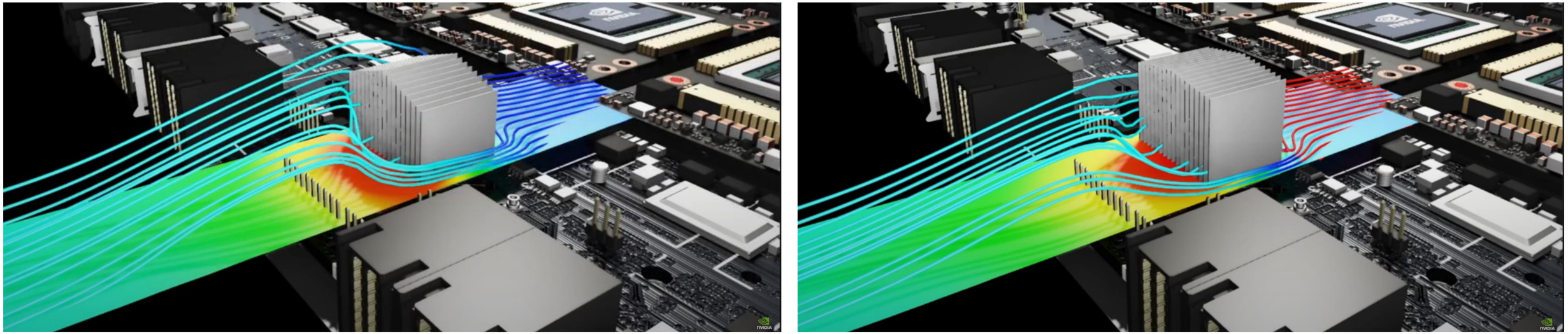
(l) σ_{VM} (Difference)

A comparison between Modulus and commercial solver results for a bracket deflection example. Linear elasticity equations are solved here.

What is Modulus?

Modulus is a tool for efficient design optimization for multi-physics problems

- With Modulus, professionals in Manufacturing and Product Development can explore different configurations and scenarios of a model, in near-real time by, changing its parameters, allowing them to gain deeper insights about the system or product, and to perform efficient design optimization of their products.

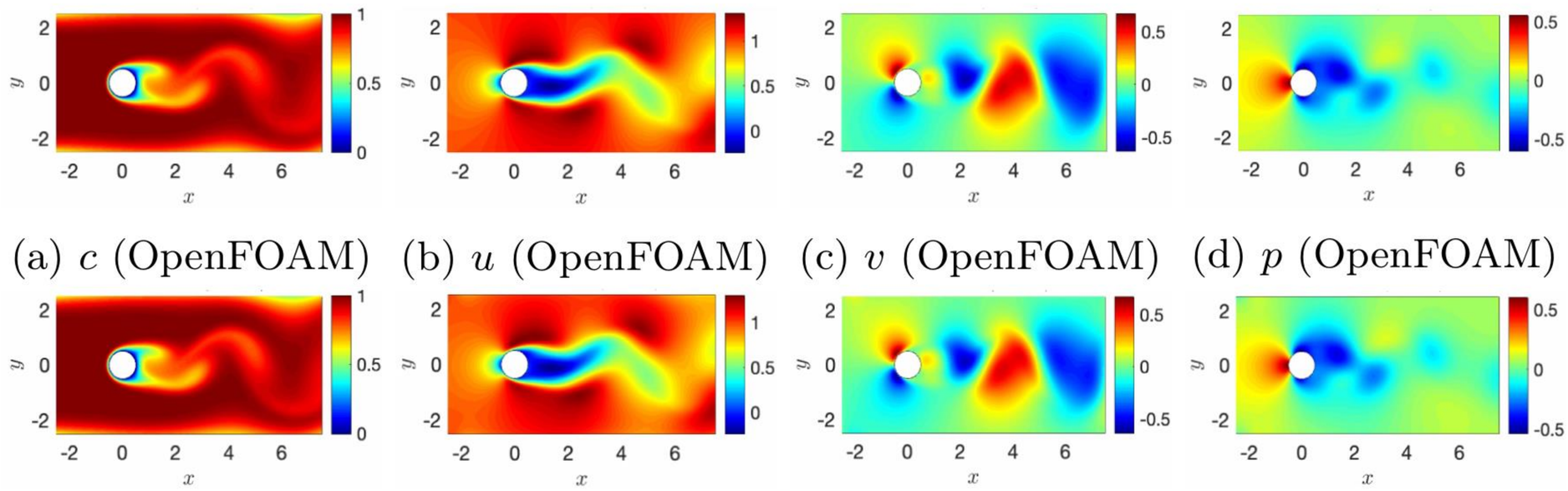


Efficient design space exploration of the heatsink of a Field-Programmable Gate Array (FPGA) using Modulus.

What is Modulus?

Modulus is a solver for inverse problems

- Many applications in science and engineering involve inferring unknown system characteristics given measured data from sensors or imaging.
- By combining data and physics, Modulus can effectively solve inverse problems.

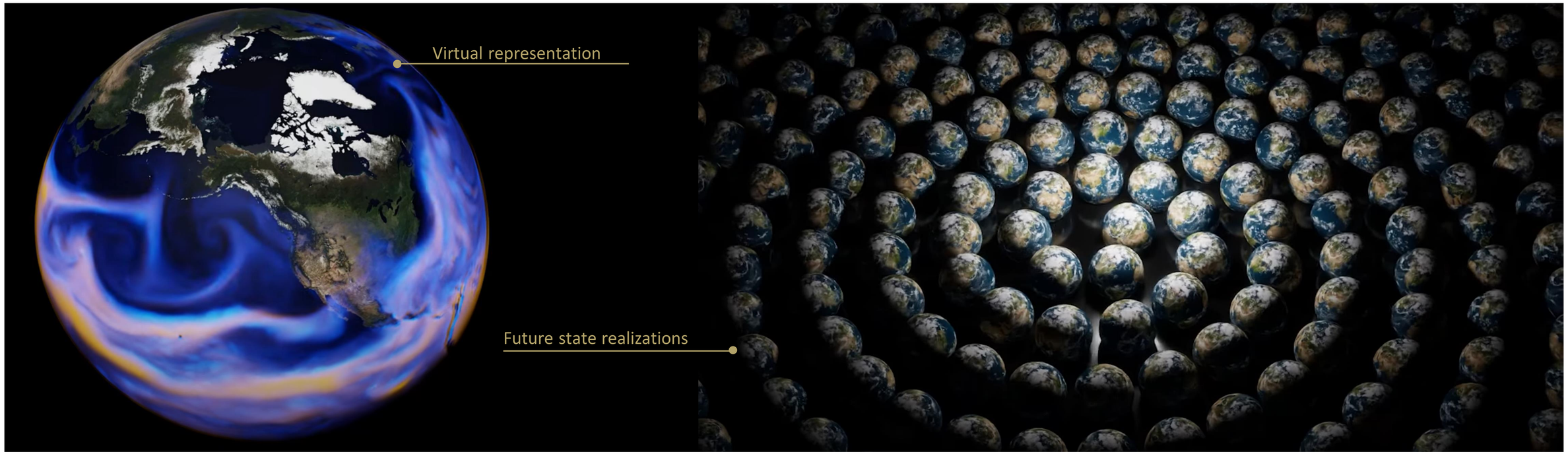


A comparison between Modulus and OpenFOAM results for the flow velocity, pressure and passive scalar concentration fields. Modulus has inferred the velocity and pressure fields using scattered data from passive scalar concentration.

What is Modulus?

Modulus is a tool for developing digital twins

- A digital twin is a virtual representation (a true-to-reality simulation of physics) of a real-world physical asset or system, which is continuously updated via stream of data.
- Digital twin predicts the future state of the real-world system under varying conditions.



What is Modulus?

Modulus is a tool for developing data-driven solutions to engineering problems

- Modulus contains a variety of APIs for developing data-driven machine learning solutions to challenging engineering systems, including:
  - Data-driven modeling of physical systems
  - Super resolution of low-fidelity results computed by traditional solvers

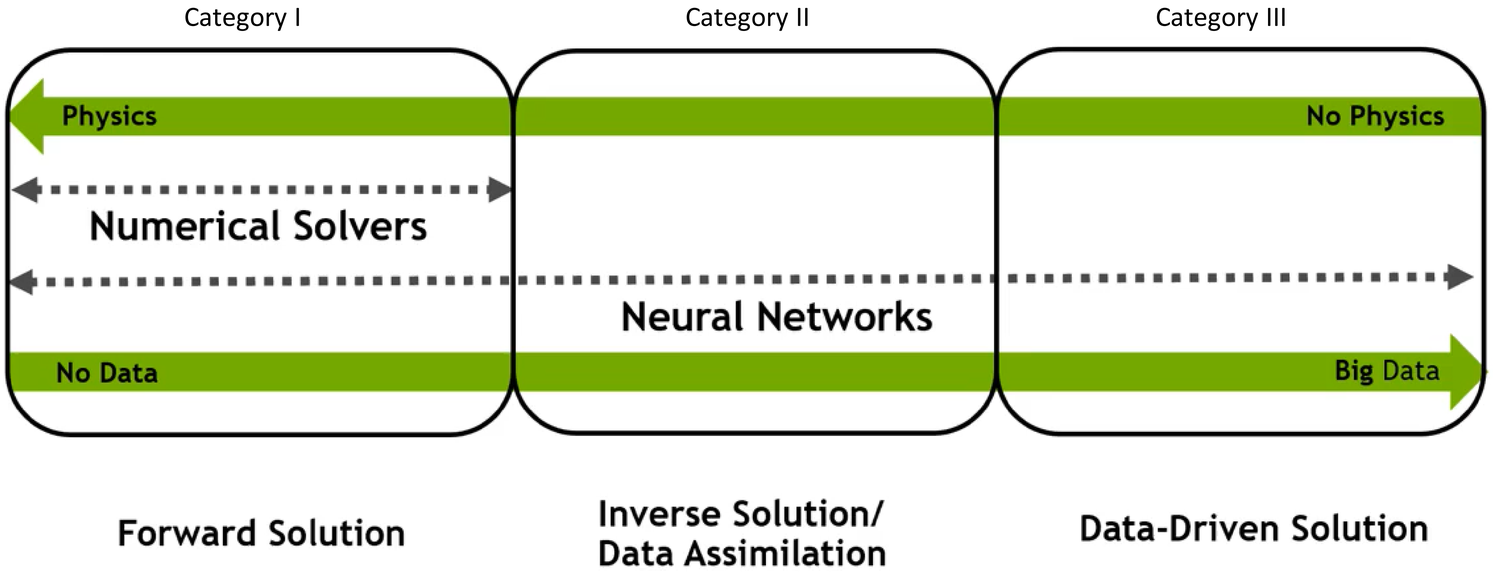
Super-resolution of flow in a wind farm using Modulus

What is Modulus?

Putting it all together

- Modulus is a PDE solver (category I)
- Modulus is a tool for efficient design optimization & design space exploration (category I)
- Modulus is a solver for inverse problems (category II)
- Modulus is a tool for developing digital twins (category II)
- Modulus is a tool for developing AI solutions to engineering problems (category III)

These are all done by developing deep neural network models in Modulus that are physics-informed and/or data-informed.



Agenda

- What is Modulus?
- Modulus Architecture, Training
- Physics informed neural networks in Modulus
- Data informed neural networks in Modulus
- Modulus other features and advancements

Modulus Architecture

Geometry and Data

Geometry
Parameterization of the physical geometry / problem. Described with geometric primitives or tessellated geometries.

Data
Training and validation data from either simulation solutions or measured data / observations. Supports point-wise data, integral and grid data (images).

Modular Nodal Structures

Nodes
Abstracted model building blocks of Modulus

Neural Network Architectures
Model zoo containing *optimized* networks such as MLP, Fourier feature, Sirens, FNO, DeepOnet, PINO, AFNO…

Physical Laws / PDEs
Symbolic representation of governing equations. E.g. Navier Stokes, Conjugate Heat Transfer, EM, combustion, Normalization…

Constraint / Objectives

Constraints
Modular blocks to represent constraints/ objectives used during training

Node Graph
Optimized execution order of nodes for each training objective. Built in optimizations: JIT, CUDA graph, etc.

Loss Functions
Loss functions for data-driven and physics-constrained models.

Train / Optimization

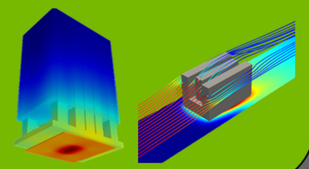
Solver
High performance training and inference. TF32 computation, AMP, Multi-GPU/Node

Domain
Contains all needed constraints solved for a given problem

- **Monitor** — Monitor quantities during training
- **Validator** — Validate results against test data
- **Inferencer** — Inference trained model
- **Optimizer** — All torch.optim optimizers and beyond

Deployment

Optimization and Exploration
Deploy surrogate for design optimization, exploration and inverse problems

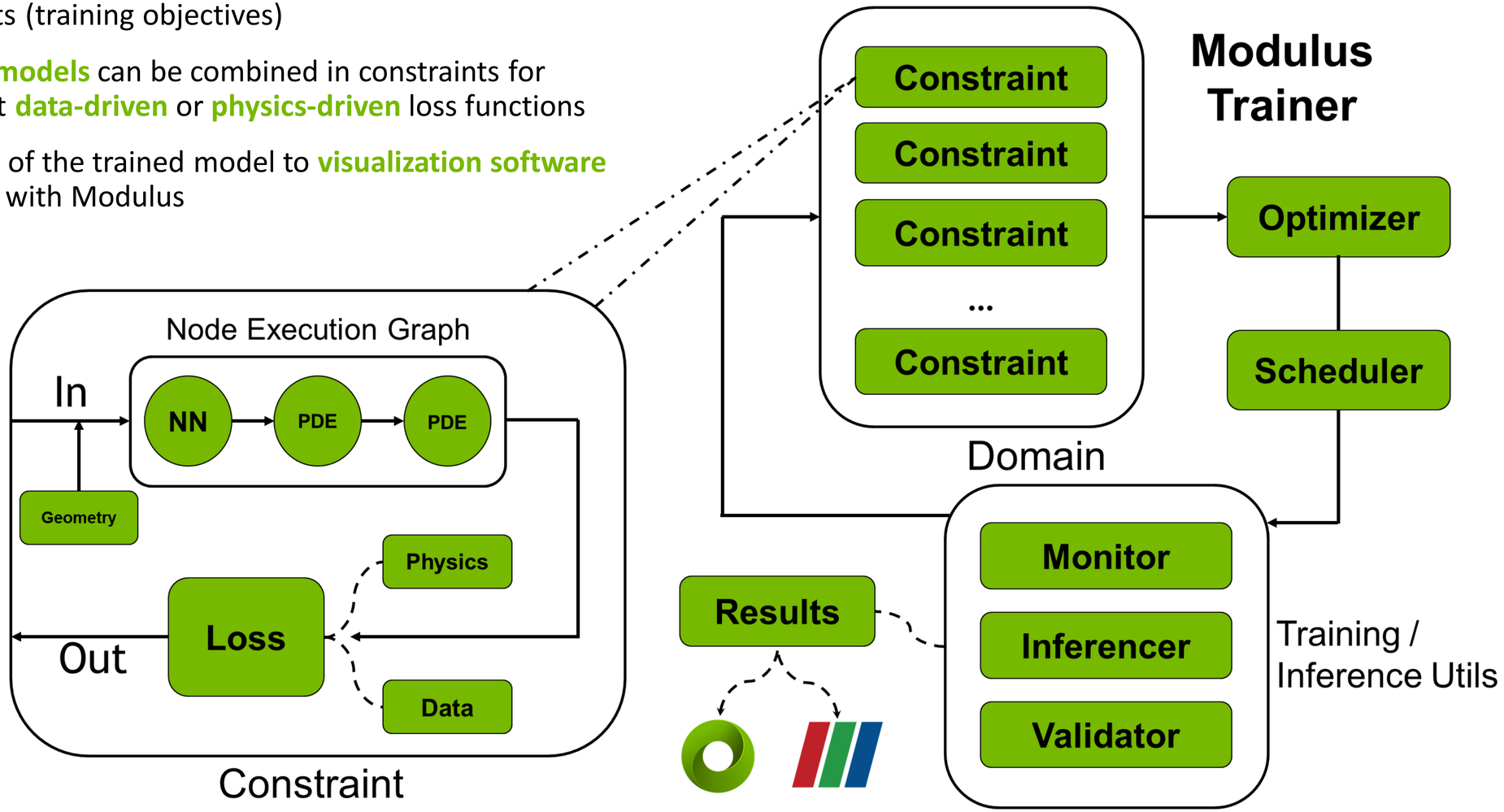


Results and Visualizations
Export results to Omniverse, Paraview, Tensorboard

Hydra Configuration

Modulus Training

- Modulus allows for **complex problems** to be described through sets of constraints (training objectives)
- Multiple **nodes/models** can be combined in constraints for learning different **data-driven** or **physics-driven** loss functions
- Exporting results of the trained model to **visualization software** is then effortless with Modulus



