Robust and Interpretable Learning for Modern Healthcare

Peirong Liu

Harvard Medical School & Massachusetts General Hospital

Robust and Interpretable Learning for Modern Healthcare

Robust and Interpretable Learning for Modern Healthcare

Medical Imaging in Patient Care

Patient Intake & Screening

Medical Imaging in Patient Care

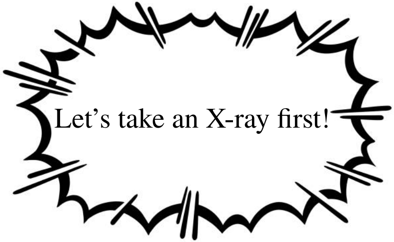
Patient Intake & Screening

Assessment & Diagnosis

Treatment Planning

Intervention & Follow-ups

Medical Imaging in Patient Care



Patient Intake & Screening

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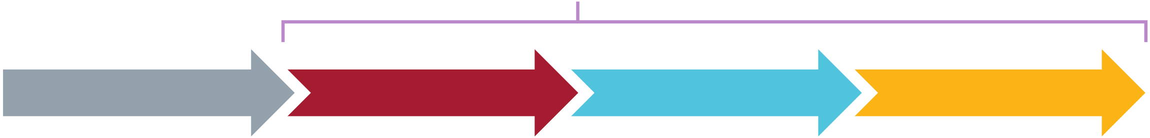
Medical Imaging in Patient Care

The Importance of Medical Imaging in Patient Care



Patient Intake & Screening

Assessment & Diagnosis

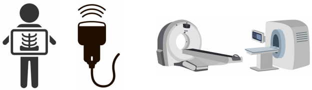
Treatment Planning

Intervention & Follow-ups

Medical Image Analysis × AI → ***AI-Powered*** Diagnosis & Treatment

Medical Imaging

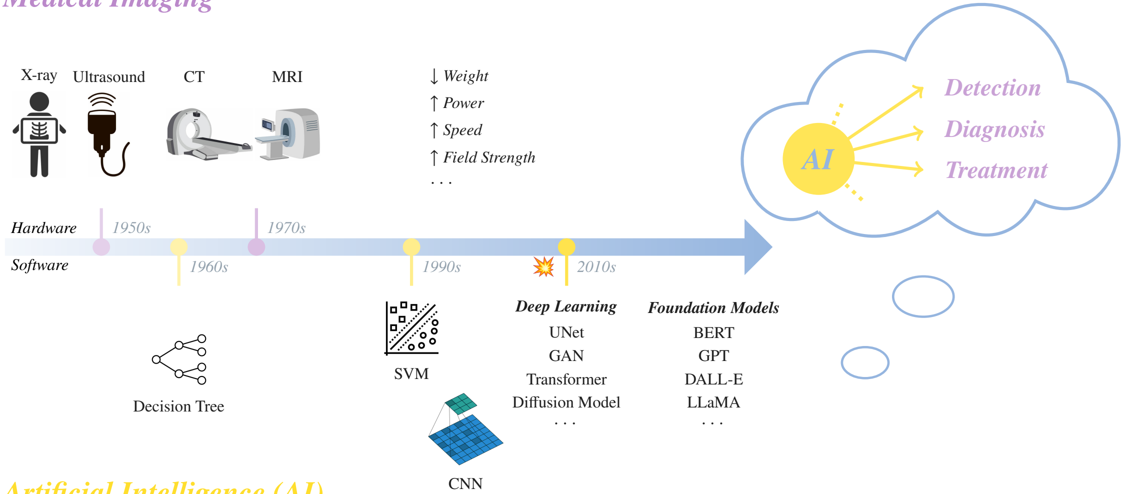
X-ray Ultrasound CT MRI



$\downarrow$ *Weight*
$\uparrow$ *Power*
$\uparrow$ *Speed*
$\uparrow$ *Field Strength*
...

Medical Image Analysis × AI → ***AI-Powered*** Diagnosis & Treatment

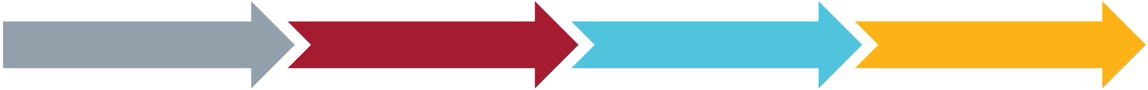
Medical Imaging



Artificial Intelligence (AI)

AI-Powered Diagnosis & Treatment in Modern Healthcare

AI-Powered Healthcare



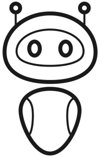
Patient Intake & Screening

Assessment & Diagnosis

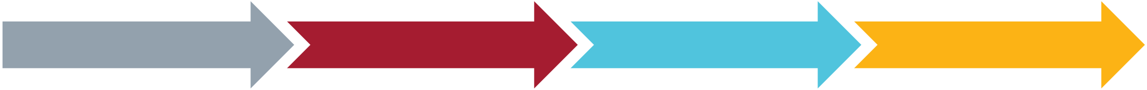
Treatment Planning

Intervention & Follow-ups

AI-Powered Diagnosis & Treatment in Modern Healthcare



AI-Powered Healthcare



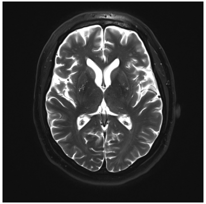
Patient Intake & Screening

Assessment & Diagnosis

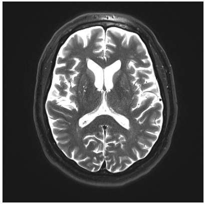
Treatment Planning

Intervention & Follow-ups

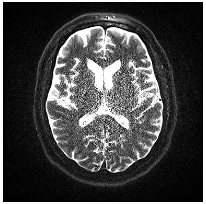
Challenges of *Data-Driven* Modeling for Medical Image Analysis



No Acceleration



Acceleration = 3



Acceleration = 6

Noise in Parallel MR Imaging (***Faster*** Acquisition ~ ***Lower*** Quality)

Patient-Induced Motion Artifacts

Physics-Induced Metallic Artifacts

Data Acquisition

Noise, ***Artifacts***, ...

100

Physics, Biology, ...
Ground Truth Anatomy

Challenges of *Data-Driven* Modeling for Medical Image Analysis

Data Access

Data Acquisition

😕 Noise, Artifacts, ...

💯

🌎 Physics, Biology, ...
Ground Truth Anatomy

Challenges of ***Data-Driven*** Modeling for Medical Image Analysis

Data Access

💰 $ $ $ $

The 1st 7T MRI scanner for clinical use (Siemens)

↑ ***Field Strength***	↑ ***Price***
1.5 T	> $1,000,000
3 T	> $3,000,000
7 T	> $7,000,000

Data Acquisition

😕 Noise, Artifacts, ...

💯

🌎 Physics, Biology, ...
Ground Truth Anatomy

Challenges of ***Data-Driven*** Modeling for Medical Image Analysis

Data Access

$ $ $ $

Patient Conditions

Data Acquisition

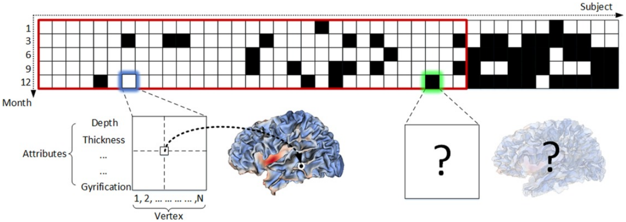
Noise, Artifacts, ...

