Physics-informed machine learning – Hype or new trend in computational engineering?

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6th Short Course & Forum on Computational Fluid Dynamics in Rotary Positive Displacement Machines

City, University of London, 10-09-2023



ChatGPT

Can you explain to me the working principle of a twin screw compressor?

ChatGPT

Can you explain to me the working principle of a twin screw compressor?

Certainly! A twin-screw compressor is a type of positive displacement compressor used to compress gases, most commonly air and refrigerant gases. It's called "twin-screw" because it consists of two interlocking helical rotors, usually referred to as the male rotor and the female rotor, that rotate in opposite directions within a tightly fitted casing. The working principle of a twin-screw compressor can be broken down into several key steps:

- 1. **Intake**: The process begins with the rotation of the male and female rotors. As they turn, their helical lobes create expanding cavities between them and the compressor casing. This causes gas to be drawn into the compressor through the inlet port.
- 2. **Compression**: As the rotors continue to rotate, the interlocking lobes of the rotors reduce the volume of the cavities. This reduction in volume compresses the gas trapped in the cavities. The compression process occurs continuously as the gas is carried from the intake side towards the discharge side of the compressor.
- 3. Intermeshing: ...
- 4. Compression Ratio: ...
- 5. Discharge: ...
- 6. Oil Injection: ...
- 7. Cooling and Control: ...

The design of a twin-screw compressor allows for continuous and relatively pulsation-free compression, making it well-suited for applications where a steady flow of compressed gas is required. Its efficiency, reliability, and ability to handle a wide range of operating conditions make it a popular choice in various industries.

Stable Diffusion (text-to-image generator)





"A sunny summer day in London"



Stable Diffusion (text-to-image generator)





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"A twin screw compressor"



Stable Diffusion (text-to-image generator)





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"A twin screw compressor"



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Terminology Deep learning 101

2 Physics-informed machine learning

Physics-informed neural networks Deep Operator neural networks

3 IgANets

Concept and preliminary applications





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Concept and preliminary applications



- Artificial Intelligence (AI)
- Machine Learning (ML)
- Deep Learning (DL)
- Scientific Machine Learning (SciML)



So what is what? And what is physics-informed machine learning?





- statistical modelling often w/o using process-knowledge
- empirical discovery of new knowledge from (big) data
- Examples:
 - linear regression
 - PCA/SVD, POD
 - reduced-order models
 - self-driving cars
 - large language models (ChatGPT, Bard, Co-pilot)
 - text-to-image generators (Stable Diffusion)



- "effort to automate intellectual tasks normally performed by humans" – François Chollet, creator of Keras
- Example: rule/label-based automatic packing machine





- "field of study that gives computers the ability to learn without being explicitly programmed" – Arthur Samuel, ML pioneer
- Example: classification-based waste sorting machine





- next-level ML based on deep artificial neural networks
- Example: self-driving cars





- mathematical formulas based on **physics laws**
- derived from observational studies and experiments
- solved by numerical methods







In a nutshell

Scientific Machine Learning [Baker et al., 2019] is *not* the replacement of physics-based modelling by statistical modelling but the clever combination of process-knowledge (i.e. mechanistic models) with the capability of ML/DL to *'learn'* from (big) data.



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Synonyms

- Theory-guided data science [Karpatne et al., 2017]
- Physically informed neural networks [Raissi et al., 2019]
- Universal differential equations [Rackauckas et al., 2020]
- Physics-informed machine learning [Karniadakis et al., 2021a]
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Note: Other AI/ML/DL approaches are not 'bad'. We just don't consider them here.



Timeline



Figure from: *Physics-informed machine learning: A survey on problems, methods and applications* [Hao et al., 2022]



Notation

scalar variable f(x) function G(f)(x) operator $\mathbf{x} = \begin{bmatrix} x_1 & \dots & x_n \end{bmatrix}$ vector $\mathbf{A} = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} \quad \mathsf{matrix}$

x



Artificial neural network (ANN)



Output layer \mathbf{y}

Single-layer network



Output layer
$$\mathbf{y} \in \{+1(\text{'dog'}), -1(\text{'cat'})\}$$



Linear regression

$$\mathbf{A}\mathbf{X} = \mathbf{Y} \quad \rightarrow \quad \begin{bmatrix} a_1 & a_2 & \dots & a_n \end{bmatrix} \begin{bmatrix} | & | & \dots & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \dots & \mathbf{x}_s \\ | & | & \dots & | \end{bmatrix} = \begin{bmatrix} y_1 & y_1 & \dots & y_s \end{bmatrix}$$