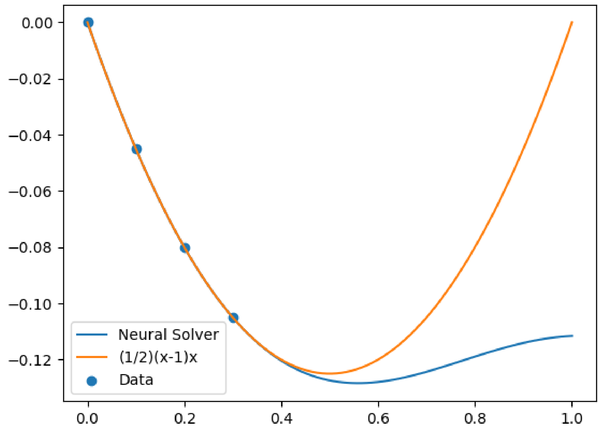
Physics Informed Neural Networks (PINNs) in Modulus

A problem with NNs and the promise of PINNs

Data Only

$$L_{data} = \sum_{x_i \in data} (u_{net}(x_i) - u_{true}(x_i))^2$$

$$L_{total} = L_{data}$$

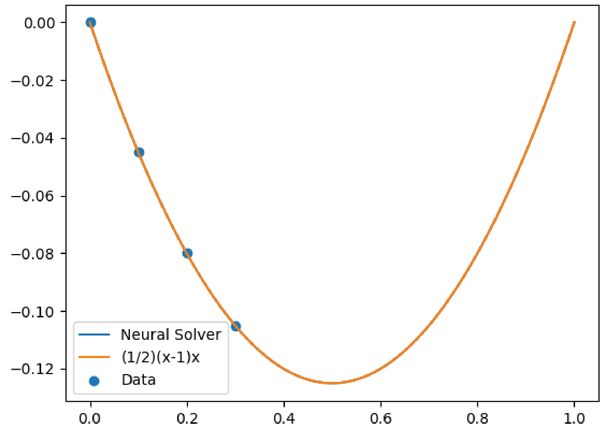


Data + Physics

$$\frac{\delta^2 u}{\delta x^2}(x) = 1$$

$$L_{physics} = \sum_{x_j \in domain} \left(\frac{\delta^2 u_{net}}{\delta x^2}(x_i) - f(x_i) \right)^2$$

$$L_{total} = L_{data} + L_{physics}$$

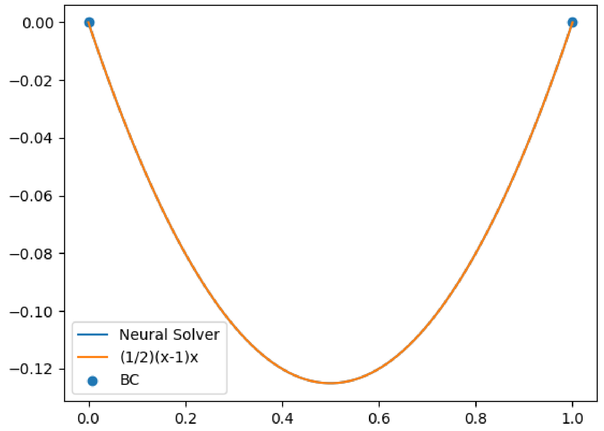


Physics only

$$\frac{\delta^2 u}{\delta x^2}(x) = 1 \qquad u(0) = u(1) = 0$$

$$L_{physics} = L_{residual} + L_{BC}$$

$$L_{total} = L_{physics}$$



NVIDIA

PINNs Theory: Neural Network Solver

Problem description

- Goal: Train a neural network to satisfy the boundary conditions and differential equations by constructing an appropriate loss function
- Consider an example problem:

$$\mathbf{P}: \begin{cases} \dfrac{\delta^2 u}{\delta x^2}(x) = f(x) \\ u(0) = u(1) = 0 \end{cases}$$

- We construct a neural network $u_{net}(x)$ which has a single value input $x \in \mathbb{R}$ and single value output $u_{net}(x) \in \mathbb{R}$.
- We assume the neural network is infinitely differentiable $u_{net} \in C^{\infty}$ - Use activation functions that are infinitely differentiable

PINNs Theory: Neural Network Solver

Loss formulation

- Construct the loss function. We can compute the second order derivatives $\left(\frac{\delta^2 u_{net}}{\delta x^2}(x)\right)$ using Automatic differentiation

$$L_{BC} = u_{net}(0)^2 + u_{net}(1)^2$$

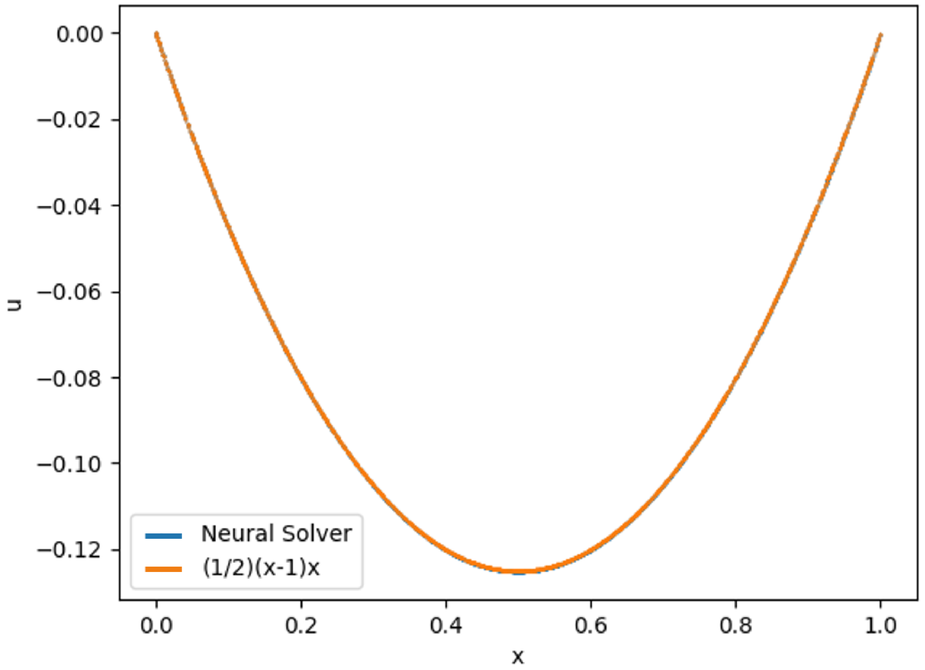
$$L_{Residual} = \int_0^1 \left(\frac{\delta^2 u_{net}}{\delta x^2}(x) - f(x)\right)^2 dx \approx \left(\int_0^1 dx\right)\frac{1}{N}\sum_{i=0}^{N}\left(\frac{\delta^2 u_{net}}{\delta x^2}(x_i) - f(x_i)\right)^2$$

- Where x_i are a batch of points in the interior $x_i \in (0, 1)$. Total loss becomes $L = L_{BC} + L_{Residual}$
- Minimize the loss using optimizers like Adam

PINNs Theory: Neural Network Solver

Results

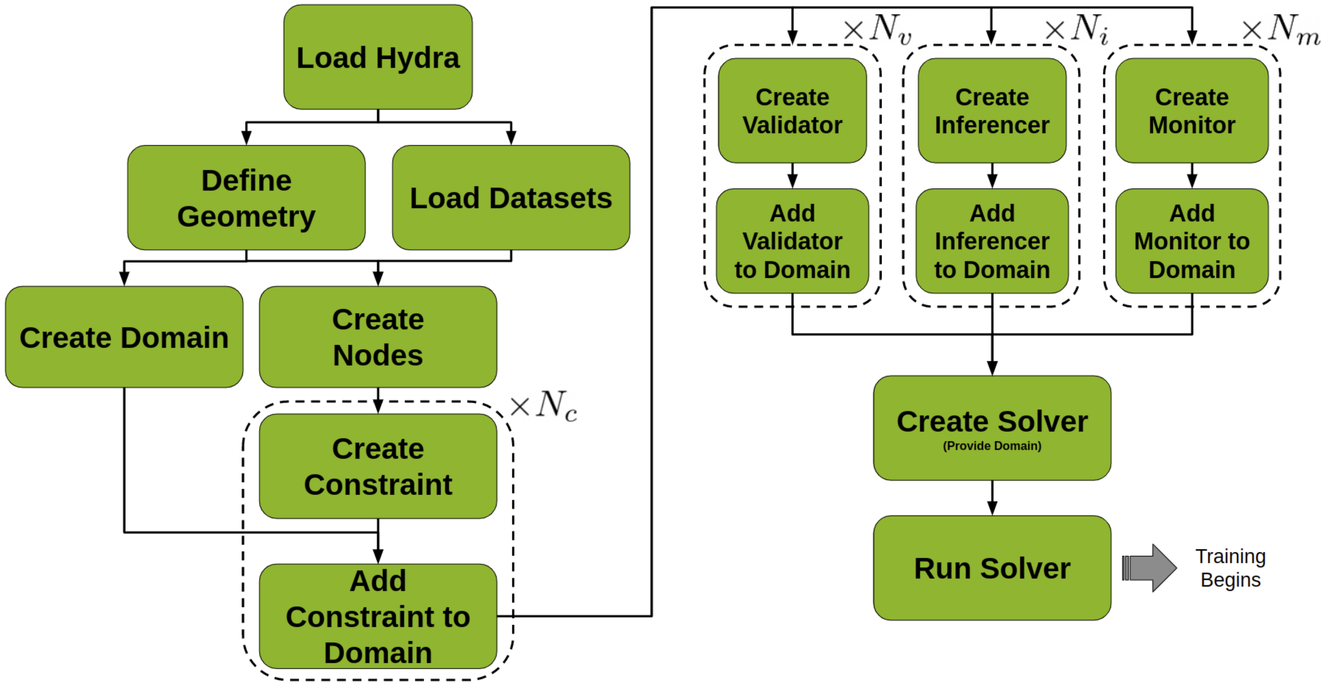
- For $f(x) = 1$, the true solution is $\frac{1}{2}(x-1)x$. After sufficient training we have,



Comparison of the solution predicted by Neural Network with the analytical solution

Modulus: Anatomy of a project

Overview

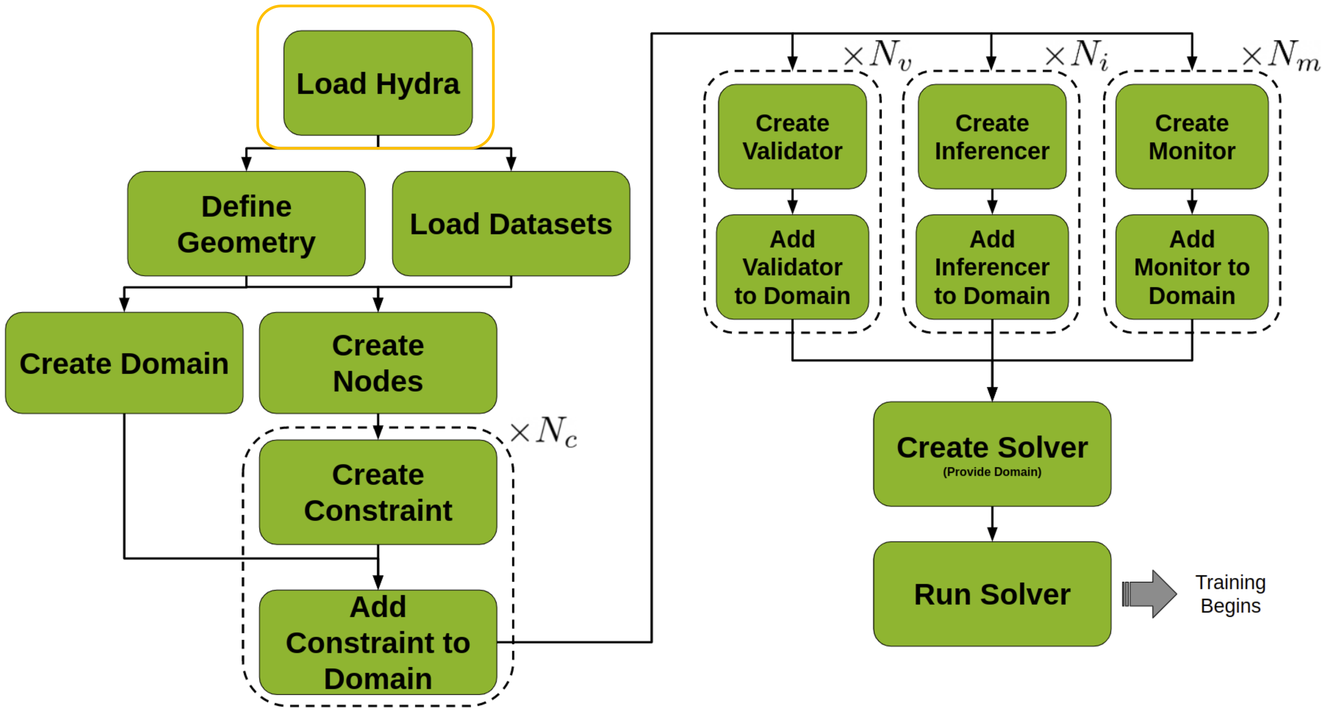


Modulus works by:

- Writing models which include at least one adaptable function (a NN)
- Writing objective functions as a combination of these models
- Describing the geometry/dataset where the models should be evaluated
- Minimizing the objective functions by using the provided data, by sampling the geometry, or both
- Running the models to obtain the desired effect

Modulus: Anatomy of a project

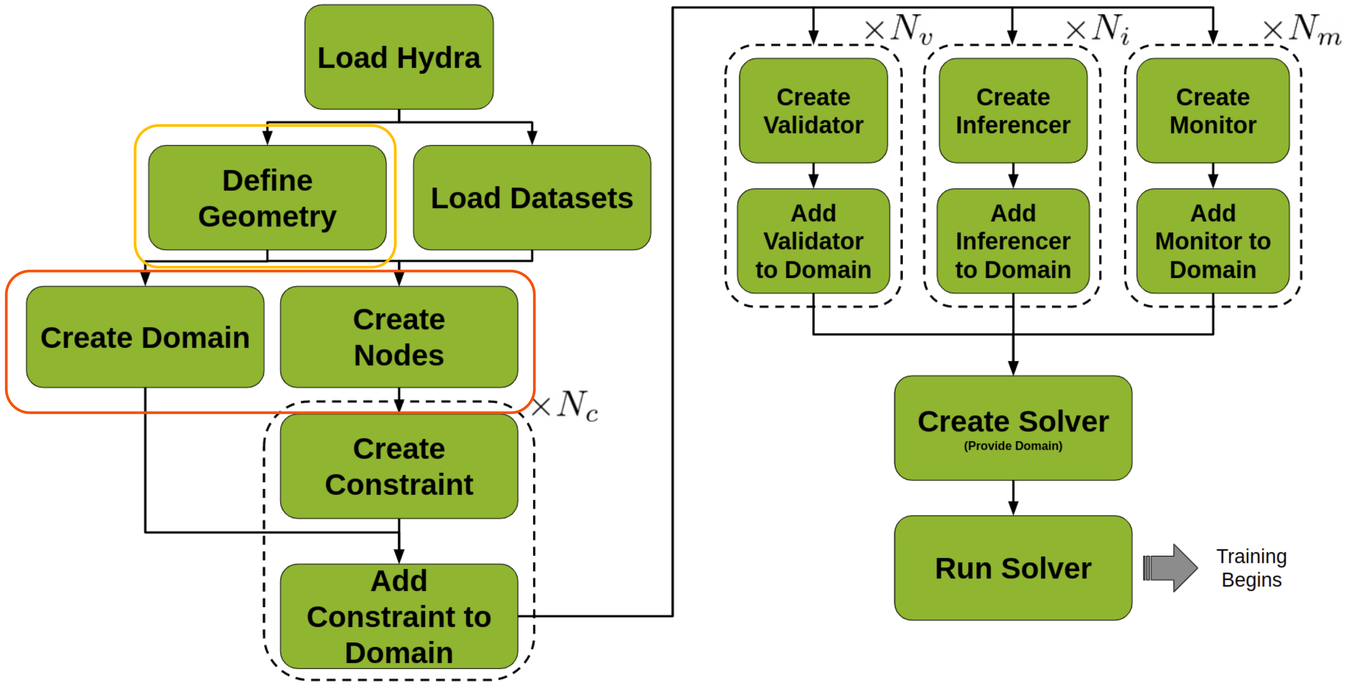
Load Hydra




```
defaults :
  - modulus_default
  - scheduler: tf_exponential_lr
  - optimizer: adam
  - loss: sum
  - _self_

scheduler:
  decay_rate: 0.95
  decay_steps: 200

save_filetypes : "vtk,npz"

training:
  rec_results_freq : 1000
  rec_constraint_freq: 1000
  max_steps : 5000
```