Physics, Biology, ...
Ground Truth Anatomy

Challenges of *Data-Driven* Modeling for Medical Image Analysis

Data Access

- $ $ $ $
- Patient Conditions
- ✕ *Missing Data*



Missing data in longitudinal study of infant cortical growth
(P. Liu et al., IPMI'19 (Oral))

Data Acquisition

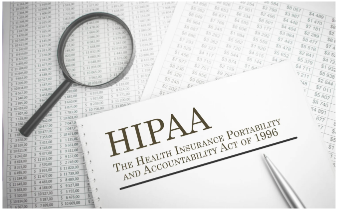
Noise, Artifacts, ...

Physics, Biology, ...
Ground Truth Anatomy

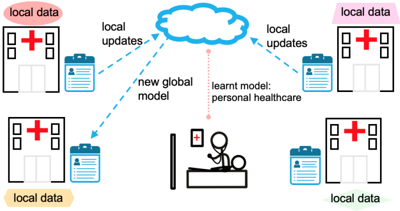
Challenges of *Data-Driven* Modeling for Medical Image Analysis

Data Access

- 💰 $ $ $ $
- 🚑 Patient Conditions
- ❌ Missing Data
- 🔒 ***Data Privacy***



HIPAA for Patient Privacy



Federated Learning for Healthcare

Data Acquisition

🤒 Noise, Artifacts, ...

💯

🌎 Physics, Biology, ...
Ground Truth Anatomy

Challenges of *Data-Driven* Modeling for Medical Image Analysis

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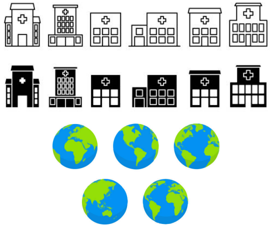
Data Analysis

- 🔀 *Varied Protocols*
- ⚖️ *Group Variances*



Data Acquisition

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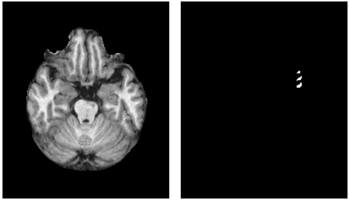
Data Analysis

- 🔀 Varied Protocols
- ⚖️ Group Variances
- 📝 *Annotations*
  - 💦 *Labor-Intensive*
  - 🔎 *Non-Inclusive*



T1 MRI *Gold-Standard Stroke Lesion*

Expertise + Hours ⟶

Data Acquisition

😕 Noise, Artifacts, ...

💯

🌎 Physics, Biology, ...
Ground Truth Anatomy

Challenges of *Data-Driven* Modeling for Medical Image Analysis

Data Access

- $ $ $ $
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Data Analysis

- Varied Protocols
- Group Variances
- ***Annotations***
  - *Labor-Intensive*
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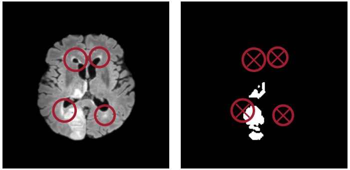

FLAIR MRI *Gold-Standard*
No WMH Annotated → *Stroke Lesion*
(WMH: white matter hyperintensities)

Data Acquisition

Noise, Artifacts, ...

100

Physics, Biology, ...
Ground Truth Anatomy

Challenges of *Data-Driven* Modeling for Medical Image Analysis

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- ⚖️ Group Variances
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  - 💦 *Labor-Intensive*
  - 🔎 *Non-Inclusive*

Data-Driven Models

🚩 ***Accuracy*** & ***Speed***

Data Acquisition

🤥 Noise, Artifacts, ...

💯

🌎 Physics, Biology, ...
Ground Truth Anatomy

Challenges of *Data-Driven* Modeling for Medical Image Analysis

Data Access

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- Data Privacy

Data Analysis

- Varied Protocols
- Group Variances
- Annotations
  - *Labor-Intensive*
  - *Non-Inclusive*

Data-Driven Models

- Accuracy & Speed
- *Interpretability*

Data Acquisition

Noise, Artifacts, ...

Physics, *Biology*, ...
Ground Truth *Anatomy*

Challenges of *Data-Driven* Modeling for Medical Image Analysis

Data Access

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Data Analysis

- 🔀 Varied Protocols
- ⚖️ Group Variances
- 📝 Annotations
  - 💦 *Labor-Intensive*
  - 🔎 *Non-Inclusive*

Data-Driven Models

- 🚩 Accuracy & Speed
- 🚩 Interpretability
- 🚩 ***Robustness***
- 🚩 ***Generalizability***

Data Acquisition

🤥 Noise, Artifacts, ...

💯

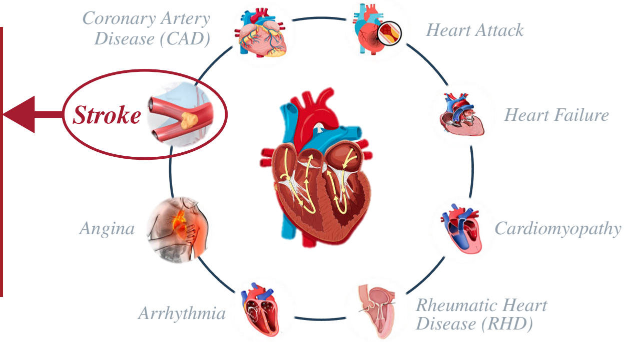
🌎 Physics, Biology, ...
Ground Truth Anatomy

Robust and Interpretable Learning for Modern Healthcare

Cardiovascular Diseases (CVDs) | *Stroke*

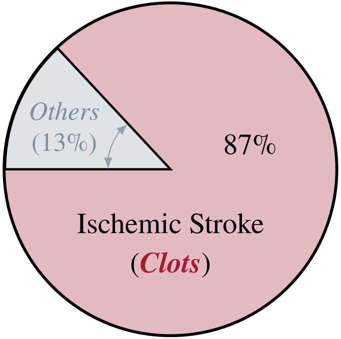
No. 2 Cause of Death Worldwide

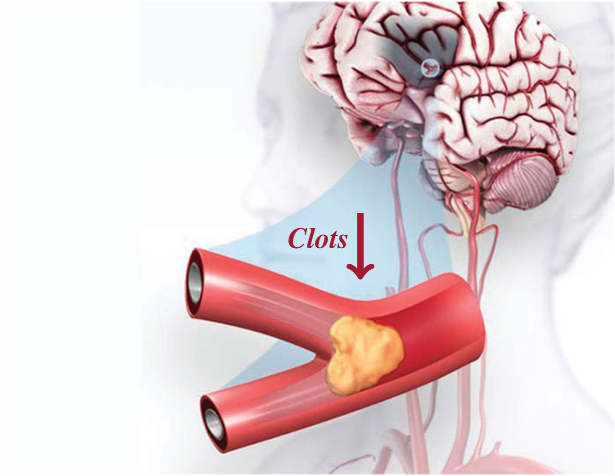
A Stroke Occurs Every *40 Seconds*



Common Type of *Cardiovascular Diseases (CVDs)*

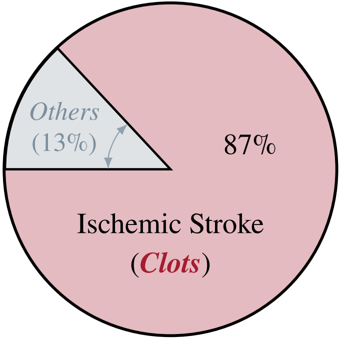
Stroke | *Ischemic Stroke*



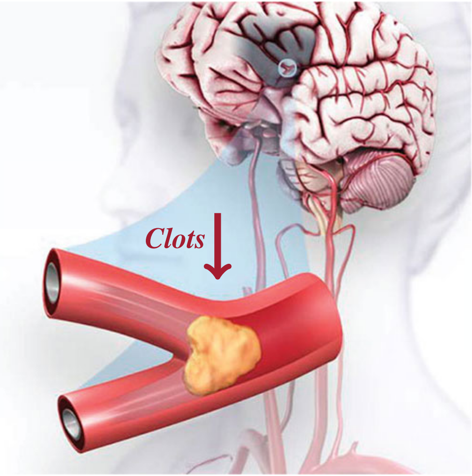


American Heart Association (AHA) and American Stroke Association (ASA): Stroke and Treatment