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Common solution approaches

Pseudo-inverseLASSO regression $\mathbf{A} = \mathbf{Y}\mathbf{X}^{\dagger}$ $\mathbf{A} = \operatorname{argmin}_{\mathbf{A}'} \|\mathbf{A}'\mathbf{X} - \mathbf{Y}\|_2 + \lambda \|\mathbf{A}'\|_1$



Multi-layer network



Output layer $\mathbf{y} \in \{+1(\text{`dog'}), -1(\text{`cat'})\}$

Input layer \mathbf{x}

Beyond linear regression

$$\begin{array}{rcl} \mathbf{A}_1 \mathbf{X} &=& \mathbf{X}^{(1)} \\ \mathbf{A}_2 \mathbf{X}^{(1)} &=& \mathbf{Y} \end{array} \right\} \quad \Leftrightarrow \quad \mathbf{A}_2 \mathbf{A}_1 \mathbf{X} = \mathbf{Y} \quad \Leftrightarrow \quad \tilde{\mathbf{A}} \mathbf{X} = \mathbf{Y} \end{array}$$



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Enrichment of functional responses by nonlinear activation functions

$$\begin{cases} f_1(\mathbf{A}_1, \mathbf{X}) &= \mathbf{X}^{(1)} \\ f_2(\mathbf{A}_2, \mathbf{X}^{(1)}) &= \mathbf{Y} \end{cases} \Rightarrow f_2(\mathbf{A}_2, f_1(\mathbf{A}_1, \mathbf{X})) = \mathbf{Y}$$



Activation functions

$$\begin{array}{lll} f(x) &=& x, & \mbox{linear} \\ f(x) &=& \left\{ \begin{array}{ll} 0 & \mbox{for } x \leq 0, \\ 1 & \mbox{for } x > 0, \end{array} \right. & \mbox{binary step} \\ f(x) &=& \frac{1}{1 + \exp(-x)}, & \mbox{logistic (soft step)} \\ f(x) &=& \mbox{tanh}(x), & \mbox{tanh} \\ f(x) &=& \left\{ \begin{array}{ll} 0 & \mbox{for } x \leq 0, \\ x & \mbox{for } x > 0, \end{array} \right. & \mbox{rectified linear unit (ReLU)} \end{array}$$

Elementwise application

$$\mathbf{Y} = f(\mathbf{A}, \mathbf{X}) \quad :\Leftrightarrow \quad \mathbf{Y} = (y_{ij}), \ y_{ij} = f(\tilde{y}_{ij}) \ \forall i, j, \quad \tilde{\mathbf{Y}} = \mathbf{A}\mathbf{X}$$



Nonlinear optimization problem

$$\begin{bmatrix} \mathbf{A}_1 & \mathbf{A}_2 \end{bmatrix} = \operatorname*{argmin}_{\mathbf{A}_1', \mathbf{A}_2'} E(\mathbf{A}_1', \mathbf{A}_2')$$

In words: find network weights A_1 and A_2 that minimize the mean-square error (MSE)

$$E(\mathbf{A}_1, \mathbf{A}_2) = \frac{1}{s} \sum_{\ell=1}^{s} \left(f_2(\mathbf{A}_2, f_1(\mathbf{A}_1, \mathbf{x}^{\ell})) - \mathbf{y}^{\ell} \right)^2$$

over the set of input-output pairs $(\mathbf{x}^\ell;\mathbf{y}^\ell)$ from the training data set



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Solving nonlinear optimization problems is not new. A common approach in SciML is based on backpropagation and the stochastic gradient descent algorithm.









MSE $E=(y-\hat{y})^2$ between target output y and network output \hat{y} is minimal if

Λ

$$\frac{\partial E}{\partial a} = 0$$
$$\frac{\partial E}{\partial b} = 0$$





MSE $E = (y - \hat{y})^2$ between target output y and network output \hat{y} is minimal if

$$\frac{\partial E}{\partial a} = 2(y - \hat{y}) \left[\frac{dy}{da} - \frac{d\hat{y}}{da} \right] = 0$$

$$\land \quad \frac{\partial E}{\partial b} = 2(y - \hat{y}) \left[\frac{dy}{db} - \frac{d\hat{y}}{db} \right] = 0$$