Modulus: Anatomy of a project

Create geometry, domain and nodes

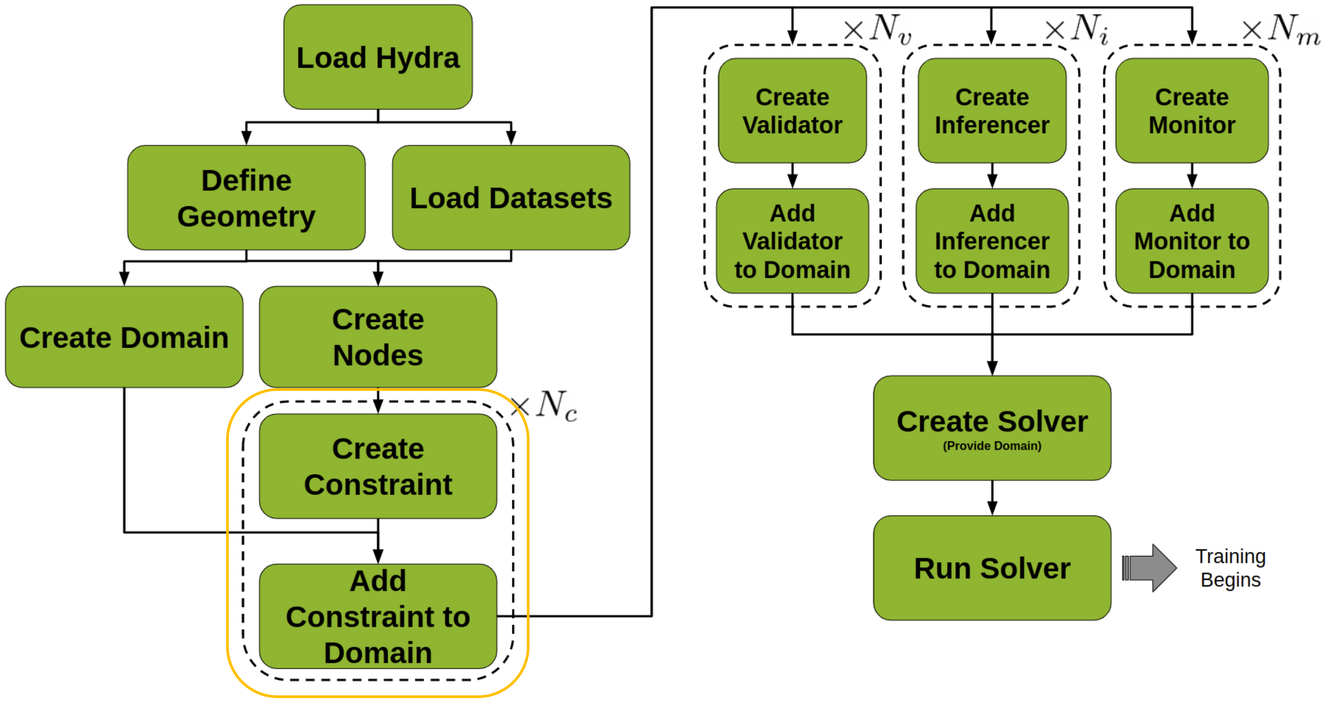



```python
@modulus.main(config_path="conf", config_name="config")
def run(cfg: ModulusConfig) -> None:

    # make geometry
    x = Symbol("x")
    geo = Line1D(0, 1)
```

```python
    # make list of nodes to unroll graph on
    eq = CustomPDE(f=1.0)
    u_net = FullyConnectedArch(
        input_keys=[Key("x")],
        output_keys=[Key("u")],
        nr_layers=3,
        layer_size=32
    )

    nodes = eq.make_nodes() + [u_net.make_node(name="u_network")]

    # make domain
    domain = Domain()
```

Modulus: Anatomy of a project

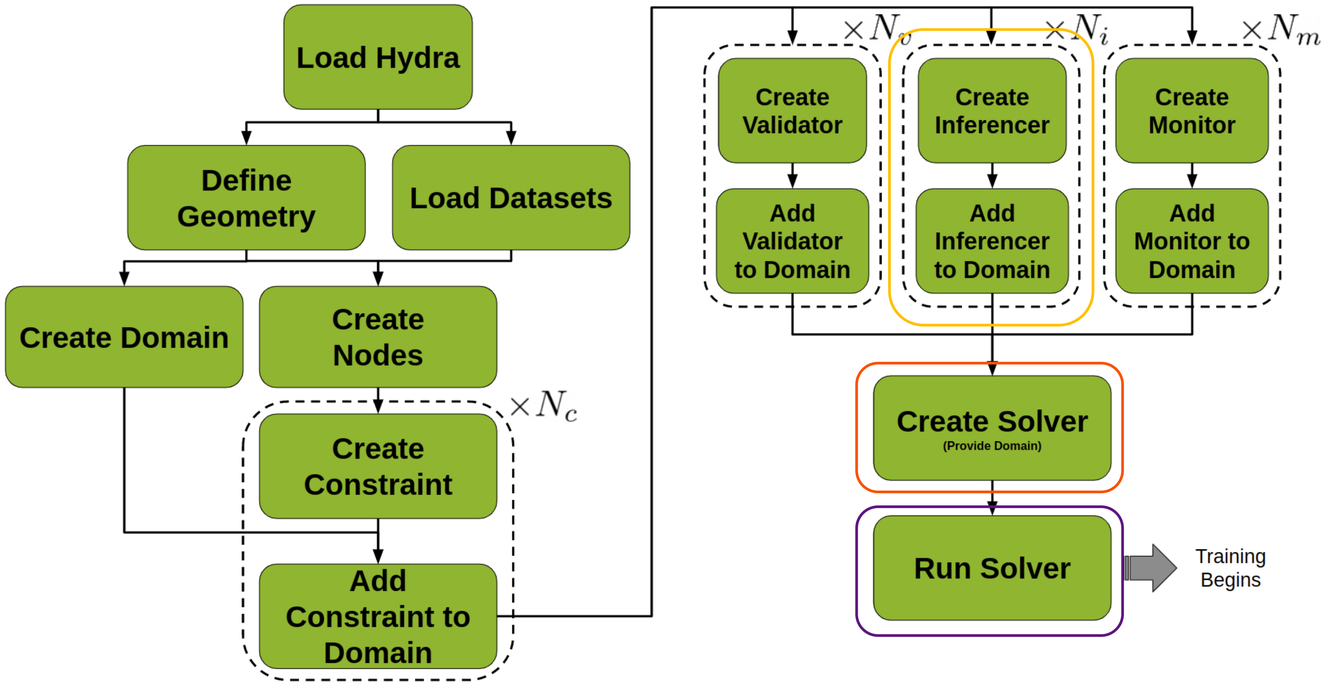
Add constraints




```python
# add constraints to solver

# bcs
bc = PointwiseBoundaryConstraint(
    nodes=nodes,
    geometry=geo,
    outvar={"u": 0},
    batch_size=2,
)
domain.add_constraint(bc, "bc")

# interior
interior = PointwiseInteriorConstraint(
    nodes=nodes,
    geometry=geo,
    outvar={"custom_pde": 0},
    batch_size=100,
    bounds={x: (0, 1)},
)
domain.add_constraint(interior, "interior")
```

Modulus: Anatomy of a project

Create utils to visualize the results and run the solver




```python
    # add inferencer
    inference = PointwiseInferencer(
        nodes=nodes,
        invar={"x": np.linspace(0, 1.0, 100).reshape(-1,1)},
        output_names=["u"],
    )
    domain.add_inferencer(inference, "inf_data")
```

```python
    # make solver
    slv = Solver(cfg, domain)

    # start solver
    slv.solve()

if __name__ == "__main__":
    run()
```

```
python <script_name>.py
mpirun –np <#GPU> <script_name>.py
```

Solving Parameterized Problems

Problem definition

- Consider the parameterized version of the same problem as before. Suppose we want to determine how the solution changes as we move the position on the boundary condition $u(l) = 0$
- Parameterize the position by variable $l \in [1, 2]$ and the problem now becomes:

$$\mathbf{P}: \begin{cases} \dfrac{\delta^2 u}{\delta x^2}(x) = f(x) \\ u(0) = u(l) = 0 \end{cases}$$

- This time, we construct a neural network $u_{net}(x, l)$ which has x and l as input and single value output $u_{net}(x, l) \in \mathbb{R}$.
- The losses become

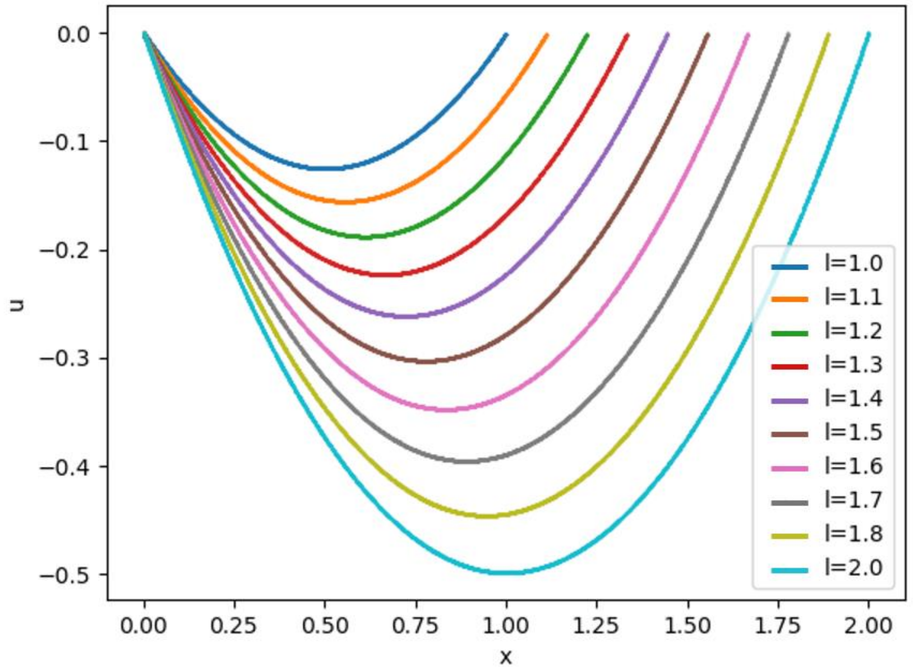
$$L_{Residual} = \int_1^2 \int_0^1 \left(\frac{\delta^2 u_{net}}{\delta x^2}(x) - f(x) \right)^2 dx dl \approx \left(\int_1^2 \int_0^1 dx\, dl \right) \frac{1}{N} \sum_{i=0}^{N} \left(\frac{\delta^2 u_{net}}{\delta x^2}(x_i, l_i) - f(x_i) \right)^2$$

$$L_{BC} = \int_1^2 \big(u_{net}(0, l)\big)^2 + \big(u_{net}(l, l)\big)^2 dl \approx \left(\int_1^2 dl \right) \frac{1}{N} \sum_{i=0}^{N} (u_{net}(0, l_i))^2 + (u_{net}(l_i, l_i))^2$$

Solving Parameterized Problems

Results

- For $f(x) = 1$, for different values of l we have different solutions



Solution to the parametric problem

Solving Inverse Problems

Problem definition

- For inverse problems, we start with a set of observations and then calculate the causal factors that produced them
- For example, suppose we are given the solution $u_{true}(x)$ at 100 random points between 0 and 1 and we want to determine the $f(x)$ that is causing it
- Train two networks $u_{net}(x)$ and $f_{net}(x)$ to approximate $u(x)$ and $f(x)$

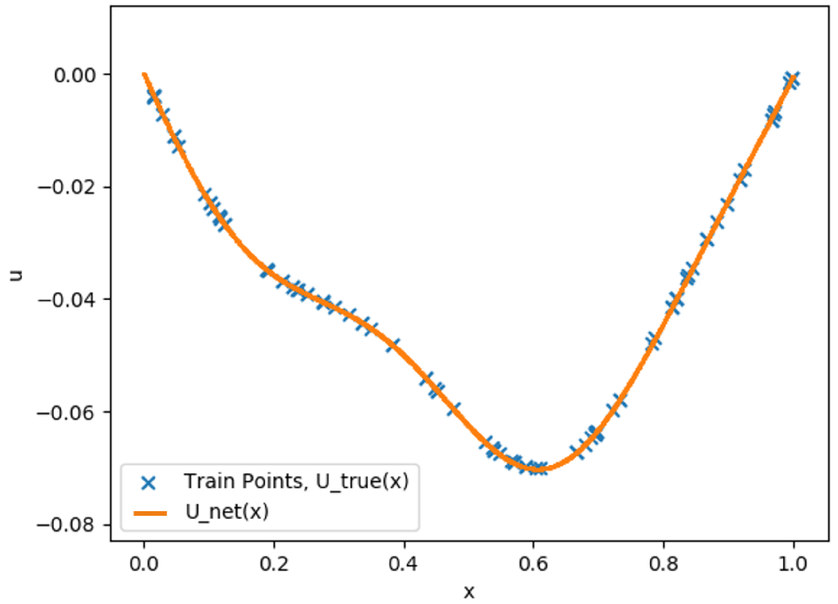
$$L_{Residual} \approx \left(\int_0^1 dx\right)\frac{1}{N}\sum_{i=0}^{N}\left(\frac{\delta^2 u_{net}}{\delta x^2}(x_i) - f(x_i)\right)^2$$

$$L_{Data} = \frac{1}{100}\sum_{i=0}^{100}\left(u_{net}(x_i) - u_{true}(x_i)\right)^2$$

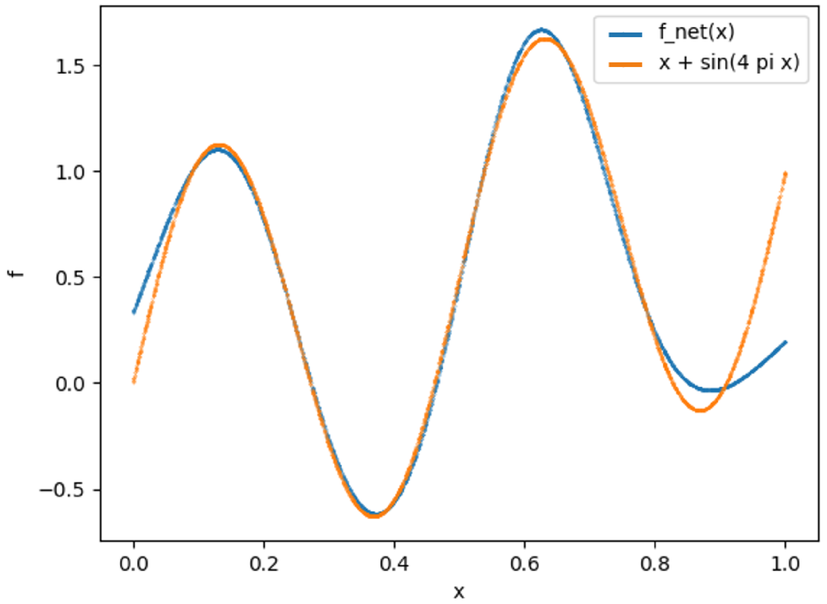
Solving Inverse Problems

Results

- For $u_{true}(x) = \frac{1}{48}\left(8x(-1+x^2) - \frac{3\sin(4\pi x)}{\pi^2}\right)$ the solution for $f(x)$ is $x + \sin(4\pi x)$



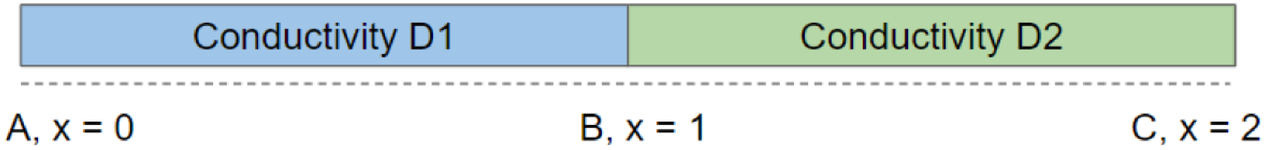
Comparison of $u\_net\ (x)$ and train points from u_true



Comparison of the true solution for $f(x)$ and the $f_{net}(x)$ inverted out

Solution to 1D diffusion

Problem description



- Composite bar with material of conductivity $D_1 = 10$ for $x \in (0,1)$ and $D_2 = 0.1$ for $x \in (1,2)$. Point A and C are maintained at temperatures of 0 and 100 respectively
- Equations: Diffusion equation in $1D$

$$\frac{d}{dx}\left(D_1 \frac{dU_1}{dx}\right) = 0 \qquad \text{When } 0 < x < 1$$

$$\frac{d}{dx}\left(D_2 \frac{dU_2}{dx}\right) = 0 \qquad \text{When } 1 < x < 2$$

- Flux and field continuity at interface (x=1)

$$\left(D_1 \frac{dU_1}{dx}\right) = \left(D_2 \frac{dU_2}{dx}\right)$$
$$U_1 = U_2$$

Solution to 1D diffusion

Code snippets – Custom symbolic PDE

```python
from sympy import Symbol, Eq, Function, Number
from modulus.eq.pde import PDE
```

```python
class Diffusion(PDE):
    name = "Diffusion"
```

Create a child class from Modulus' PDE class

```python
    def __init__(self, T="T", D="D", Q=0, dim=3, time=True):
        # set params
        self.T = T
        self.dim = dim
        self.time = time
```