Stroke | *Ischemic Stroke*

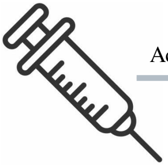


Quick Treatment
=
Less Brain Damage



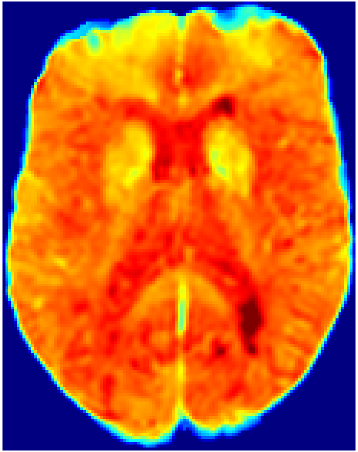
American Heart Association (AHA) and American Stroke Association (ASA): Stroke and Treatment

Stroke | Ischemic Stroke | Perfusion Imaging ***Records*** Blood Flow



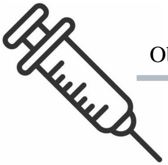
Acquire (CT/MR): 4D Perfusion ***Time-Series***

Inject: ***Tracer***



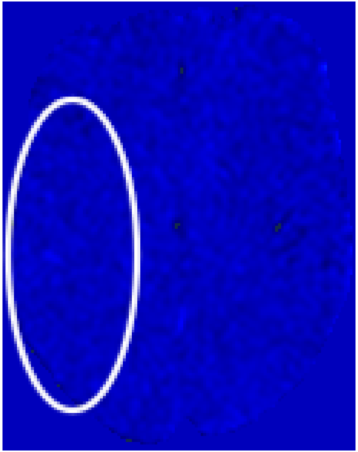
J. Demeestere el al.: Review of Perfusion Imaging in Acute Ischemic Stroke: From Time to Tissue. *Stroke* (2020)

Stroke | Ischemic Stroke | Perfusion Imaging ***Records*** Blood Flow



Inject: ***Tracer***

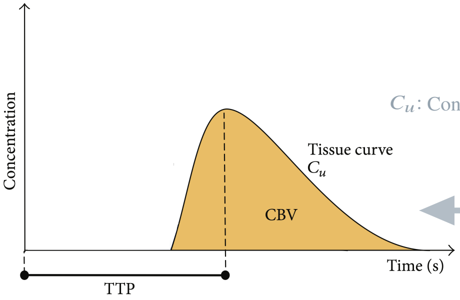
Obtain: Tracer ***Concentration Dynamics***



J. Demeestere el al.: Review of Perfusion Imaging in Acute Ischemic Stroke: From Time to Tissue. *Stroke* (2020)

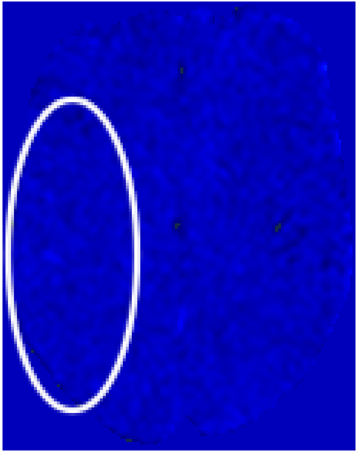
Stroke | Ischemic Stroke | Perfusion Imaging - Conventional *Voxel-Wise* Analysis

✗ *No Spatiotemporal Relations*



C_u: Concentration in Tissue

Voxel-Wise Time-Series



TTP: Time To Peak | CBV: Cerebral Blood Volume

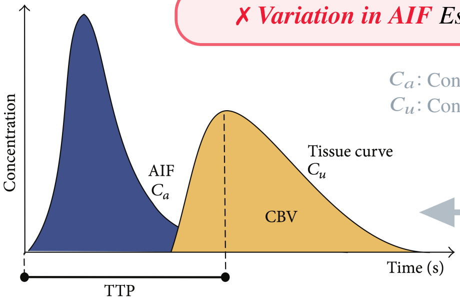
F. Scalzo & D. Liebeskind: Perfusion Angiography in Acute Ischemic Stroke. *Computational and Mathematical Methods in Medicine* (2016)

Stroke | Ischemic Stroke | Perfusion Imaging - Conventional *Voxel-Wise* Analysis

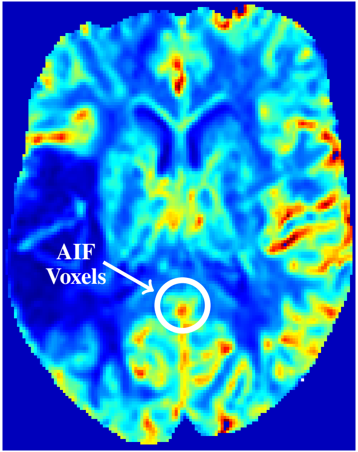
✗ ***No Spatiotemporal*** *Relations*

✗ ***Variation in AIF*** *Estimation*

C_a: Concentration in **AIF**
C_u: Concentration in Tissue



Voxel-Wise Time-Series



TTP: Time To Peak | CBV: Cerebral Blood Volume | AIF: Arterial Input Function

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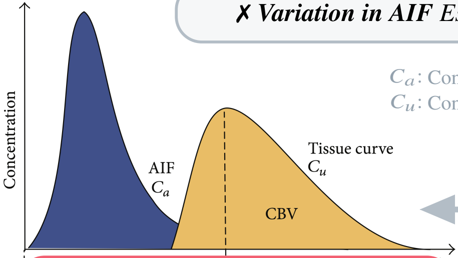
Stroke | Ischemic Stroke | Perfusion Imaging - Conventional *Voxel-Wise* Analysis

✗ ***No Spatiotemporal*** *Relations*

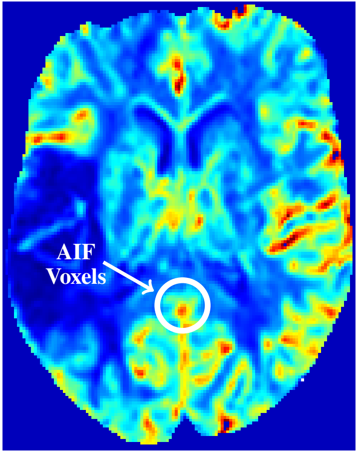
✗ ***Variation in AIF*** *Estimation*



✗ ***Within-Subject*** *Relative Units*

C_a: Concentration in **AIF**
C_u: Concentration in Tissue

Voxel-Wise Time-Series



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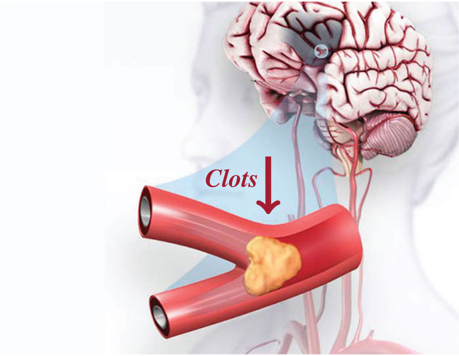
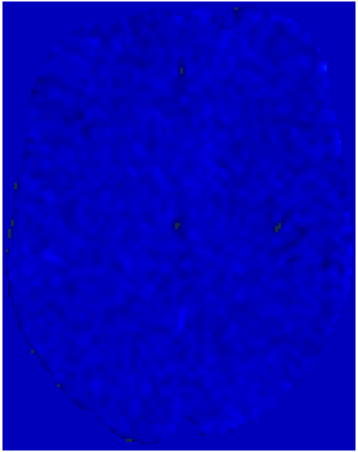
Perfusion Imaging ***Records*** Blood Flow ~ ***Fluid Dynamics***