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Iterative update of the network weights

$$a_{k+1} = a_k - \delta_k \frac{\partial E}{\partial a_k} \quad \wedge \quad b_{k+1} = b_k - \delta_k \frac{\partial E}{\partial b_k} \quad \text{with learning rate } \delta_k > 0$$

Example: z = tanh(ax) and y = bz

$$\frac{\partial E}{\partial a_k} = -2(y-\hat{y})\frac{\mathrm{d}\hat{y}}{\mathrm{d}z}\frac{\mathrm{d}z}{\mathrm{d}a_k} = -2(y-\hat{y})b_k\left[1-\tanh^2(a_kx)\right]x$$
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We are not there yet. This is for *scalar* input x and output y and for a *single* input-output pair (x; y). In practice we have multiple possibly vector-valued input-output pairs $(\mathbf{X}; \mathbf{Y})$.









Optimization problem

 $\operatorname*{argmin}_{\mathbf{A}'_j} E(\mathbf{A}'_1,\mathbf{A}'_2,\mathbf{A}'_3),$





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Stochastic gradient descent algorithm with a single randomly chosen $(\mathbf{x}^\ell;\mathbf{y}^\ell)$ pair

$$\begin{bmatrix} \mathbf{A}_1 & \mathbf{A}_2 & \mathbf{A}_3 \end{bmatrix}_{k+1} = \begin{bmatrix} \mathbf{A}_1 & \mathbf{A}_2 & \mathbf{A}_3 \end{bmatrix}_k - \delta_k \nabla \left(f_3(\mathbf{A}_3, f_2(\mathbf{A}_2, f_1(\mathbf{A}_1, \mathbf{x}^{\ell}))) - \mathbf{y}^{\ell} \right)^2$$



- Activation functions enable nonlinear network responses
- Backpropagation yields the gradient of the error w.r.t. the network weights
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$$\mathbf{y} = f(\mathbf{A}, \mathbf{b}, \mathbf{x}) = f(\mathbf{A}\mathbf{x} + \mathbf{b})$$



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• Short hand notations

$$\mathbf{W} = (\mathbf{A}_1, \dots, \mathbf{A}_L, \mathbf{b}_1, \dots, \mathbf{b}_L), \qquad \mathcal{N}(\mathbf{x}) = f_L(\mathbf{A}_L, \mathbf{b}_L, \dots, f_1(\mathbf{A}_1, \mathbf{b}_1, \mathbf{x}))$$



Introduction

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Concept and preliminary applications



Learning from	data	physics
given	$(\mathbf{x};\mathbf{y})$	$(\mathbf{x}; L(u(\mathbf{x})) = f)$
predict	$\mathbf{\hat{y}} = \mathcal{N}(\mathbf{x})$	$\hat{u} = \mathcal{N}(\mathbf{x})$
compare	$E = \ \mathbf{y} - \hat{\mathbf{y}}\ ^2$	$E = \ L(\hat{u}) - f\ ^2$
update	$\mathbf{W}_{k+1} = \mathbf{W}_k - \delta_k \nabla E$	$\mathbf{W}_{k+1} = \mathbf{W}_k - \delta_k \nabla E$



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Universal approximation theorem [Cybenko, 1989, Hornik et al., 1989]: For every continuous function $f : \mathbb{R}^n \to \mathbb{R}^m$ there exists an ANN that approximates it with given accuracy. [This does not say that it is easy to find this ANN in practice.]



Example: Poisson's equation in 1d

Compute derivatives w.r.t. to x by the same backpropagation algorithm as for the weights

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History

• Neural networks for DEs [Dissanayake and Phan-Thien, 1994, Lagaris et al., 1998]



Example: Poisson's equation in 1d

$$u_{xx}(x) = f(x) \text{ in } (0,1) \qquad \qquad E = \|\mathcal{N}_{xx}(x) - f(x)\|^2$$
$$u(x) = g(x) \text{ at } 0,1 \qquad \qquad \rightarrow \qquad \qquad + \|\mathcal{N}(x) - g(x)\|^2$$

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- Rediscovery as physics-informed neural networks [Raissi et al., 2017a,b, 2019]
- Since then applied to many problems (forward, inverse, ...), extended in various ways (distributed PINNs, adaptive PINNs, ...), and made available as easy-to-use software packages (DeepXDE, SciANN, NVIDIA Modulus, NeuroDiffEq, NeuralPDE, ...)