Add the __init__() function to define any PDE specific arguments

```python
        # coordinates
        x, y, z = Symbol("x"), Symbol("y"), Symbol("z")

        # time
        t = Symbol("t")

        # make input variables
        input_variables = {"x": x, "y": y, "z": z, "t": t}
        if self.dim == 1:
            input_variables.pop("y")
            input_variables.pop("z")
        elif self.dim == 2:
            input_variables.pop("z")
        if not self.time:
            input_variables.pop("t")
```

Symbolic input variables using sympy's Symbol

```python
        # Temperature
        assert type(T) == str, "T needs to be string"
        T = Function(T)(*input_variables)

        # Diffusivity
        if type(D) is str:
            D = Function(D)(*input_variables)
        elif type(D) in [float, int]:
            D = Number(D)

        # Source
        if type(Q) is str:
            Q = Function(Q)(*input_variables)
        elif type(Q) in [float, int]:
            Q = Number(Q)
```

Dependent variables defined using sympy's Function

Any additional terms that potentially need to be parameterized can also be specified as dependent variables

```python
        # set equations
        self.equations = {}
        self.equations["diffusion_" + self.T] = (
            T.diff(t) - (D * T.diff(x)).diff(x) - (D * T.diff(y)).diff(y) - (D * T.diff(z)).diff(z) - Q
        )
```

Symbolic PDE. Derivatives are computed using sympy's functions

$$T_t = \nabla \cdot (D \nabla T) + Q$$

Solution to 1D diffusion

Code snippets

```python
@modulus.main(config_path="conf", config_name="config")
def run(cfg: ModulusConfig) -> None:
```

Loading hydra configs

```python
    # make list of nodes to unroll graph on
    diff_u1 = Diffusion(T="u_1", D=D1, dim=1, time=False)
    diff_u2 = Diffusion(T="u_2", D=D2, dim=1, time=False)
    diff_in = DiffusionInterface("u_1", "u_2", D1, D2, dim=1, time=False)

    diff_net_u_1 = instantiate_arch(
        input_keys=[Key("x")],
        output_keys=[Key("u_1")],
        cfg=cfg.arch.fully_connected,
    )
    diff_net_u_2 = instantiate_arch(
        input_keys=[Key("x")],
        output_keys=[Key("u_2")],
        cfg=cfg.arch.fully_connected,
    )

    nodes = (
        diff_u1.make_nodes()
        + diff_u2.make_nodes()
        + diff_in.make_nodes()
        + [diff_net_u_1.make_node(name="u1_network", jit=cfg.jit)]
        + [diff_net_u_2.make_node(name="u2_network", jit=cfg.jit)]
    )
```

Equation and neural network nodes

```python
    # make domain add constraints to the solver
    domain = Domain()

    # sympy variables
    x = Symbol("x")

    # right hand side (x = 2) Pt c
    rhs = PointwiseBoundaryConstraint(
        nodes=nodes,
        geometry=L2,
        outvar={"u_2": Tc},
        batch_size=cfg.batch_size.rhs,
        criteria=Eq(x, 2),
    )
    domain.add_constraint(rhs, "right_hand_side")
```

Domain and Constraints

```python
    # left hand side (x = 0) Pt a
    lhs = PointwiseBoundaryConstraint(
        nodes=nodes,
        geometry=L1,
        outvar={"u_1": Ta},
        batch_size=cfg.batch_size.lhs,
        criteria=Eq(x, 0),
    )
    domain.add_constraint(lhs, "left_hand_side")
```

Sample the boundary of geometry

```python
    # interface 1-2
    interface = PointwiseBoundaryConstraint(
        nodes=nodes,
        geometry=L1,
        outvar={
            "diffusion_interface_dirichlet_u_1_u_2": 0,
            "diffusion_interface_neumann_u_1_u_2": 0,
        },
        batch_size=cfg.batch_size.interface,
        criteria=Eq(x, 1),
    )
    domain.add_constraint(interface, "interface")
```

Criteria for sub-sampling

```python
    # interior 1
    interior_u1 = PointwiseInteriorConstraint(
        nodes=nodes,
        geometry=L1,
        outvar={"diffusion_u_1": 0},
        bounds={x: (0, 1)},
        batch_size=cfg.batch_size.interior_u1,
    )
    domain.add_constraint(interior_u1, "interior_u1")
```

Sample the interior of geometry

```python
    # interior 2
    interior_u2 = PointwiseInteriorConstraint(
        nodes=nodes,
        geometry=L2,
        outvar={"diffusion_u_2": 0},
        bounds={x: (1, 2)},
        batch_size=cfg.batch_size.interior_u2,
    )
    domain.add_constraint(interior_u2, "interior_u2")
```

Solution to 1D diffusion

Code snippets

```python
# validation data
x = np.expand_dims(np.linspace(0, 1, 100), axis=-1)
u_1 = x * Tb + (1 - x) * Ta
invar_numpy = {"x": x}
outvar_numpy = {"u_1": u_1}
val = PointwiseValidator(nodes=nodes, invar=invar_numpy, true_outvar=outvar_numpy)
domain.add_validator(val, name="Val1")

# make validation data line 2
x = np.expand_dims(np.linspace(1, 2, 100), axis=-1)
u_2 = (x - 1) * Tc + (2 - x) * Tb
invar_numpy = {"x": x}
outvar_numpy = {"u_2": u_2}
val = PointwiseValidator(nodes=nodes, invar=invar_numpy, true_outvar=outvar_numpy)
domain.add_validator(val, name="Val2")
```

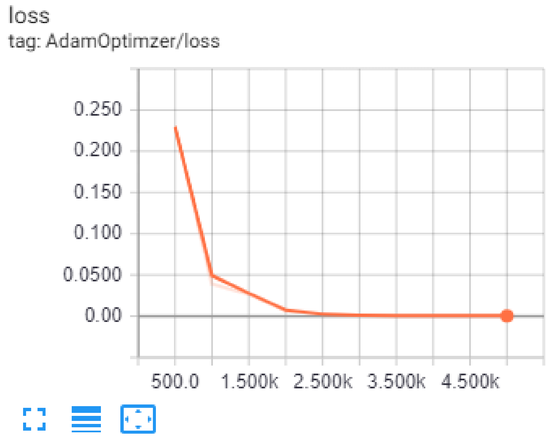
Validators to compare with experimental/analytical /solver data

```python
# make monitors
invar_numpy = {"x": [[1.0]]}
monitor = PointwiseMonitor(
    invar_numpy,
    output_names=["u_1__x"],
    metrics={"flux_u1": lambda var: torch.mean(var["u_1__x"])},
    nodes=nodes,
    requires_grad=True,
)
domain.add_monitor(monitor)

monitor = PointwiseMonitor(
    invar_numpy,
    output_names=["u_2__x"],
    metrics={"flux_u2": lambda var: torch.mean(var["u_2__x"])},
    nodes=nodes,
    requires_grad=True,
)
domain.add_monitor(monitor)
```

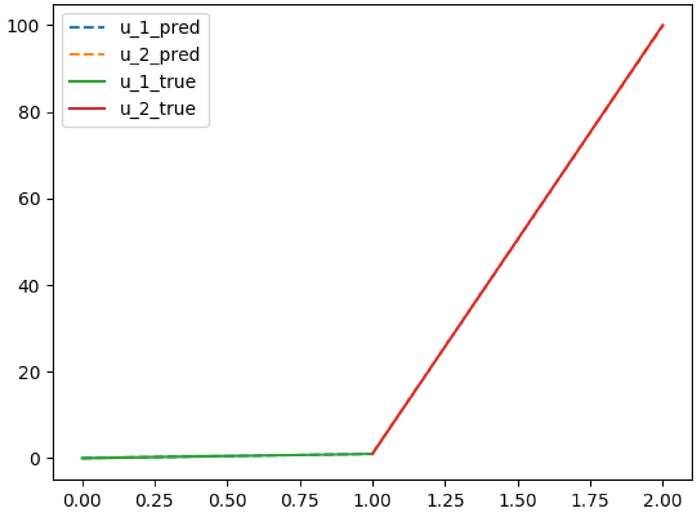
Monitor the quantities of interest during the runtime

```python
# make solver
slv = Solver(cfg, domain)

# start solver
slv.solve()
```

Solver



Tensorboard visualization of loss curves



Results generated from numpy output

Parameterized Solution to 1D diffusion

Problem description and code snippets

- Composite bar with material of conductivity D_1 for $x \in (0,1)$ and $D_2 = 0.1$ for $x \in (1,2)$.
- Solve the problem for multiple values of D_1 in the range $(5, 25)$ in a single training
- Same boundary and interface conditions as before

```python
# params for domain
L1 = Line1D(0, 1)
L2 = Line1D(1, 2)
```

```python
D1 = Symbol("D1")
D1_range = {D1: (5, 25)}
```

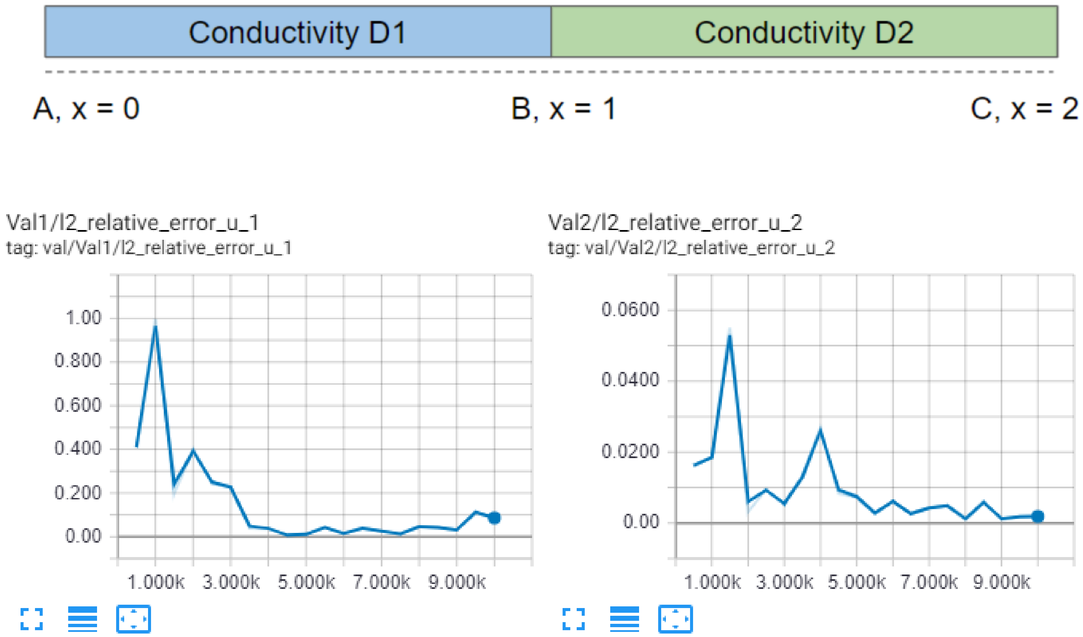
```python
@modulus.main(config_path="conf", config_name="config_param")
def run(cfg: ModulusConfig) -> None:
    # make list of nodes to unroll graph on
    diff_u1 = Diffusion(T="u_1", D="D1", dim=1, time=False)
    diff_u2 = Diffusion(T="u_2", D=D2, dim=1, time=False)
    diff_in = DiffusionInterface("u_1", "u_2", "D1", D2, dim=1, time=False)

    diff_net_u_1 = instantiate_arch(
        input_keys=[Key("x"), Key("D1")],
        output_keys=[Key("u_1")],
        cfg=cfg.arch.fully_connected,
    )
    diff_net_u_2 = instantiate_arch(
        input_keys=[Key("x"), Key("D1")],
        output_keys=[Key("u_2")],
        cfg=cfg.arch.fully_connected,
    )
```

Symbolically parameterize the variables of choice (geometric/physical) and setup the architecture

```python
    # right hand side (x = 2) Pt c
    rhs = PointwiseBoundaryConstraint(
        nodes=nodes,
        geometry=L2,
        outvar={"u_2": Tc},
        batch_size=cfg.batch_size.rhs,
        criteria=Eq(x, 2),
        parameterization=Parameterization(D1_range),
    )
    domain.add_constraint(rhs, "right_hand_side")
```

Specify the appropriate parameterization to the constraints

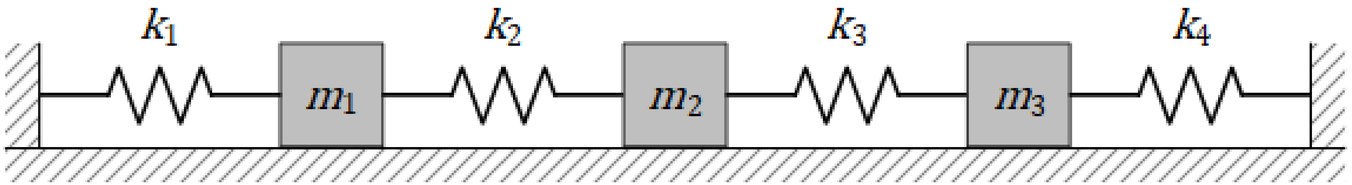
Fairly simple changes to go from single forward simulation to parameterized simulation



Validation error for $D_1 = 10$

Solution to ODEs – Coupled Spring Mass System

Problem description



- Three masses connected by four springs
- System's equations (ordinary differential equations):

$$m_1 x_1''(t) = -k_1 x_1(t) + k_2\big(x_2(t) - x_1(t)\big)$$
$$m_2 x_2''(t) = -k_2\big(x_2(t) - x_1(t)\big) + k_3\big(x_3(t) - x_2(t)\big)$$
$$m_3 x_3''(t) = -k_3\big(x_3(t) - x_2(t)\big) - k_4 x_3(t)$$

- For given values masses, spring constants and boundary conditions

$$[m_1, m_2, m_3] = [1, 1, 1]$$
$$[k_1, k_2, k_3, k_4] = [2, 1, 1, 2]$$
$$[x_1(0), x_2(0), x_3(0)] = [1, 0, 0]$$
$$[x_1'(0), x_2'(0), x_3'(0)] = [0, 0, 0]$$

Solution to ODEs – Coupled Spring Mass System

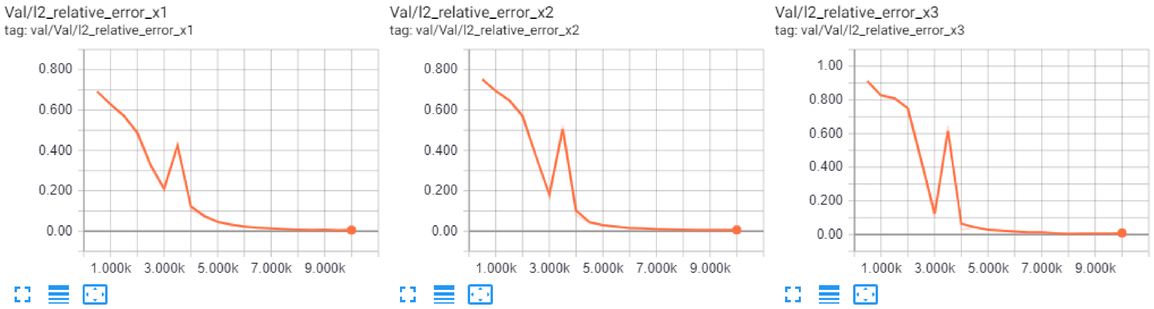
Code snippets

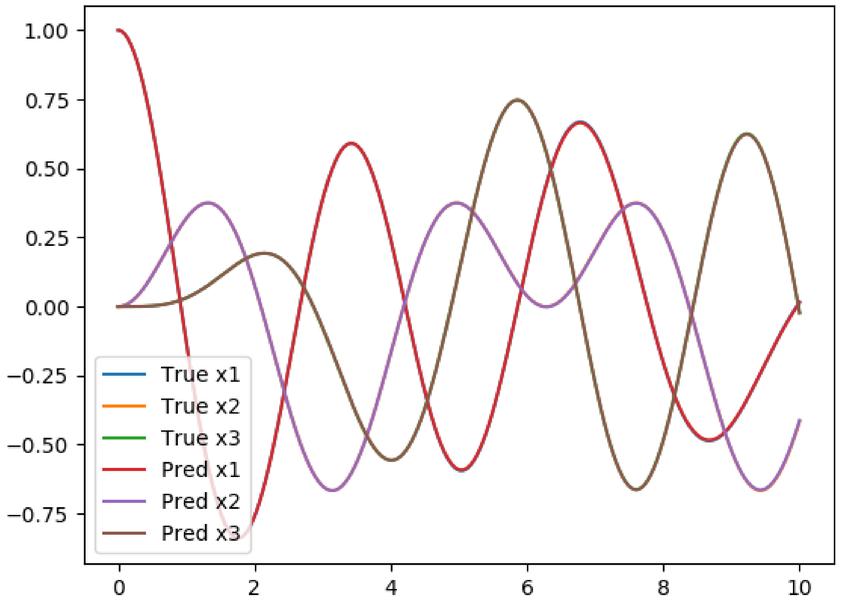
```python
@modulus.main(config_path="conf", config_name="config")
def run(cfg: ModulusConfig) -> None:
    # make list of nodes to unroll graph on
    sm = SpringMass(k=(2, 1, 1, 2), m=(1, 1, 1))
    sm_net = instantiate_arch(
        input_keys=[Key("t")],
        output_keys=[Key("x1"), Key("x2"), Key("x3")],
        cfg=cfg.arch.fully_connected,
    )
    nodes = sm.make_nodes() + [
        sm_net.make_node(name="spring_mass_network", jit=cfg.jit)
    ]
```