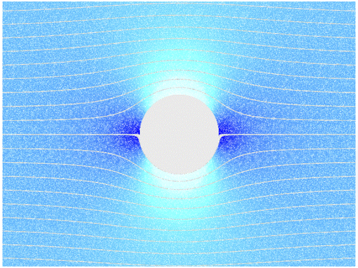


Clots Obstructing Blood Flow

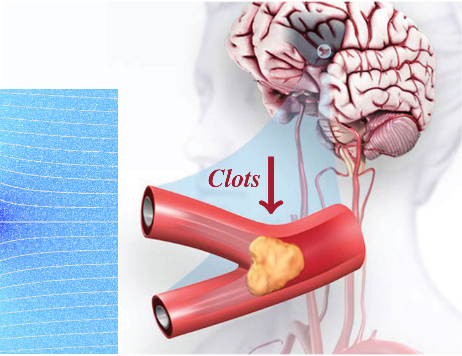


BACK

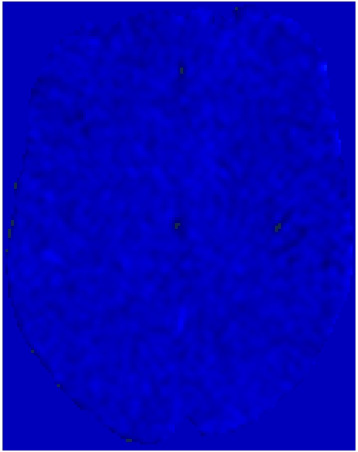
Perfusion Imaging ***Records*** Blood Flow ~ ***Fluid Dynamics***



Fluid Flow Around an Obstacle



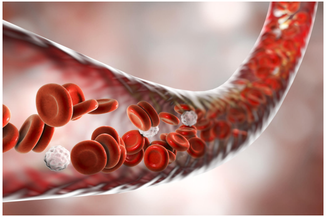
Clots Obstructing Blood Flow

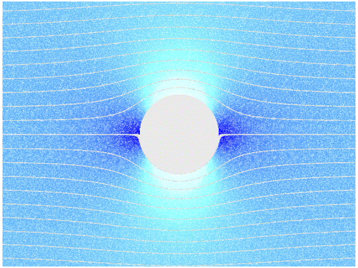


BACK

Perfusion Imaging *Records* Blood Flow ~ *Fluid Dynamics*

Blood Cells Tracking





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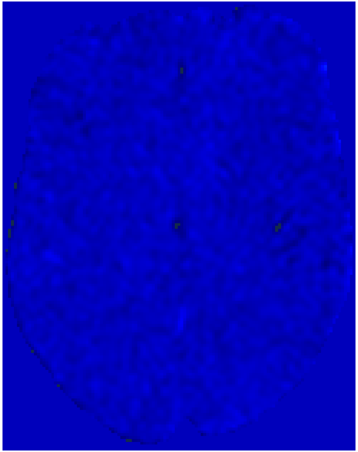
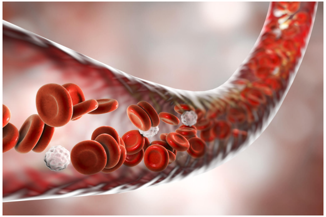


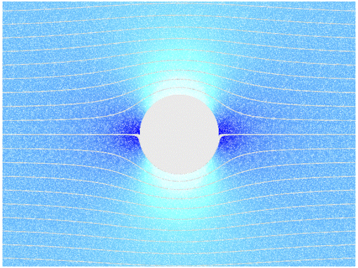
BACK

Perfusion Imaging ***Records*** Blood Flow ~ ***Fluid Dynamics***

Blood Cells Tracking



Optical Flow for Object Tracking

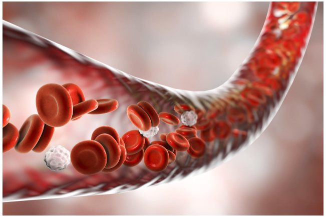


Fluid Flow Around an Obstacle

BACK

Perfusion Imaging *Records* Blood Flow ~ *Fluid Dynamics*

Blood Cells Tracking



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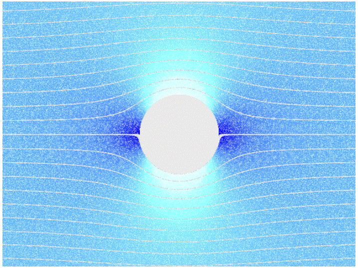

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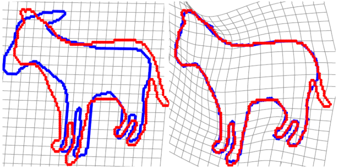
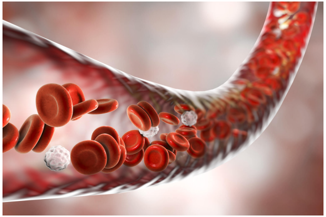


Non-Rigid Image Registration

BACK

Perfusion Imaging *Records* Blood Flow ~ *Fluid Dynamics*

Blood Cells Tracking



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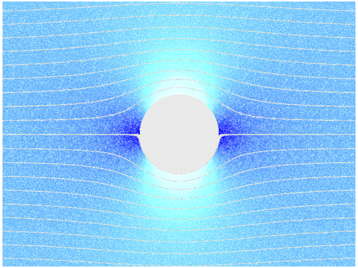
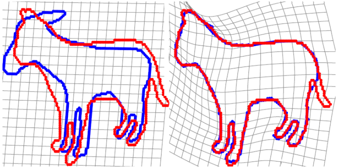
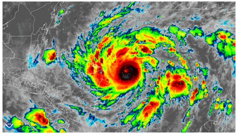


Fluid Flow Around an Obstacle



Non-Rigid Image Registration



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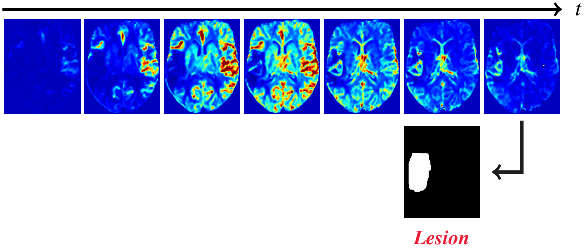
Weather and Climate Forecast

BACK

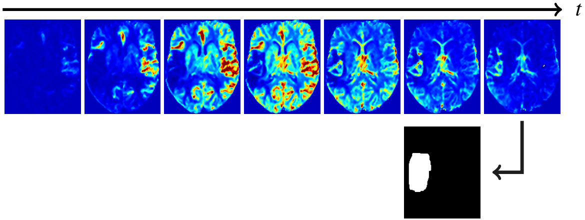
[*Preview*] *End-to-End* & *Interpretable* Stroke Lesion Detection



	Conventional	*Ours*
Preprocessing	*AIF Computation Per Subject*	–
Model Type	Voxel-Wise	*Spatiotemporal*

P. Liu et al.: `PIANO`: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)
P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)
P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)
P. Liu et al.: Deep Decomposition for Stochastic Normal-Abnormal Transport. ***CVPR*** (2022) (★ *Oral*)
P. Liu et al.: Disentangling Normal and Abnormal Perfusion via Stochastic Advection-Diffusion. *Under Review at **IEEE TPAMI*** (2024)