Examples of PINNs



Figure from: Physics-informed neural networks for high-speed flows [Mao et al., 2020]

Examples of PINNs



Figure from: *Physics-informed data based neural networks for two-dimensional turbulence* [Kag et al., 2022]



Examples of PINNs



Figure from: Physics-informed machine learning [Karniadakis et al., 2021b]



⊕ Easy to implement for 'any' physical model



 $E = MSE_{\mathsf{NSE-u}}(u \ , v \ , p \) + MSE_{\mathsf{NSE-v}}(u \ , v \ , p \) + MSE_{\mathsf{NSE-p}}(u \ , v \ , p \)$

 $+MSE_{\mathsf{BDR}}(u,v,p)$



- $\oplus\,$ Easy to implement for 'any' physical model
- ⊕ Simulation/experimental data can be included



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$$+MSE_{BDR}(u, v, p) + ||u| - u_{ref}||^2 + ||v| - v_{ref}||^2 + ||p| - p_{ref}||^2$$



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- ⊕ Simulation/experimental data can be included
- $\oplus\,$ Easy prediction of derived quantities of interest or model parameters $\theta \rightarrow$ inverse problems



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$$+ MSE_{\mathsf{BDR}}(u^{\theta}, v^{\theta}, p^{\theta}) + \|u^{\theta} - u_{\mathsf{ref}}^{\theta}\|^{2} + \|v^{\theta} - v_{\mathsf{ref}}^{\theta}\|^{2} + \|p^{\theta} - p_{\mathsf{ref}}^{\theta}\|^{2}$$



- ⊕ Easy to implement for 'any' physical model
- ⊕ Simulation/experimental data can be included
- \oplus Easy prediction of derived quantities of interest or model parameters $\theta \rightarrow$ inverse problems
- \oplus Flexibility to 'tune' network architecture to problem structure (e.g., separate $\mathcal{N}_u, \mathcal{N}_v, \mathcal{N}_p$)



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Challenge: How to feed 'designs' into the PINN framework?



Parameterized PINNs



Note: Impractical if the number of design parameters is large (curse of dimensionality)



Auto encoders



Train network so that $x \equiv y$. Then separate the encoder from the decoder and use the latter to generate designs y from the latent space variables z serving as network inputs.

Latent space parameterized PINNs



Physics-informed deep learning for computational fluid flow analysis [Kakkar, 2022]

Collaboration between TU Delft and Monolith AI Limited, UK



Latent space parameterized PINNs: NACA 4812 at 5 deg AoA









TUDelft

Latent space parameterized PINNs: NACA 4812 at 5 deg AoA













TUDelft

From function to operator learning

Function learning: learn the input-output relation of a function

 $f:x\in X\to Y$


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$$f = \sin, \quad X = \mathbb{R}, \quad Y = [-1, 1] \quad \rightarrow \quad \text{learn} \quad y = \sin(x)$$



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e.g., learn $\mathcal{N}_{sin}(0) = 0$, $\mathcal{N}_{sin}(\pi/2) = 1$, $\mathcal{N}_{sin}(\pi) = 0$, ...



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e.g., learn $\mathcal{N}_{\sin}(0) = 0, \quad \mathcal{N}_{\sin}(\pi/2) = 1, \quad \mathcal{N}_{\sin}(\pi) = 0, \quad \dots$

Operator learning¹: learn the action of an operator on a function, e.g.,

 $G: f \mapsto G(f), \quad G(f): x \in X \to Y$

¹Universal approximation theorem for operators [Chen and Chen, 1993]

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Function learning: learn the input-output relation of a function

$$f = \sin, \quad X = \mathbb{R}, \quad Y = [-1, 1] \quad \rightarrow \quad \text{learn} \quad y = \sin(x)$$

e.g., learn $\mathcal{N}_{sin}(0) = 0$, $\mathcal{N}_{sin}(\pi/2) = 1$, $\mathcal{N}_{sin}(\pi) = 0$, ...

Operator learning¹: learn the action of an operator on a function, e.g.,

$$G = \frac{\partial \cdot}{\partial x}, \quad f = \sin \quad \rightarrow \quad \text{learn} \quad y = G(f)(x) = \cos(x)$$

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e.g., learn $\mathcal{N}(\sin, 0) = 1$, $\mathcal{N}(\sin, \pi) = -1$, $\mathcal{N}(\cos, \pi/2) = -1$,...