Nodes for a simple transient problem using **continuous time approach**

```python
    # add constraints to solver
    # make geometry
    geo = Point1D(0)
    t_max = 10.0
    t_symbol = Symbol("t")
    x = Symbol("x")
    time_range = {t_symbol: (0, t_max)}

    # make domain
    domain = Domain()

    # initial conditions
    IC = PointwiseBoundaryConstraint(
        nodes=nodes,
        geometry=geo,
        outvar={"x1": 1.0, "x2": 0, "x3": 0, "x1__t": 0, "x2__t": 0, "x3__t": 0},
        batch_size=cfg.batch_size.IC,
        lambda_weighting={
            "x1": 1.0,
            "x2": 1.0,
            "x3": 1.0,
            "x1__t": 1.0,
            "x2__t": 1.0,
            "x3__t": 1.0,
        },
        parameterization=Parameterization({t_symbol: 0}),
    )
    domain.add_constraint(IC, name="IC")

    # solve over given time period
    interior = PointwiseBoundaryConstraint(
        nodes=nodes,
        geometry=geo,
        outvar={"ode_x1": 0.0, "ode_x2": 0.0, "ode_x3": 0.0},
        batch_size=cfg.batch_size.interior,
        parameterization=Parameterization(time_range),
    )
    domain.add_constraint(interior, "interior")
```

Under **continuous time approach,** time can be modeled as any other parametrized variable



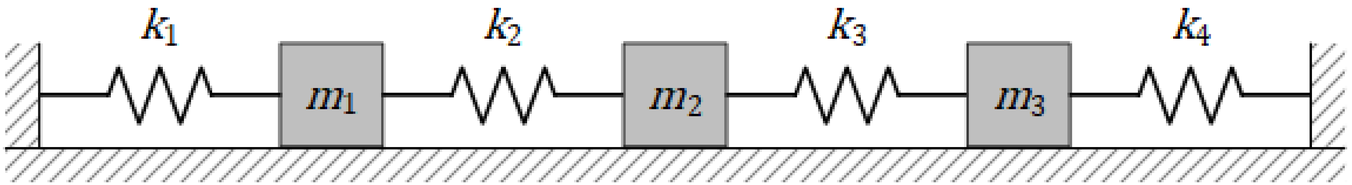


Validation error for each mass

Simple transient problem using **continuous time approach**. Advanced approaches like **moving-time-window** etc. also available for more complex problems.

Inverse Problem – Coupled Spring Mass System

Problem description



- For the same system, assume we know the analytical solution which is given by:

$$x_1(t) = \frac{1}{6}\cos(t) + \frac{1}{2}\cos\left(\sqrt{3}t\right) + \frac{1}{3}\cos(2t)\,;$$
$$x_2(t) = \frac{2}{6}\cos(t) - \frac{1}{3}\cos(2t)\;;$$
$$x_3(t) = \frac{1}{6}\cos(t) - \frac{1}{2}\cos\left(\sqrt{3}t\right) + \frac{1}{3}\cos(2t)$$

- With the above data and the values for m_2, m_3, k_1, k_2, k_3 same as before, use the neural network to find the values of m_1 and k_4

Inverse Problem – Coupled Spring Mass System

Code snippets

```python
@modulus.main(config_path="conf", config_name="config_inverse")
def run(cfg: ModulusConfig) -> None:
    # prepare data
    t_max = 10.0
    deltaT = 0.01
    t = np.arange(0, t_max, deltaT)
    t = np.expand_dims(t, axis=-1)
```

```python
    invar_numpy = {"t": t}
    outvar_numpy = {
        "x1": (1 / 6) * np.cos(t)
        + (1 / 2) * np.cos(np.sqrt(3) * t)
        + (1 / 3) * np.cos(2 * t),
        "x2": (2 / 6) * np.cos(t)
        + (0 / 2) * np.cos(np.sqrt(3) * t)
        - (1 / 3) * np.cos(2 * t),
        "x3": (1 / 6) * np.cos(t)
        - (1 / 2) * np.cos(np.sqrt(3) * t)
        + (1 / 3) * np.cos(2 * t),
    }
    outvar_numpy.update({"ode_x1": np.full_like(invar_numpy["t"], 0)})
    outvar_numpy.update({"ode_x2": np.full_like(invar_numpy["t"], 0)})
    outvar_numpy.update({"ode_x3": np.full_like(invar_numpy["t"], 0)})
```

Analytical data

```python
    # make list of nodes to unroll graph on
    sm = SpringMass(k=(2, 1, 1, "k4"), m=("m1", 1, 1))
    sm_net = instantiate_arch(
        input_keys=[Key("t")],
        output_keys=[Key("x1"), Key("x2"), Key("x3")],
        cfg=cfg.arch.fully_connected,
    )
    invert_net = instantiate_arch(
        input_keys=[Key("t")],
        output_keys=[Key("m1"), Key("k4")],
        cfg=cfg.arch.fully_connected,
    )
```

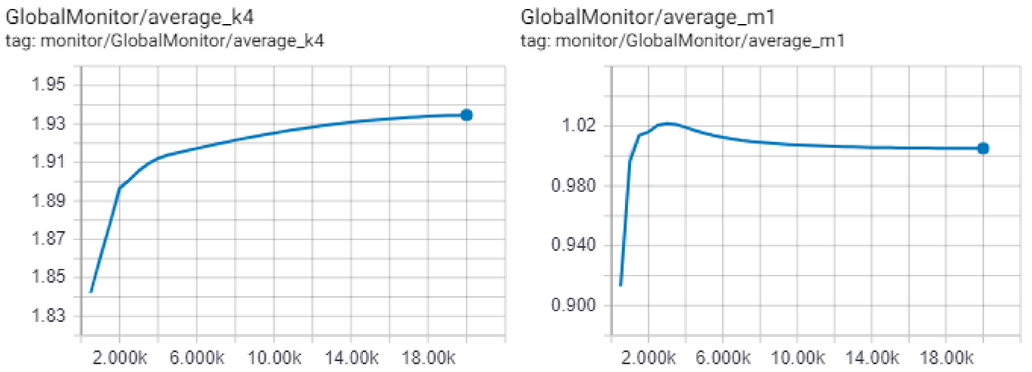
Additional network to invert out the unknowns

```python
    # data and pdes
    data = PointwiseConstraint.from_numpy(
        nodes=nodes,
        invar=invar_numpy,
        outvar=outvar_numpy,
        batch_size=cfg.batch_size.data,
    )
    domain.add_constraint(data, name="Data")
```

Assimilate the data using PointwiseConstraint

```python
    # add monitors
    monitor = PointwiseMonitor(
        invar_numpy,
        output_names=["m1"],
        metrics={"mean_m1": lambda var: torch.mean(var["m1"])},
        nodes=nodes,
    )
    domain.add_monitor(monitor)

    monitor = PointwiseMonitor(
        invar_numpy,
        output_names=["k4"],
        metrics={"mean_k4": lambda var: torch.mean(var["k4"])},
        nodes=nodes,
    )
    domain.add_monitor(monitor)
```

Monitors to infer the inverted quantities



Results

Data-driven analysis – Surrogate Model for Darcy Flow

Problem description

- Use Fourier Neural Operator (FNO) and its variants to develop a surrogate model that learns a mapping between a permeability field and pressure field, $\mathbf{K} \rightarrow \mathbf{U}$, for a distribution of permeability fields $\mathbf{K} \sim p(\mathbf{K})$.
- The Darcy PDE is a second order, elliptical PDE with the following form:

$$-\nabla \cdot \big(k(\mathbf{x}) \nabla u(\mathbf{x}) \big) = f(\mathbf{x}), \qquad \mathbf{x} \in D,$$

- Where, $u(\mathbf{x})$ is the flow pressure, $k(\mathbf{x})$ is the permeability field and $f(\cdot)$ is the forcing function.
- The Darcy flow can parameterize a variety of systems including flow through porous media, elastic materials and heat conduction.
- Here, we will define the domain as a 2D unit square $D = \{x, y \in (0,1)\}$ with the boundary condition $u(\mathbf{x}) = 0, \mathbf{x} \in \partial D$.
- Both the permeability and flow fields are discretized into a 2D matrix $\mathbf{K}, \mathbf{u} \in \mathbb{R}^{N \times N}$.

Darcy Flow – Fourier Neural Operators (FNO)

Theory

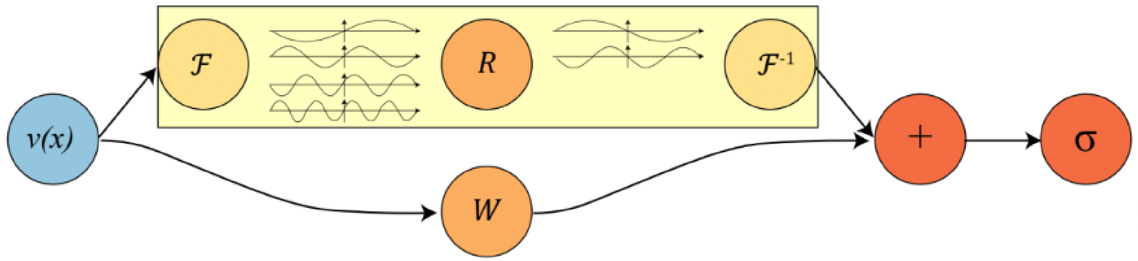
- FNO can be used to parameterize solutions for a distribution of PDE solutions. The key feature of FNO is the spectral convolutions: operations that place the integral kernel in Fourier space:

$$(K(\mathbf{w})\phi)(x) = F^{-1}(R_{\mathbf{W}} \cdot (F)\phi)(x), \qquad \forall x \in D$$

- $R_{\mathbf{w}}$ is the transformation containing the learnable parameters $\mathbf{w}$. This operator is calculated over the entire *structured Euclidean* domain D. Fast Fourier Transform (FFT) is used to perform the Fourier transforms efficiently and the resulting transformation $R_{\mathbf{w}}$ is a finite size matrix of learnable weights.
- In spectral convolution, the Fourier coefficients are truncated to only the lower modes which allows explicit control over the dimensionality of the spectral space and linear operator.
- The FNO model is a composition of a fully-connected "lifting" layer, L spectral convolutions with point-wise linear skip connections and a decoding point-wise fully-connected neural network at the end:

$$u_{net}(\Phi{:}\,\theta) = Q \circ \sigma(\boldsymbol{W}_L + \boldsymbol{K}_L) \circ \cdots \circ \sigma(\boldsymbol{W}_1 + \boldsymbol{K}_1) \circ P(\Phi), \qquad \Phi = \{\phi(x); \forall x \in D\}$$

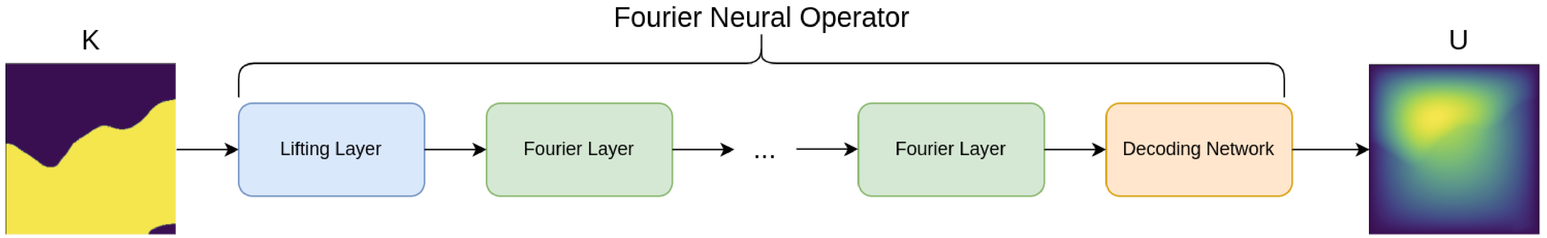
- Here, $\sigma(\boldsymbol{W}_i + \boldsymbol{K}_i)$ is the spectral convolution layer i with the point-wise linear transform $\boldsymbol{W}_i$ and activation function $\sigma(\cdot)$. P is the point-wise lifting network that projects the input into a higher dimensional latent space. *Q* is the point-wise fully-connected decoding network.
- Since all fully-connected components of FNO are point-wise operations, the model is invariant to the dimensionality of the input.



Source: Li et al., 2010.08895.pdf (arxiv.org)

Darcy Flow – Fourier Neural Operators (FNO)

Code Snippets




```python
@modulus.main(config_path="conf", config_name="config_FNO")
def run(cfg: ModulusConfig) -> None:

    # load training/ test data
    input_keys = [Key("coeff", scale=(7.48360e00, 4.49996e00))]
    output_keys = [Key("sol", scale=(5.74634e-03, 3.88433e-03))]

    download_FNO_dataset("Darcy_241", outdir="datasets/")
    train_path = to_absolute_path(
        "datasets/Darcy_241/piececonst_r241_N1024_smooth1.hdf5"
    )
    test_path = to_absolute_path(
        "datasets/Darcy_241/piececonst_r241_N1024_smooth2.hdf5"
    )

    # make datasets
    train_dataset = HDF5GridDataset(
        train_path, invar_keys=["coeff"], outvar_keys=["sol"], n_examples=1000
    )
    test_dataset = HDF5GridDataset(
        test_path, invar_keys=["coeff"], outvar_keys=["sol"], n_examples=100
    )
```

Lazy data loading (in addition to eager loading) available for large datasets

```python
    # make list of nodes to unroll graph on
    model = instantiate_arch(
        input_keys=input_keys,
        output_keys=output_keys,
        cfg=cfg.arch.fno,
    )
    nodes = model.make_nodes(name="FNO", jit=cfg.jit)
```

Instantiate the FNO model. Network parameters handled in configs.

```yaml
defaults :
  - modulus_default
  - arch:
      - fno
  - scheduler: tf_exponential_lr
  - optimizer: adam
  - loss: sum
  - _self_

jit: false

arch:
  fno:
    dimension: 2
    nr_fno_layers: 4
    fno_layer_size: 32
    fno_modes: 12
    padding: 9
    output_fc_layer_sizes:
      - 128

scheduler:
  decay_rate: 0.95
  decay_steps: 1000

training:
  rec_results_freq : 1000
  max_steps : 10000

batch_size:
  grid: 32
  validation: 32
```

Hydra configs for the Darcy FNO problem

Darcy Flow – Fourier Neural Operators (FNO)

Code Snippets

```python
# make domain
domain = Domain()

# add constraints to domain
supervised = SupervisedGridConstraint(
    nodes=nodes,
    dataset=train_dataset,
    batch_size=cfg.batch_size.grid,
    num_workers=4,  # number of parallel data loaders
)
domain.add_constraint(supervised, "supervised")
```

Supervised grid constraints

```python
# add validator
val = GridValidator(
    nodes,
    dataset=test_dataset,
    batch_size=cfg.batch_size.validation,
    plotter=GridValidatorPlotter(n_examples=5),
)
domain.add_validator(val, "test")
```

Grid Validators

```python
# make solver
slv = Solver(cfg, domain)

# start solver
slv.solve()
```

- Note
  - The constraint will constraint will construct the data loader
  - Modulus constraints can instantly be scaled to multi-node/multi-GPU training
  - Optimizations such as torch script/CUDA graphs will be performed under-the-hood.
  - Batch size is controlled in the Hydra configuration file.
- These are the two core components of setting up basic data-driven problem in Modulus

Darcy Flow – Fourier Neural Operators (FNO)

Results and discussion

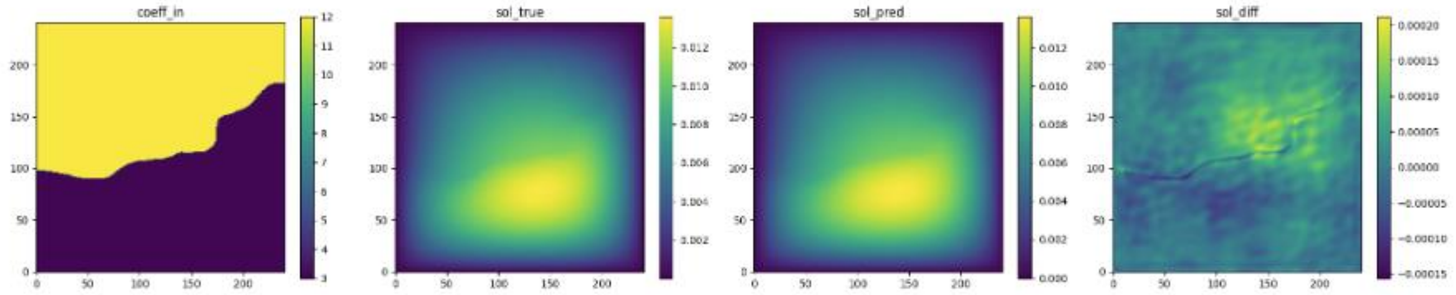


Fig. 61 *FNO validation prediction 1. (Left to right) Input permeability, true pressure, predicted pressure, error.*

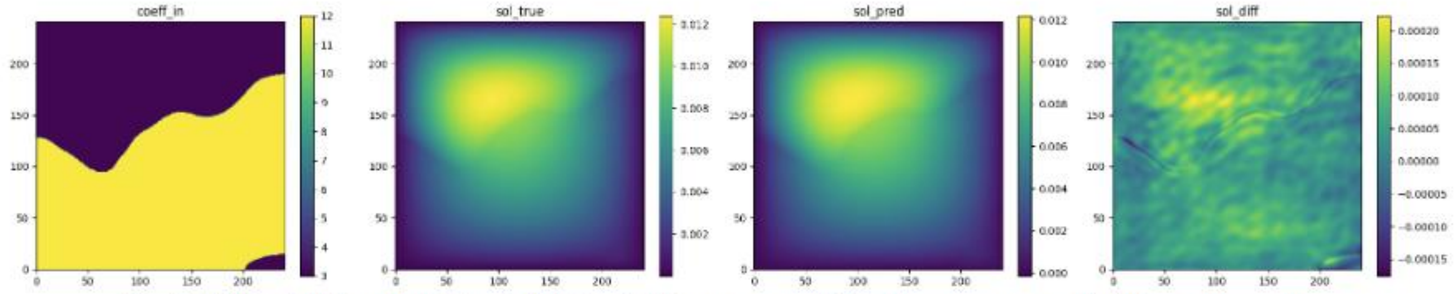


Fig. 62 *FNO validation prediction 2. (Left to right) Input permeability, true pressure, predicted pressure, error.*

FNO accurately learns the solution of this system.