[*Preview*] ***End-to-End*** & ***Interpretable*** Stroke Lesion Detection



Lesion

Accuracy
Speed

	Conventional	***Ours***
Preprocessing	*AIF Computation Per Subject*	–
Model Type	Voxel-Wise	***Spatiotemporal***
Inference Time	> 1 hour	< ***5 seconds***
Lesion Detection AUC	0.65	***0.79*** (↑ 20%)

(AUC: area under the curve — Higher (↑) = Better)

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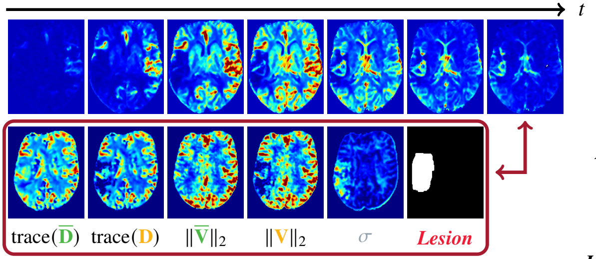
[*Preview*] ***End-to-End*** & ***Interpretable*** Stroke Lesion Detection



✓ *Interpretable* Physics: $\mathbf{V}$, $\mathbf{D}$

✓ *Normal* Physics: $\overline{\mathbf{V}}$, $\overline{\mathbf{D}}$

✓ *Lesion* Segmentation

Accuracy
Speed

	Conventional	***Ours***
Preprocessing	*AIF Computation Per Subject*	–
Model Type	Voxel-Wise	***Spatiotemporal***
Inference Time	> 1 hour	***< 5 seconds***
Lesion Detection AUC	0.65	***0.79*** (↑ 20%)

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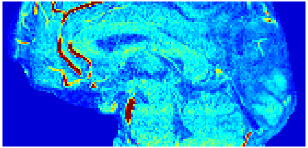
Physics-Driven Formulation for Tracer Dynamics | *Advection-Diffusion PDE*



Mass Transport of Tracer

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (\mathbf{D}\, \nabla C)$$

C: Tracer **Concentration**

P. Liu et al.: `PIANO`: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)
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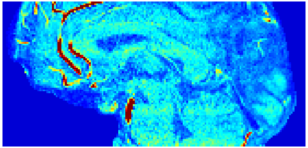
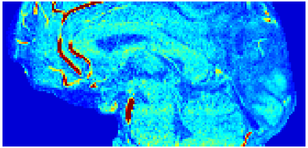
Physics-Driven Formulation for Tracer Dynamics | *Advection-Diffusion PDE*



Mass Transport of Tracer

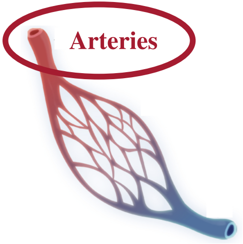


via ***Advection***

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (\mathbf{D}\, \nabla C)$$

C: Tracer Concentration

$\mathbf{V}$: **Velocity** Field



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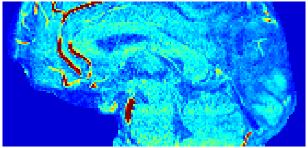
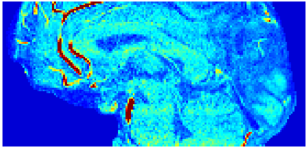
Physics-Driven Formulation for Tracer Dynamics | *Advection-Diffusion PDE*



Mass Transport of Tracer

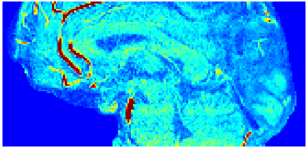
$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (\mathbf{D}\, \nabla C)$$

C: Tracer Concentration
V: Velocity Field
D: **Diffusion** Field

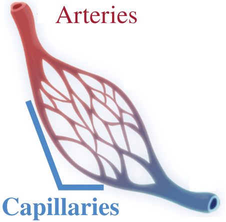


via ***Advection***

+



via ***Diffusion***



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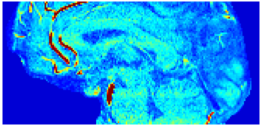
P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

Perfusion Imaging via Advection-Diffusion | *Synthetic Brain Perfusion Samples*

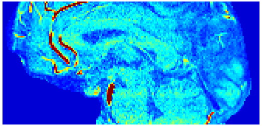
Advection-Diffusion Solvers Toolbox in PyTorch



Mass Transport of Tracer

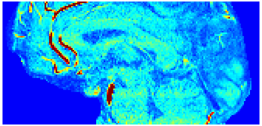
$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (\mathbf{D}\, \nabla C)$$

C: Tracer Concentration
$\mathbf{V}$: Velocity Field
$\mathbf{D}$: Diffusion Field

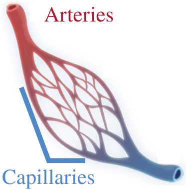


via ***Advection***

+



via ***Diffusion***



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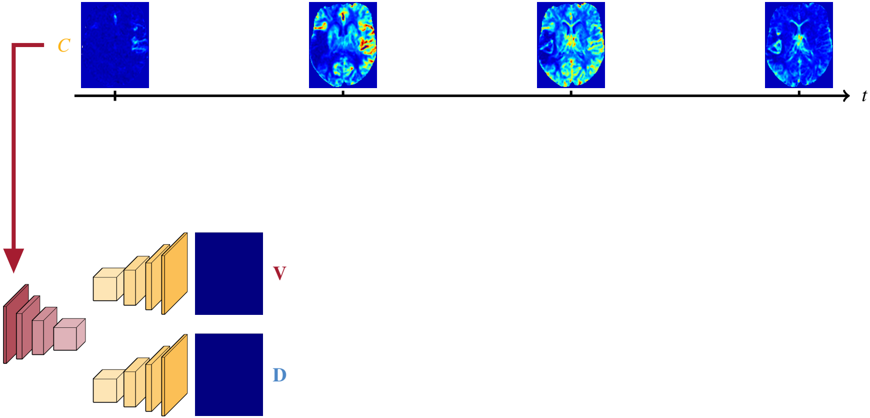
Perfusion Imaging via Advection-Diffusion | *Time-Series Input*



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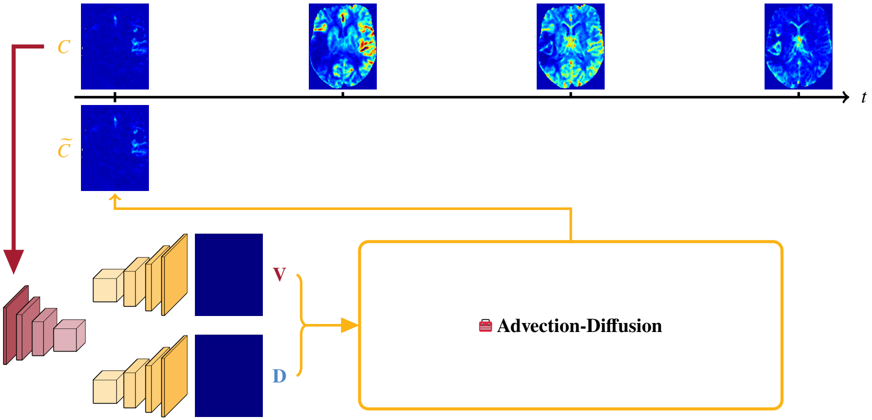
Perfusion Imaging via Advection-Diffusion | *Forward in Time*