¹Universal approximation theorem for operators [Chen and Chen, 1993]

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Deep operator networks

DeepONets: Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators [Lu et al., 2021], many follow-up papers, e.g. *Physics-informed deep operator networks* [Goswami et al., 2022]



Figure from: Improved architectures and training algorithms for deep operator networks [Wang et al., 2022]



Simplified interpretation of DeepONets

Trunk network: learns a set of basis functions $(b_i(\mathbf{x}))_i$

Branch network: learns the basis coefficients $(c_i)_i$ (relative to this basis)

Cross product: combines basis coefficients and functions to produce solution values

$$u(\mathbf{x}) = \sum_{i} c_i b_i(\mathbf{x})$$



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IgANets [Möller et al., 2021]: learn basis coefficients relative to a *fixed* B-spline basis



Introduction

Terminology Deep learning 101

Physics-informed machine learning Physics-informed neural networks Deep Operator neural networks

3 IgANets

Concept and preliminary applications



B-spline basis functions



Figure from: Geometrically nonlinear isogeometric analysis of laminated composite plates based on higher-order shear deformation theory [Tran et al., 2015]



B-spline geometry models



Figure from: *Reduced order isogeometric analysis approach for PDEs in parametrized domains* [Garotta et al., 2020]



(geometry)
$$\mathbf{x}_h(\xi,\eta) = \sum_{i=1}^n B_i(\xi,\eta) \cdot \mathbf{x}_i \quad \forall (\xi,\eta) \in [0,1]^2$$

(load vector)
$$f_h \circ \mathbf{x}_h(\xi, \eta) = \sum_{i=1}^n B_i(\xi, \eta) \cdot f_i \quad \forall (\xi, \eta) \in [0, 1]^2$$

(boundary conditions)
$$g_h \circ \mathbf{x}_h(\xi, \eta) = \sum_{i=1}^n B_i(\xi, \eta) \cdot \underline{g_i} \quad \forall (\xi, \eta) \in \partial [0, 1]^2$$

(solution)
$$u_h \circ \mathbf{x}_h(\xi, \eta) = \sum_{i=1}^n B_i(\xi, \eta) \cdot \underline{u_i} \quad \forall (\xi, \eta) \in [0, 1]^2$$



IgANet architecture





Loss function

 $\mathsf{loss} = \, \mathsf{loss}_{\mathrm{PDE}} + \mathsf{loss}_{\mathrm{BDR}}$

$$\mathsf{loss}_{\mathrm{PDE}} = \frac{1}{N_{\Omega}} \sum_{k=1}^{N_{\Omega}} \left| \Delta \left[u_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) \right] - f_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) \right|^2$$

$$\mathsf{loss}_{\mathrm{BDR}} = \frac{1}{N_{\Gamma}} \sum_{k=1}^{N_{\Gamma}} \left| u_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) - g_h \circ \mathbf{x}_h \left(\xi^{(k)}, \eta^{(k)} \right) \right|^2$$



Two-level training strategy

For
$$[\mathbf{x}_1, \dots, \mathbf{x}_n] \in \mathcal{S}_{\mathsf{geo}}$$
, $[f_1, \dots, f_n] \in \mathcal{S}_{\mathsf{rhs}}$, $[g_1, \dots, g_n] \in \mathcal{S}_{\mathsf{bcond}}$ do

For batch of Greville abscissae $(\xi_k, \eta_k) \in [0, 1]^2$ do

Train IgANet
$$\begin{pmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{bmatrix}, \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}, \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix}; (\xi_k, \eta_k)_{k=1}^{N_{\text{samples}}} \end{pmatrix} \mapsto \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}$$

EndFor

EndFor



Test case: Poisson's equation on a variable annulus

















Future application: interactive design-through-analysis



Collaboration with Scientific Visualization team at SURF NL



• FEM [Courant, 1943], FVM [Mcdonald, 1971], Neural operators for differential equations [Dissanayake and Phan-Thien, 1994] ... just give it some more time

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- PIML will not replace FEM/FVM as simulation tool but enable new analyses (inverse modelling, quick/qualitative pre-design exploration, process monitoring/steering, ...)

Call to action

• SciML is not the enemy nor a panacea. Explore its capabilities (and limitations) and combine it with today's tools where it brings added value to your workflow.



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6th Short Course & Forum on Computational Fluid Dynamics in Rotary Positive Displacement Machines

City, University of London, 10-09-2023



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