Modulus supports the visualization of results through images (matplotlib), Tensorboard, VTK files and Omniverse for select problems.

For more information, please refer to the official Modulus user guide example.

Darcy Flow – Adaptive Fourier Neural Operators (AFNO)

Theory

- AFNO combines the Fourier Neural Operator (FNO) with the powerful Vision Transformer (ViT) model for image processing. The ViT and related variants of transformer models have achieved SOTA performance in image processing tasks. The multi-head self-attention (MHSA) mechanism of the ViT is key to its impressive performance.
- The first step in the architecture involves dividing the input image into a regular grid with $h \times w$ equal sized patches of size $p \times p$. The parameter p is referred to as the patch size. For simplicity, we consider a single channel image. Each patch is embedded into a token of size d, the embedding dimension. The patch embedding operation results in a token tensor $(X_{h \times w \times d})$ of size $h \times w \times d$. The patch size and embedding dimension are user selected parameters. A smaller patch size allows the model to capture fine scale details better while increasing the computational cost of training the model. A higher embedding dimension also increases the parameter count of the model. The token tensor is then processed by multiple layers of the transformer architecture performing spatial and channel mixing. The AFNO architecture implements the following operations in each layer.
- The token tensor is first transformed to the Fourier domain with

$$Z_{m,n} = [\mathrm{DFT}(X)]_{m,n}$$

- Here, m, n is the index the patch location and DFT denotes a 2D discrete Fourier transform.

Darcy Flow – Adaptive Fourier Neural Operators (AFNO)

Code Snippets

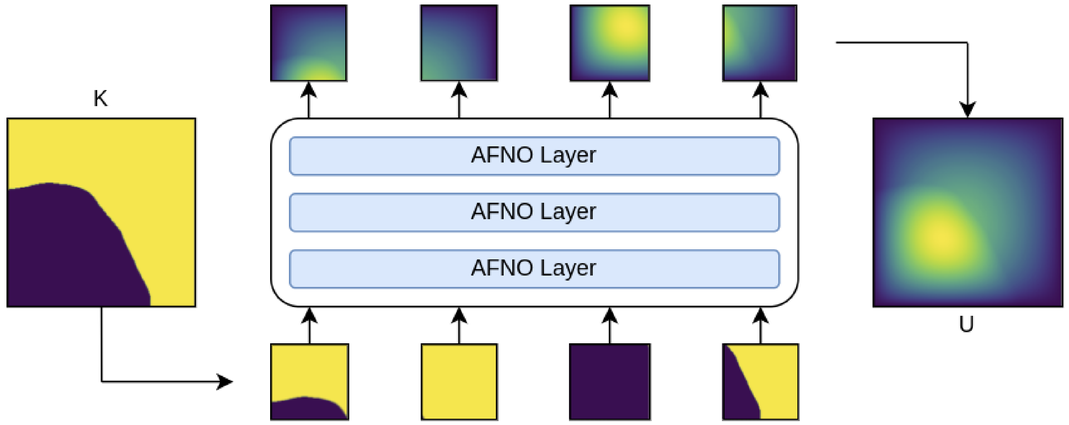
```python
@modulus.main(config_path="conf", config_name="config_AFNO")
def run(cfg: ModulusConfig) -> None:
```

```python
    # load training/ test data
    input_keys = [Key("coeff", scale=(7.48360e00, 4.49996e00))]
    output_keys = [Key("sol", scale=(5.74634e-03, 3.88433e-03))]

    download_FNO_dataset("Darcy_241", outdir="datasets/")
    invar_train, outvar_train = load_FNO_dataset(
        "datasets/Darcy_241/piececonst_r241_N1024_smooth1.hdf5",
        [k.name for k in input_keys],
        [k.name for k in output_keys],
        n_examples=1000,
    )
    invar_test, outvar_test = load_FNO_dataset(
        "datasets/Darcy_241/piececonst_r241_N1024_smooth2.hdf5",
        [k.name for k in input_keys],
        [k.name for k in output_keys],
        n_examples=100,
    )

    # get training image shape
    img_shape = [
        next(iter(invar_train.values())).shape[-2],
        next(iter(invar_train.values())).shape[-1],
    ]
```

Lazy loading like FNO example

```python
    # crop out some pixels so that img_shape is divisible by patch_size of AFNO
    img_shape = [s - s % cfg.arch.afno.patch_size for s in img_shape]
    print(f"cropped img_shape: {img_shape}")
    for d in (invar_train, outvar_train, invar_test, outvar_test):
        for k in d:
            d[k] = d[k][:, :, : img_shape[0], : img_shape[1]]
            print(f"{k}: {d[k].shape}")
```

Crop the data to make divisible by patch size




```python
    # make domain
    domain = Domain()

    # add constraints to domain
    supervised = SupervisedGridConstraint(
        nodes=nodes,
        dataset=train_dataset,
        batch_size=cfg.batch_size.grid,
        num_workers=4,  # number of parallel data loaders
    )
    domain.add_constraint(supervised, "supervised")

    # add validator
    val = GridValidator(
        nodes,
        dataset=test_dataset,
        batch_size=cfg.batch_size.validation,
        plotter=GridValidatorPlotter(n_examples=5),
    )
    domain.add_validator(val, "test")
```

Constraints and Validators same as FNO example.
Without any changes to the core constraint/validator, experiment with different architectures with ease

Darcy Flow – Adaptive Fourier Neural Operators (AFNO)

Results and discussion

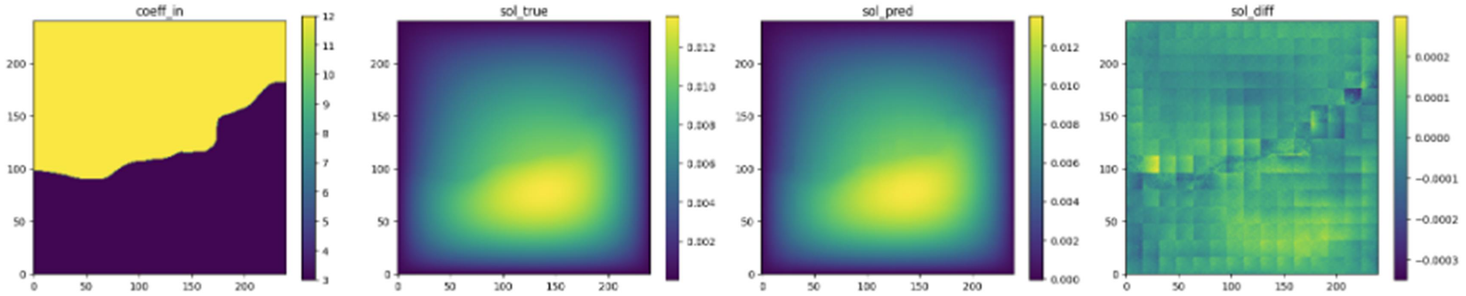


Fig. 65 AFNO validation prediction 1. (Left to right) Input permeability, true pressure, predicted pressure, error.

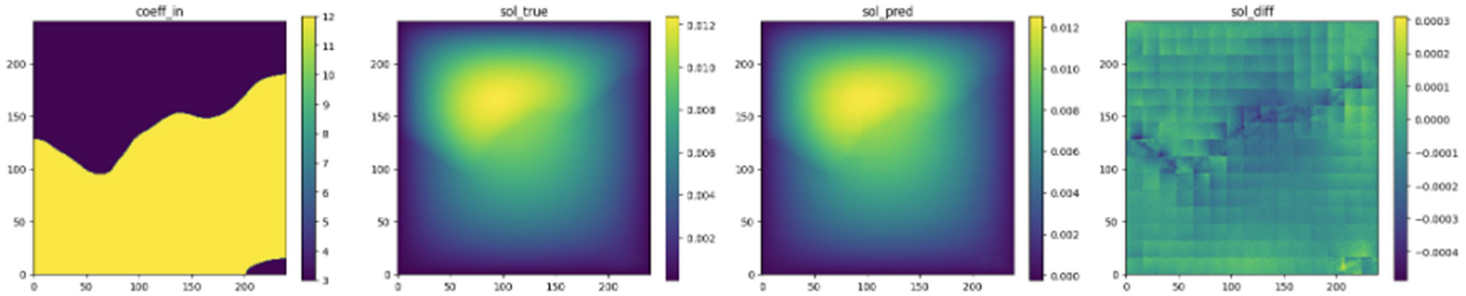
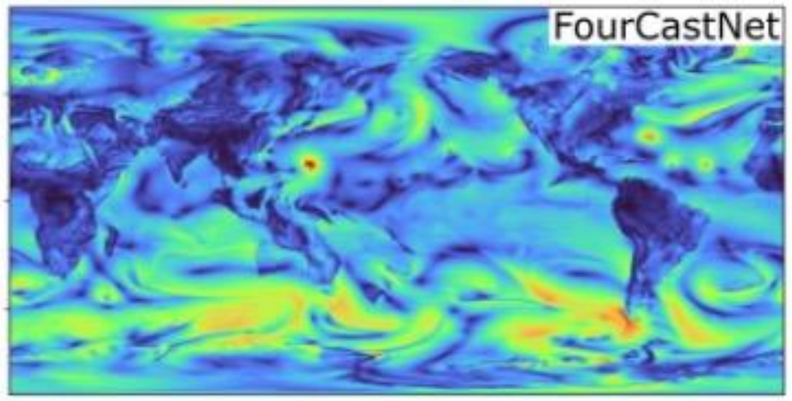


Fig. 66 AFNO validation prediction 2. (Left to right) Input permeability, true pressure, predicted pressure, error.

AFNO accurately learns the solution of this system.

For more information, please refer to the official Modulus user guide example.

AFNO is the key backboard for NVIDIA's groundbreaking FourCastNet:



Darcy Flow – Physics Informed Neural Operators (PINO)

Theory

- PINO incorporates a PDE loss to the Fourier Neural Operator. This improves interpretability and reduces the amount of data required to train a surrogate model, since the PDE loss constrains the solution space.
- In general, the PDE loss involves computing the PDE operator which in turn involves computing the partial derivatives of the Fourier Neural Operator ansatz, which is nontrivial. The key set of innovations in the PINO are the various ways to compute the partial derivatives of the operator ansatz. The PINO framework implements the differentiation in three different ways.
  - Numerical differentiation using a finite difference Method (FDM).
  - Numerical differentiation computed via spectral derivative.
  - Hybrid differentiation based on a combination of first-order “exact” and second-order FDM derivatives.

Darcy Flow – Physics Informed Neural Operators (PINO)

Code snippets

- Setting up a PINO problem in Modulus requires setting up a custom PDE loss that can compute on grid data. Readers are referred to the supplemental Jupyter notebooks for the code snippets for the Loss definition.

```python
@modulus.main(config_path="conf", config_name="config_PINO")
def run(cfg: ModulusConfig) -> None:

    # load training/ test data
    input_keys = [
        Key("coeff", scale=(7.48360e00, 4.49996e00)),
        Key("Kcoeff_x"),
        Key("Kcoeff_y"),
    ]
    output_keys = [
        Key("sol", scale=(5.74634e-03, 3.88433e-03)),
    ]
```

Load additional gradients for the loss calculation

```python
    download_FNO_dataset("Darcy_241", outdir="datasets/")
    invar_train, outvar_train = load_FNO_dataset(
        "datasets/Darcy_241/piececonst_r241_N1024_smooth1.hdf5",
        [k.name for k in input_keys],
        [k.name for k in output_keys],
        n_examples=cfg.custom.ntrain,
    )
    invar_test, outvar_test = load_FNO_dataset(
        "datasets/Darcy_241/piececonst_r241_N1024_smooth2.hdf5",
        [k.name for k in input_keys],
        [k.name for k in output_keys],
        n_examples=cfg.custom.ntest,
    )

    # add additional constraining values for darcy variable
    outvar_train["darcy"] = np.zeros_like(outvar_train["sol"])
```

Loss for physics constraint

```python
    train_dataset = DictGridDataset(invar_train, outvar_train)
    test_dataset = DictGridDataset(invar_test, outvar_test)

    # Define FNO model
    if cfg.custom.gradient_method == "hybrid":
        output_keys += [
            Key("sol", derivatives=[Key("x")]),
            Key("sol", derivatives=[Key("y")]),
        ]
    model = instantiate_arch(
        input_keys=[input_keys[0]],
        output_keys=output_keys,
        cfg=cfg.arch.fno,
        domain_length=[1.0, 1.0],
    )

    # Make custom Darcy residual node for PINO
    inputs = [
        "sol",
        "coeff",
        "Kcoeff_x",
        "Kcoeff_y",
    ]
    if cfg.custom.gradient_method == "hybrid":
        inputs += [
            "sol__x",
            "sol__y",
        ]
    darcy_node = Node(
        inputs=inputs,
        outputs=["darcy"],
        evaluate=Darcy(gradient_method=cfg.custom.gradient_method),
        name="Darcy Node",
    )
    nodes = model.make_nodes(name="FNO", jit=False) + [darcy_node]
```

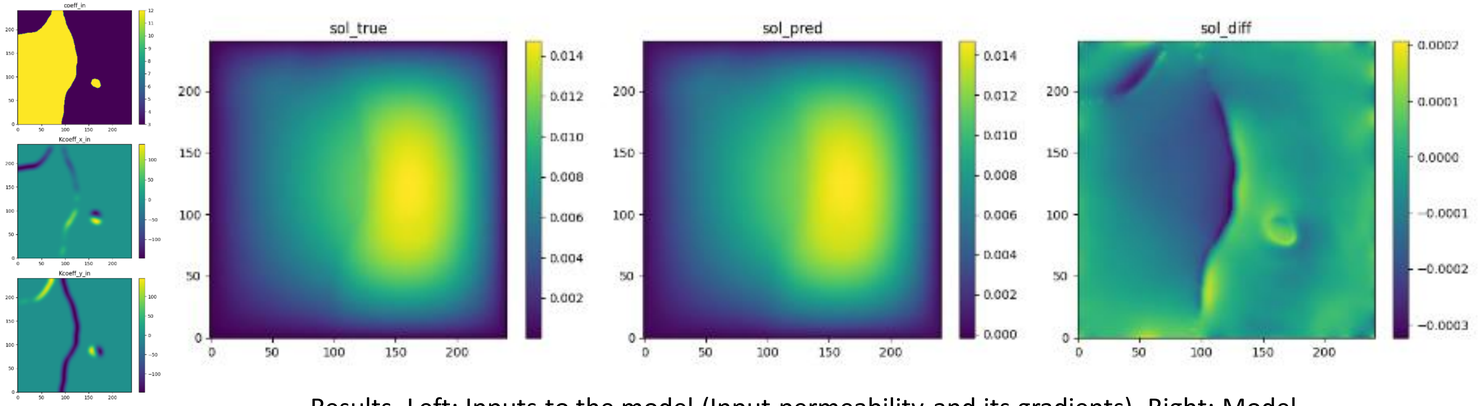
Additional nodes for physics loss

Darcy Flow – Physics Informed Neural Operators (PINO)