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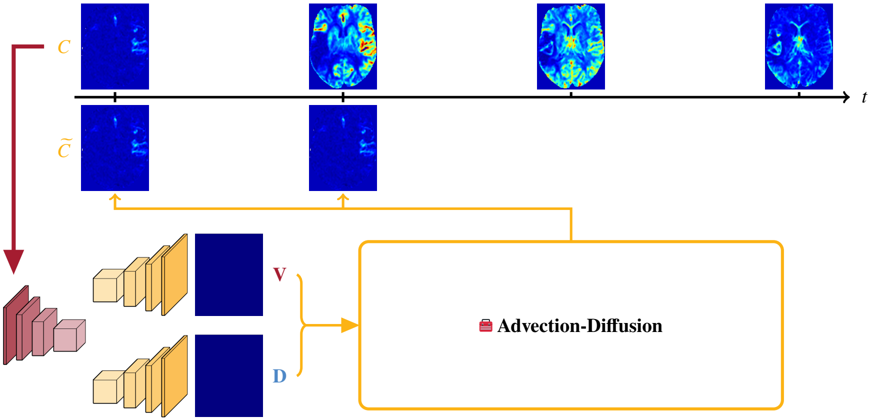
Perfusion Imaging via Advection-Diffusion | *Forward in Time*



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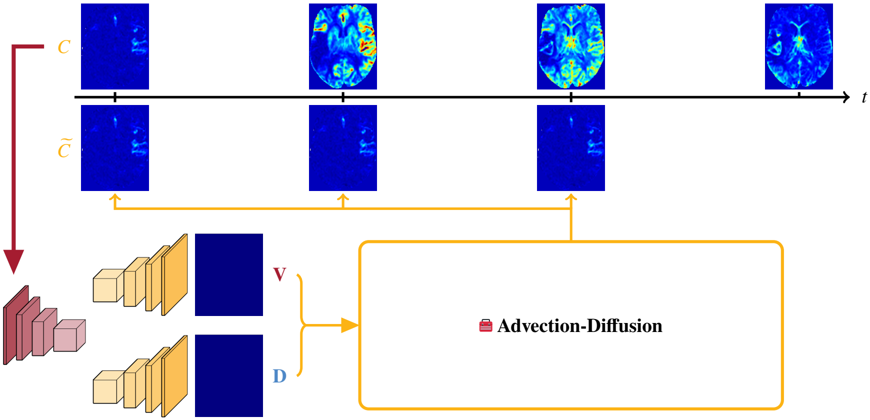
Perfusion Imaging via Advection-Diffusion | *Forward in Time*



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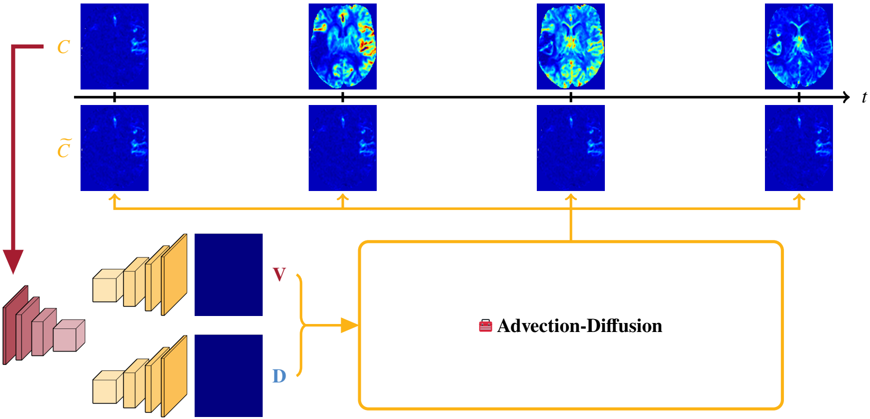
Perfusion Imaging via Advection-Diffusion | *Forward in Time*



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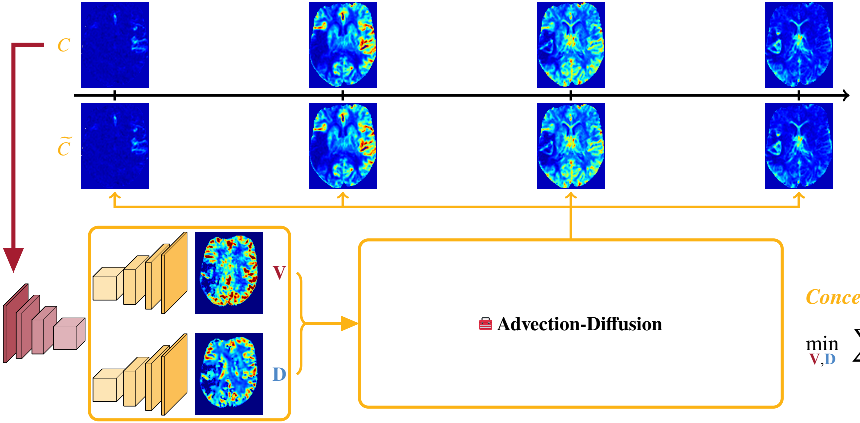
Perfusion Imaging via Advection-Diffusion | *Time-Series Regression*



Concentration Loss ($\mathcal{L}_C$)

$$\min_{\mathbf{V},\mathbf{D}} \sum_t \int_{x\in\Omega} |C - \widetilde{C}| \, dx$$

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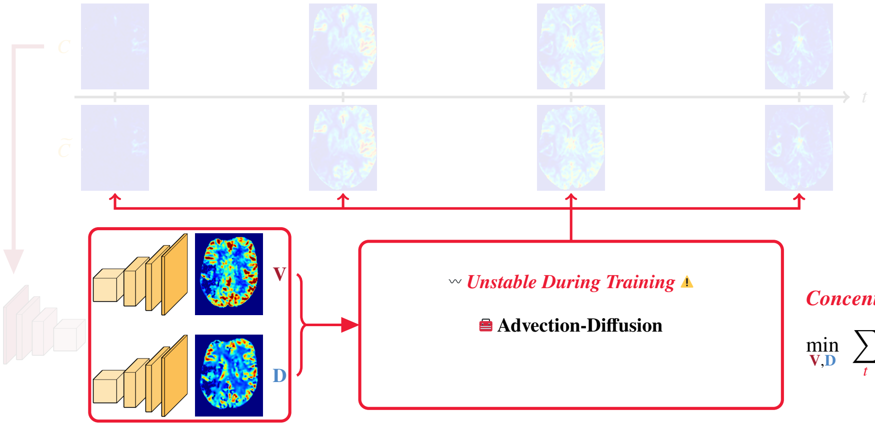
Perfusion Imaging via Advection-Diffusion | *Unstable Physics-Driven Learning*



Concentration Loss ($\mathcal{L}_C$)

$$\min_{\mathbf{V},\mathbf{D}} \sum_t \int_{x\in\Omega} |C - \widetilde{C}|\, dx$$

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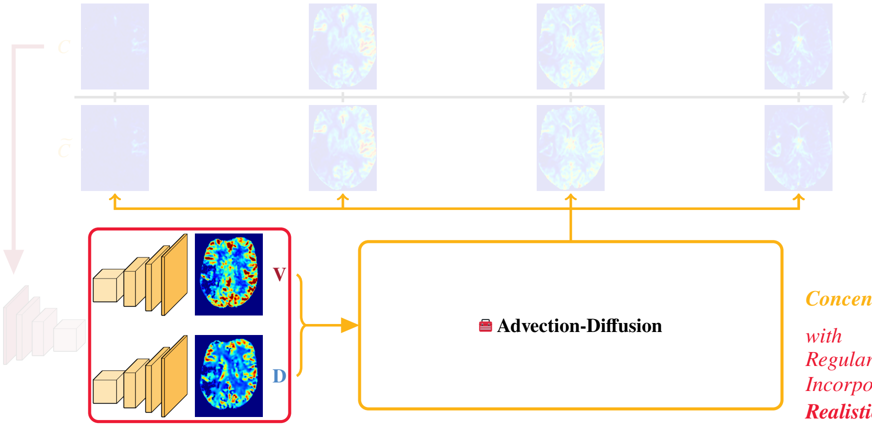
P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Perfusion Imaging via Advection-Diffusion | *Regularizations for Realistic Constraints*



Concentration Loss ($\mathcal{L}_C$)

with Regularizations Incorporating ***Realistic Constraints***

P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)

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P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularizations Incorporating Realistic Constraints

👍 Sparsity ⇔ `L1`, Smoothness ⇔ `L2` on Gradients, Bounded Values ⇔ `torch.clamp`, ...

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularizations Incorporating Realistic Constraints | *Incompressible Flow*

👍 Sparsity ⇔ `L1`, Smoothness ⇔ `L2` on Gradients, Bounded Values ⇔ `torch.clamp`, ...

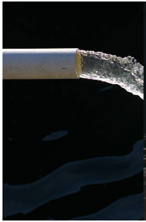
🤔 **Incompressible Flow** (Constant Flow Density)

Water Flow

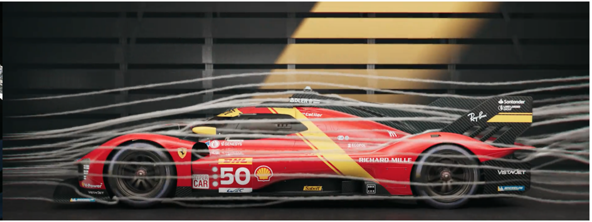
P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularizations Incorporating Realistic Constraints | *Incompressible Flow*

- 👍 Sparsity ⇔ `L1`, Smoothness ⇔ `L2` on Gradients, Bounded Values ⇔ `torch.clamp`, ...
- 🤔 **Incompressible Flow** (Constant Flow Density)



Water Flow



The Aerodynamics of Ferrari 499P

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularizations Incorporating Realistic Constraints | *Incompressible Flow*

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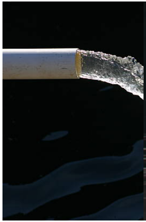
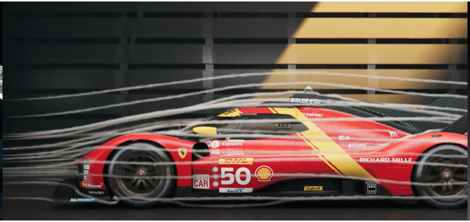


Water Flow



The Aerodynamics of Ferrari 499P

Cerebral Blood Flow

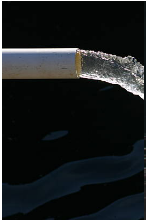
P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularizations Incorporating Realistic Constraints | *Incompressible Flow*

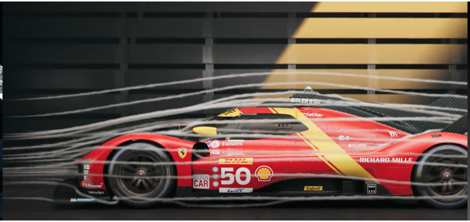
👍 Sparsity $\Leftrightarrow$ `L1`, Smoothness $\Leftrightarrow$ `L2` on Gradients, Bounded Values $\Leftrightarrow$ `torch.clamp`, ...

🤔 Incompressible Flow (Constant Flow Density) $\Leftrightarrow \nabla \cdot \mathbf{V} \equiv 0$ (**Divergence-Free Velocity**)

$$\min \int_{x \in \Omega} \|\nabla \cdot \mathbf{V}\| \, dx$$



Water Flow



The Aerodynamics of Ferrari 499P

Cerebral Blood Flow

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularizations Incorporating Realistic Constraints | ***Incompressible Flow***

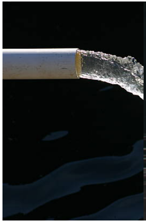
👍 Sparsity ⇔ `L1`, Smoothness ⇔ `L2` on Gradients, Bounded Values ⇔ `torch.clamp`, ...

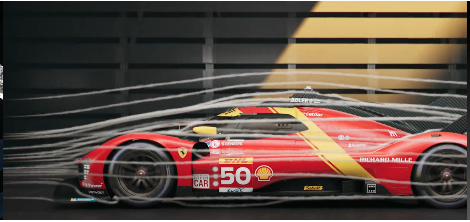
🤔 Incompressible Flow (Constant Flow Density) ⇔ $\nabla \cdot \mathbf{V} \equiv 0$ (**Divergence-Free Velocity**)

$$\min \int_{x \in \Omega} \|\nabla \cdot \mathbf{V}\| \, dx$$

✗ ***Reduce*** Time-Series Regression Performance

✗ ***Not Guaranteed*** During Inference





Water Flow | The Aerodynamics of Ferrari 499P | Cerebral Blood Flow

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

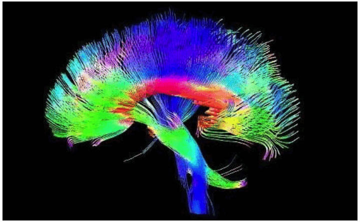
Regularizations Incorporating Realistic Constraints | *Symmetric PSD Diffusion*

- 👍 Sparsity ⇔ `L1`, Smoothness ⇔ `L2` on Gradients, Bounded Values ⇔ `torch.clamp`, ...
- 🤔 Incompressible Flow (Constant Flow Density) ⇔ $\nabla \cdot \mathbf{V} \equiv 0$ (**Divergence-Free Velocity**)

$$\min \int_{x \in \Omega} \|\nabla \cdot \mathbf{V}\| \, dx$$

- 🤔 **Symmetric Positive Semi-Definite (PSD) Diffusion**

Dye Spreading in Water



White Matter Tracts from Diffusion Tensor Imaging

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularizations Incorporating Realistic Constraints | *Symmetric PSD Diffusion*

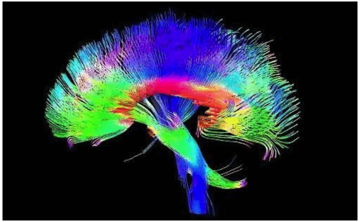
- 👍 Sparsity ⇔ `L1`, Smoothness ⇔ `L2` on Gradients, Bounded Values ⇔ `torch.clamp`, ...
- 🤔 Incompressible Flow (Constant Flow Density) ⇔ $\nabla \cdot \mathbf{V} \equiv 0$ (**Divergence-Free Velocity**)

$$\min \int_{x \in \Omega} \|\nabla \cdot \mathbf{V}\| \, dx$$

- 🤔 **Symmetric Positive Semi-Definite (PSD) Diffusion** ⇔ $q^T \mathbf{D} q \geq 0, \forall q \neq 0$

min ?