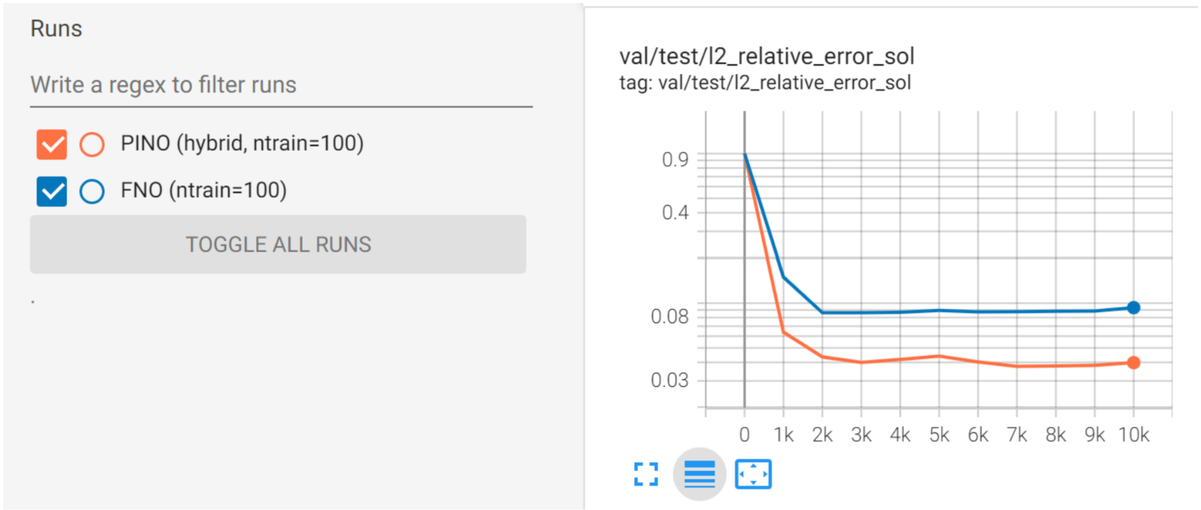
Code snippets and results and discussion

```python
# make domain
domain = Domain()

# add constraints to domain
supervised = SupervisedGridConstraint(
    nodes=nodes,
    dataset=train_dataset,
    batch_size=cfg.batch_size.grid,
)
domain.add_constraint(supervised, "supervised")

# add validator
val = GridValidator(
    nodes,
    dataset=test_dataset,
    batch_size=cfg.batch_size.validation,
    plotter=GridValidatorPlotter(n_examples=5),
    requires_grad=True,
)
domain.add_validator(val, "test")

# make solver
slv = Solver(cfg, domain)

# start solver
slv.solve()
```

Constraints and Validators same as FNO example.
Without any changes to the core constraint/validator, experiment with different architectures with ease



Results. Left: Inputs to the model (Input permeability and its gradients), Right: Model prediction and its comparison with true solution



Benefit of PINO is seen in “small data” regimes where the PDE loss regularizes the model giving better prediction than FNO when trained with only 100 samples.

Neural Operators in Modulus

Conclusions

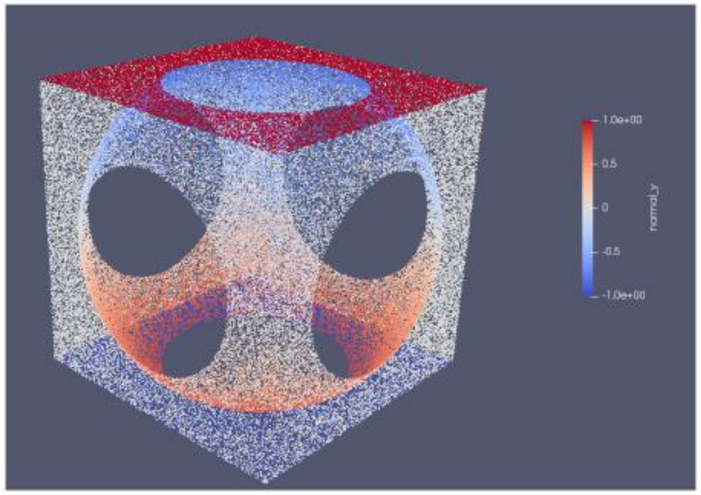
- Modulus supports several neural operators (also includes the famous DeepONets) that can easily be used out of the box.
- Modulus uses Hydra configuration for easily adjusting hyperparameters and even changing model architectures with minimal changes to Python code.
- Data-driven training can quickly be integrated into the Modulus framework.
- For more information on supported models and examples please see the Modulus documentation.

Modulus Features

Constructive Solid Geometry Module – Fully parameterizable with SymPy and allows Boolean ops

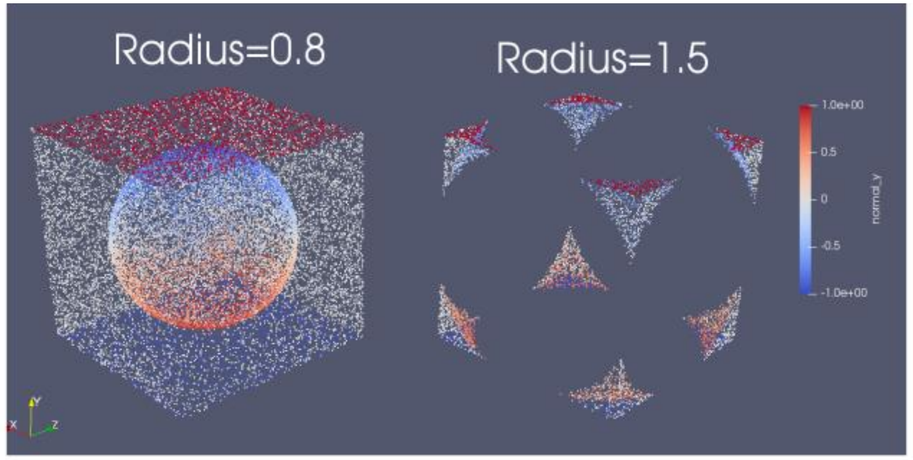
- Allows to create complex geometries using a variety of primitives (torus, cones, ellipse, etc.)
- Supports functions like translate, rotate, scale, repeat, etc.

```python
from modulus.geometry.csg.csg_3d import Sphere, Box
from modulus.plot_utils.vtk import var_to_polyvtk

# define geometry
t = Sphere((0,0,0), 1.2)
b = Box((-1,-1,-1), (1,1,1))
geo = b - t

# sample surface
surface_points = geo.sample_boundary(4096)
var_to_polyvtk(surface_points, 'surface_points')
```

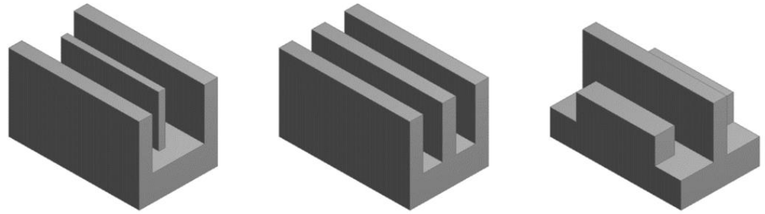


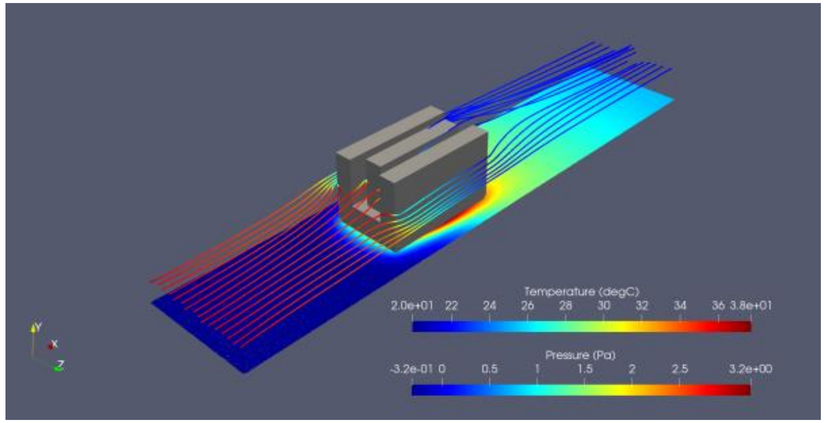
Boolean (Union, Intersection and, Subtraction) of different primitives within Modulus

```python
from modulus.geometry.csg.csg_3d import Sphere, Box
from modulus.plot_utils.vtk import var_to_polyvtk
from sympy import Symbol

# define geometry
radius = Symbol('radius')
radius_range = {radius: (1.5, 0.8)}
t = Sphere((0,0,0), radius)
b = Box((-1,-1,-1), (1,1,1))
geo = b - t

# sample surface
surface_points = geo.sample_boundary(16384, param_ranges=radius_range)
var_to_polyvtk(surface_points, 'surface_points')
```



Geometry parameterizable using SymPy



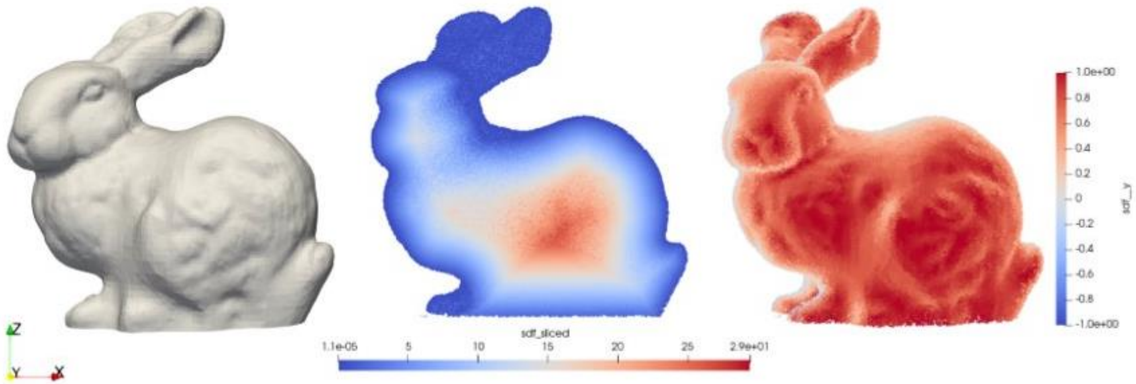


Example of a parameterized 3 Fin heatsink and solving the conjugate heat transfer problem.

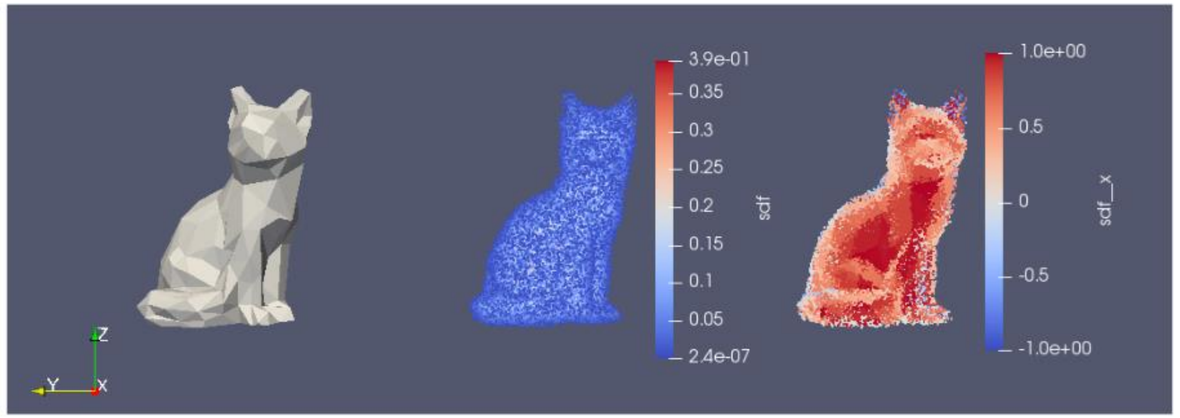
Modulus Features

PySDF library: Tessellated Geometry Module, OptiX for sampling and SDF

- Allows to import complex tessellated geometries.
- Uses ray tracing to compute SDF and its derivatives. Also computes surface normals.
- Once the geometry is imported, creates a point cloud for training.




```python
from modulus.geometry.tessellation.tessellation import Tessellation
from modulus.plot_utils.vtk import var_to_polyvtk

# read stl
geo = Tessellation.from_stl("fox.stl", airtight=True)

# sample points in interior
interior_points = geo.sample_interior(40000, compute_distance_field=True)
var_to_polyvtk(interior_points, 'interior_points')
```



NVIDIA

Modulus Features and Advancements

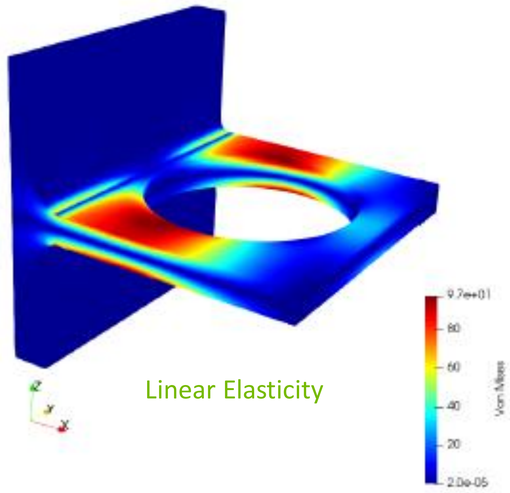
Physics types and solution of differential equations

Physics types:

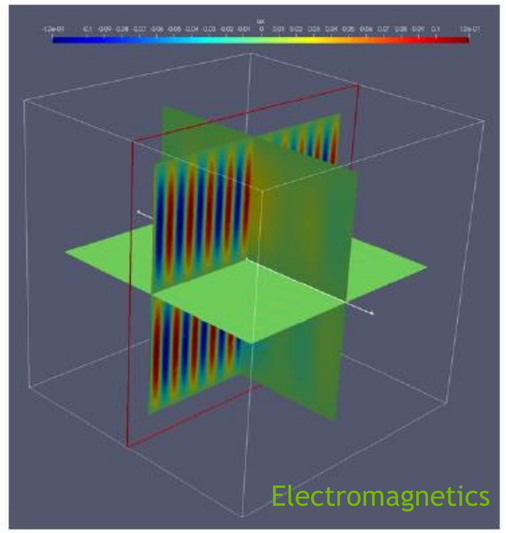
- Linear Elasticity (plane stress, plane strain and 3D)
- Fluid Mechanics
- Heat Transfer
- Coupled Fluid-Thermal
- Electromagnetics
- Wave propagation
- Examples of 2-eqn. turbulence (on fully developed channel case)

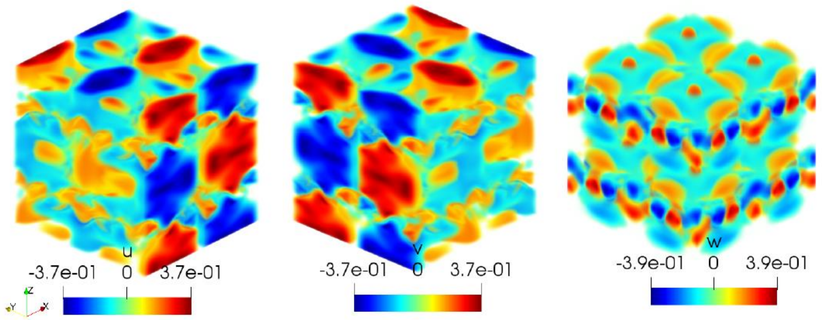
Solution of differential equations:

- Ordinary Differential Equations
- Differential (strong) Form
- Integral (weak) form of the PDEs

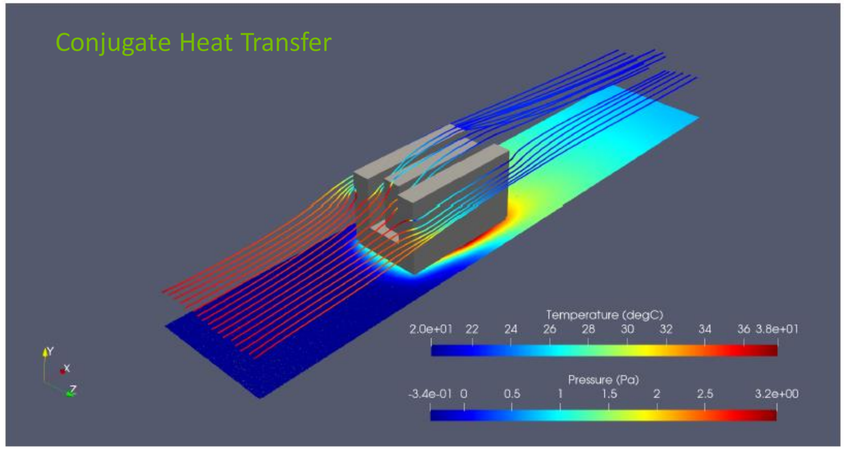


Linear Elasticity

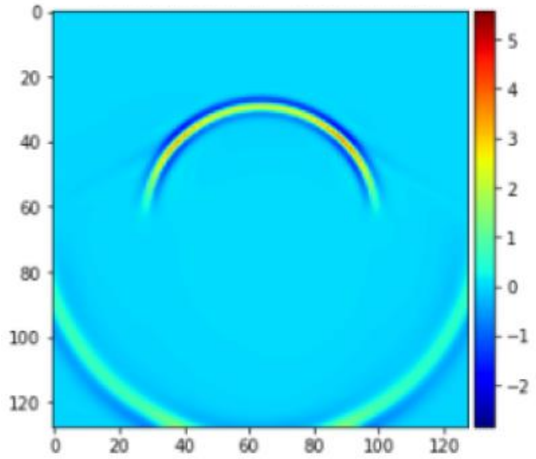




Taylor-Green vortex decay



Modulus t=600ms



Wave Propagation

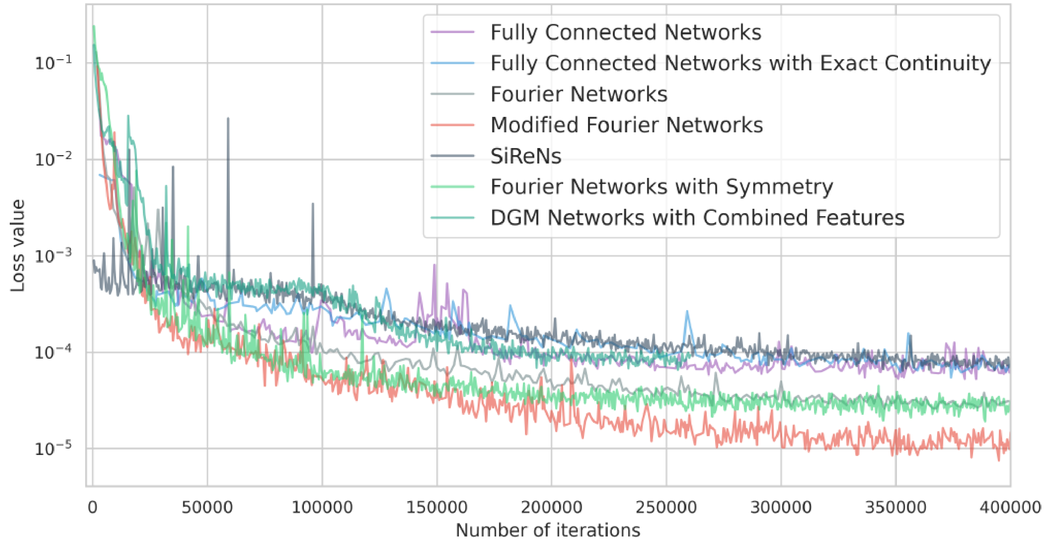
NVIDIA.

Modulus Features and Advancements

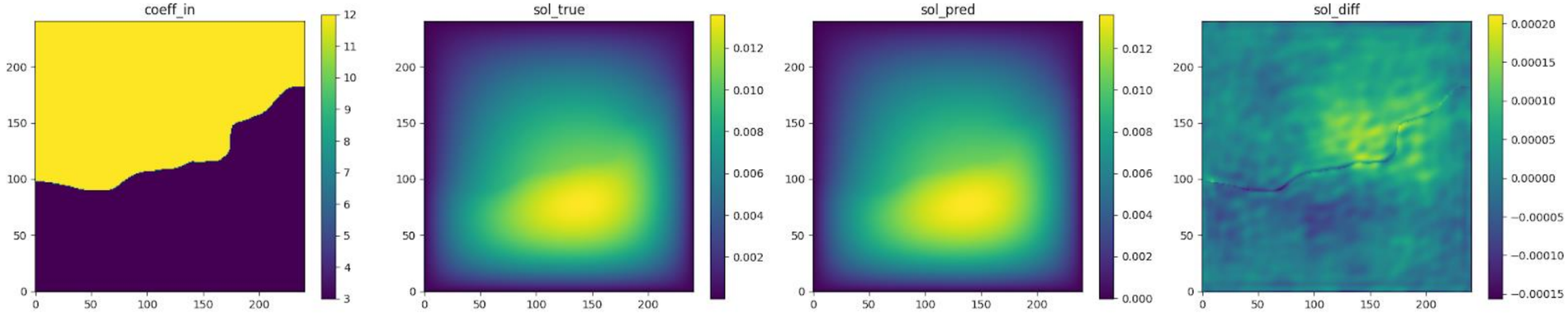
Network Architectures

Several neural network architectures:

- Fully connected Network
- Fourier Feature Network
- Sinusoidal Representation Network (SiReN)
- Modified Fourier Network
- Deep Galerkin Method Network
- Modified Highway Network
- Multiplicative Filter Networks
- Operators:
  - Fourier Neural Operator (FNO)
  - Adaptive Fourier Neural Operator (AFNO)
  - Physics Informed Fourier Neural Operator (PINO)
  - DeepONet



Comparisons of various networks in Modulus applied to solve the flow over a heatsink



Darcy Flow problem using FNO in Modulus

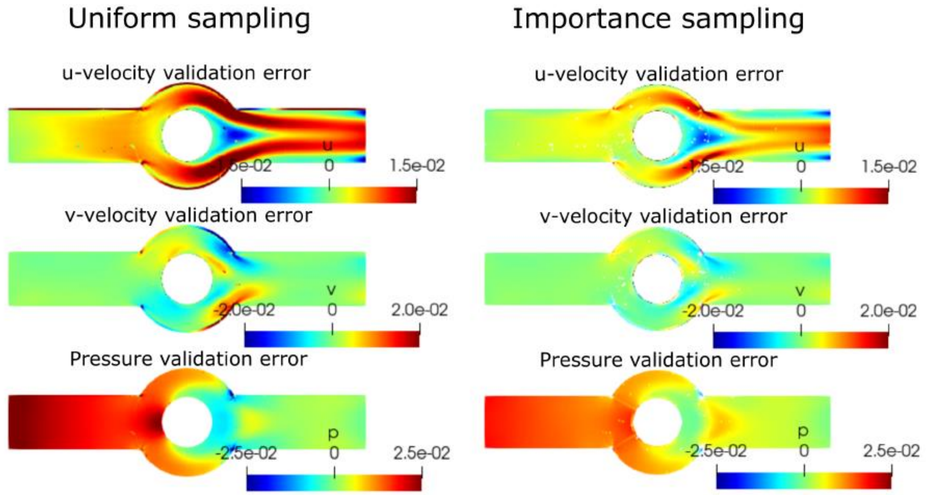
Modulus Features and Advancements

Other advanced training features

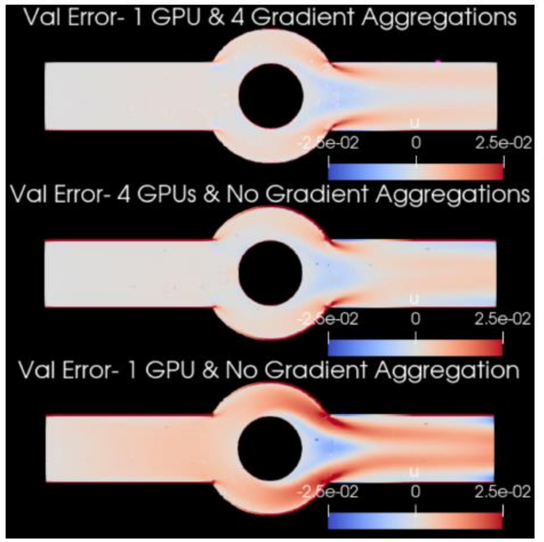
Other Features include:

- Support for new optimizers
  - AdaHessian and up to 30+ optimizers (from PyTorch's torch_optimizer library)
- New algorithms for loss balancing
  - GradNorm, ReLoBRaLo, Soft Adapt, NTK, etc.
- Sobolev (gradient-enhanced) training
- Exact boundary condition imposition
- Global and local learning rate annealing
- Global adaptive activation functions
- Halton sequences for low-discrepancy point cloud creation
- Gradient Accumulation
- Time-stepping schemes for transient problems
- Temporal loss weighting and time marching for the continuous time approach
- Importance sampling
- Homoscedastic task uncertainty quantification for loss weighting
- Hydra Configs for easy hyper-parameter tuning

Importance sampling



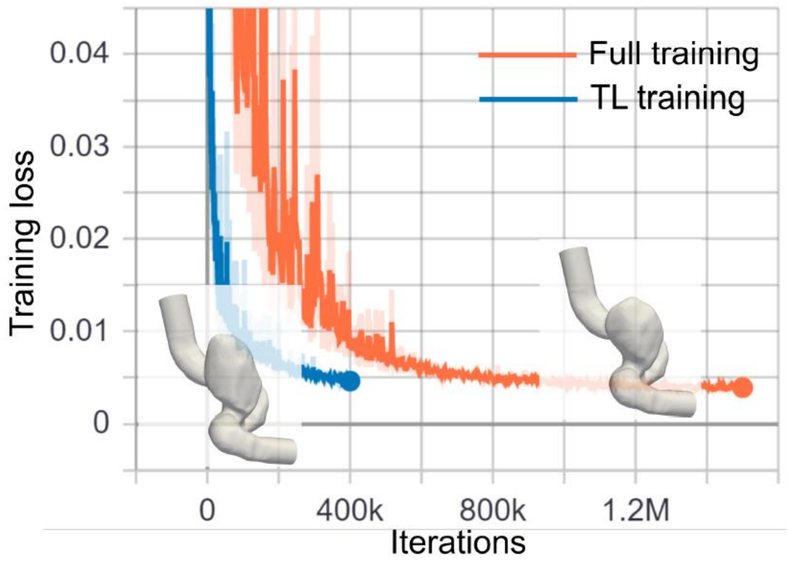
Handling larger batch sizes using Multi-GPU and/or Gradient Aggregation



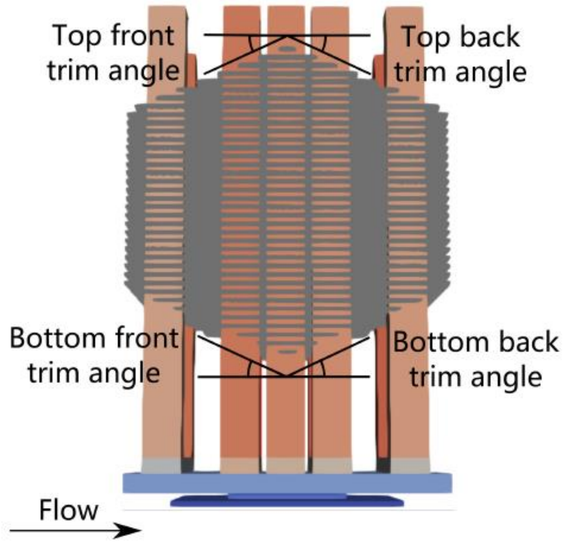
Modulus Features and Advancements

Other advanced training features

- APIs to automatically generate point clouds from Boolean compositions of geometry primitives or import point cloud for complex geometry (e.g., STL files)
- Parameterized system representation that solves several configurations concurrently for analytical geometry using Modulus CSG module
- Transfer learning for efficient surrogate-based parameterization of STL and constructive solid geometries



STL geometry and Transfer Learning

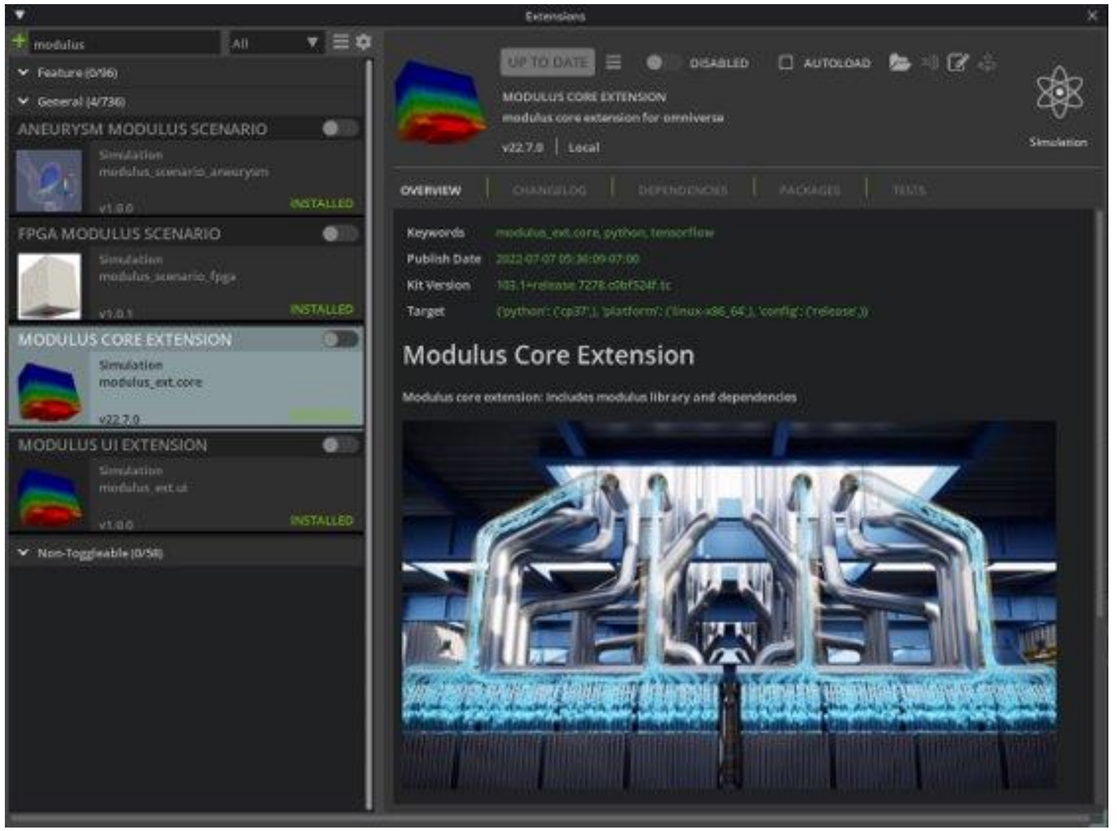


Geometry parameterization using Modulus' CSG module

Omniverse Extension for Modulus

- NVIDIA Omniverse™ is an easily extensible platform for 3D design collaboration and scalable multi-GPU, real-time, true-to-reality simulation. Omniverse revolutionizes the way we create and develop as individuals and work together as teams, bringing more creative possibilities and efficiency to 3D creators, developers and enterprises.

- Omniverse extension for Modulus enables real-time virtual-world simulation and full-design fidelity visualization. The built-in pipeline can be used for common visualizations such as streamlines and iso-surfaces for the outputs of the Modulus model. Another key feature is being able to visualize and analyze the high-fidelity simulation output in near real time as the design parameters are varied.



Modulus Resources

- Download Now: https://developer.nvidia.com/modulus-downloads
- Webpage: https://developer.nvidia.com/modulus
- Documentation: https://sw-docs-dgx-station.nvidia.com/deeplearning/modulus/index.html
- Developer Forum: https://forums.developer.nvidia.com/c/physics-simulation
- Demos:
  - Accelerating Extreme Weather Prediction with FourCastNet
  - Siemens Energy HRSG Digital Twin Simulation Using NVIDIA Modulus and Omniverse
  - Accelerating Scientific & Engineering Simulation Workflows with AI
  - Flow Physics Quantification in an Aneurysm Using NVIDIA Modulus
- Blogs:
  - AI and Machine Learning in Physics
  - Using NVIDIA Modulus and Omniverse Wind Farm Digital Twin for Siemens Gamesa (using NVIDIA Modulus and Omniverse)
  - Siemens Energy Taps NVIDIA to Develop Industrial Digital Twin of Power Plant in Omniverse and Modulus
  - Using Hybrid Physics-Informed Neural Networks for Digital Twins in Prognosis and Health Management
  - Using Physics-Informed Deep Learning for Transport in Porous Media

Modulus Resources

- Papers:
  - NVIDIA SimNet™: An AI-Accelerated Multi-Physics Simulation Framework
  - Physics-Informed Machine Learning and Uncertainty Quantification for Mechanics of Heterogeneous Materials
  - Physics Informed RNN-DCT Networks for Time-Dependent Partial Differential Equations
- Talks:
  - A Novel Framework for Physics based Machine Learning in Science & Engineering Domains
  - Accelerate HPC Simulations at Scale with Physics-informed Neural Networks and NVIDIA GPUs on AWS
  - Toward Developing High Reynolds Number, Compressible, Reacting Flows in Modulus
  - Physics-informed Neural Networks for Wave Propagation Using NVIDIA Modulus
  - Uncertainty Quantification for Transport in Porous Media Using Parameterized Physics Informed Neural Networks
  - Using Physics-Informed Neural Networks and Modulus to Accelerate Product Development
  - Physics-Informed Neural Networks for Mechanics of Heterogenous Media
  - Hybrid Physics-Informed Neural Networks for Digital Twin in Prognosis and Health Management
  - Physics-Informed Neural Network for Flow and Transport in Porous Media
  - AI-Accelerated Computational Science and Engineering Using Physics-Based Neural Networks
  - Cumulative Damage Models, Hybrid-Physics-Informed Neural Networks, and Digital TwinsWWCumulative Damage Models, Hybrid-Physics-Informed Neural Networks, and Digital Twins
  - NVIDIA Modulus - Accelerating Scientific & Engineering Simulation workflows with AI
- Podcast:
  - AI Physics Simulation Toolkit SimNet & PINNs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