Dye Spreading in Water



White Matter Tracts from Diffusion Tensor Imaging

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularizations ~~Incorporating Realistic Constraints~~

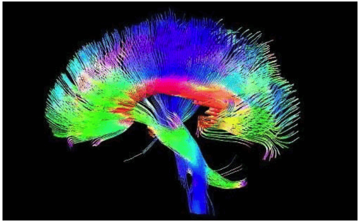
- Sparsity ⇔ `L1`, Smoothness ⇔ `L2` on Gradients, Bounded Values ⇔ `torch.clamp`, ...
- Incompressible Flow (Constant Flow Density) ⇔ $\nabla \cdot \mathbf{V} \equiv 0$ (**Divergence-Free Velocity**)

$$\cancel{\min \int_{x \in \Omega} \|\nabla \cdot \mathbf{V}\| \, dx}$$

- **Symmetric Positive Semi-Definite (PSD) Diffusion** ⇔ $q^T \mathbf{D} q \geq 0, \forall q \neq 0$

$$\cancel{\min \; ?}$$

Dye Spreading in Water

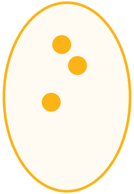


White Matter Tracts from Diffusion Tensor Imaging

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularization-Free Learning with Realistic Guarantees

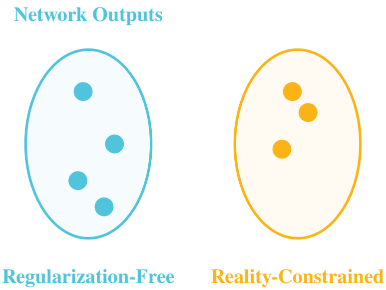
Network Outputs



Reality-Constrained

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

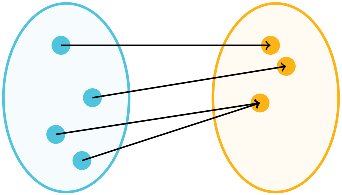
Regularization-Free Learning with Realistic Guarantees



P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularization-Free Learning with Realistic Guarantees

Network Outputs



Surjective Mapping: **Regularization-Free** $\mapsto$ **Reality-Constrained**

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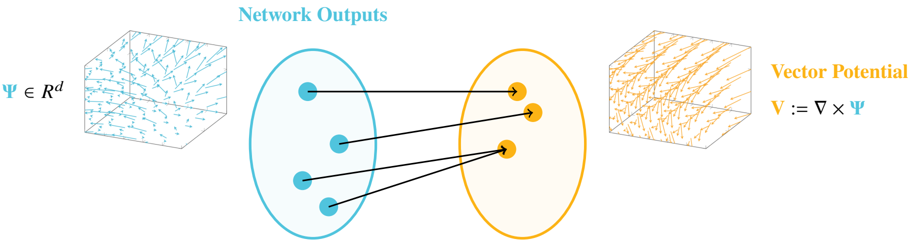
Regularization-Free Learning with Realistic Guarantees

👍 Learning ***Incompressible*** Flow, ***by Definition***



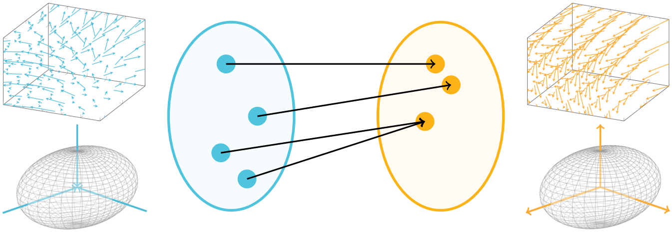
Surjective Mapping: **Regularization-Free** $\mapsto$ **Reality-Constrained**

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Regularization-Free Learning with Realistic Guarantees

👍 Learning ***Incompressible*** Flow, ***by Definition***

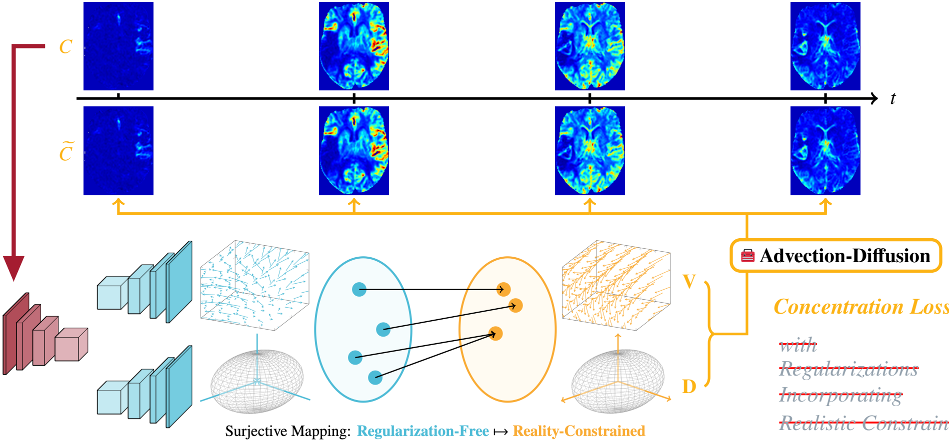
👍 Learning ***Symmetric PSD*** Diffusion, ***by Definition***



Surjective Mapping: **Regularization-Free** $\mapsto$ **Reality-Constrained**

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Perfusion Imaging via *Advection-Diffusion*: *Regularization-Free* Learning



Concentration Loss ($\mathcal{L}_C$)

~~*with Regularizations Incorporating Realistic Constraints*~~

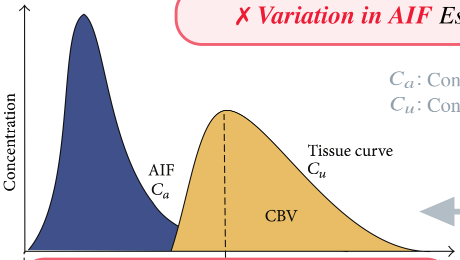
P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

[*Recap*] Perfusion Imaging - Conventional *Voxel-Wise* Analysis

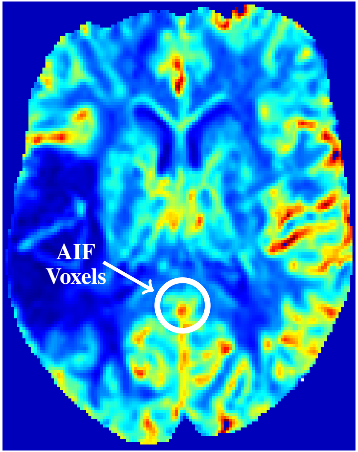
✗ *No Spatiotemporal Relations*

✗ *Variation in AIF Estimation*

C_a: Concentration in **AIF**
C_u: Concentration in Tissue



Voxel-Wise Time-Series

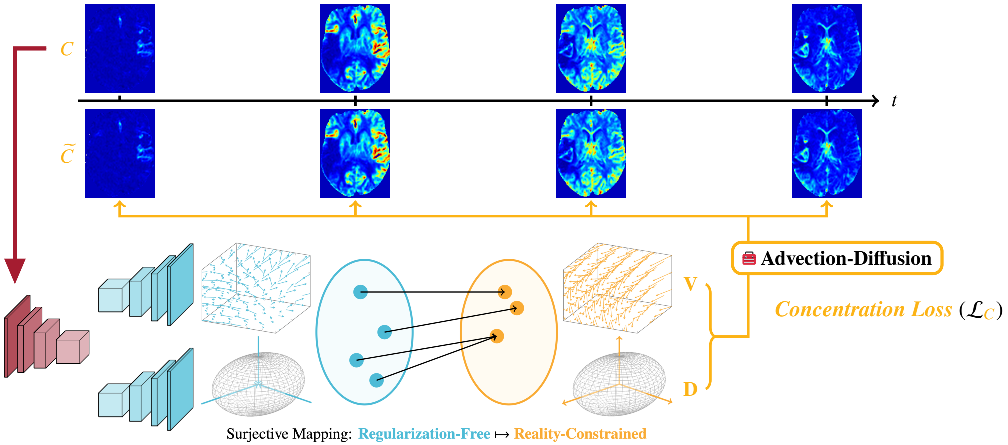


✗ *Within-Subject Relative Units*

TTP: Time To Peak | CBV: Cerebral Blood Volume | AIF: Arterial Input Function

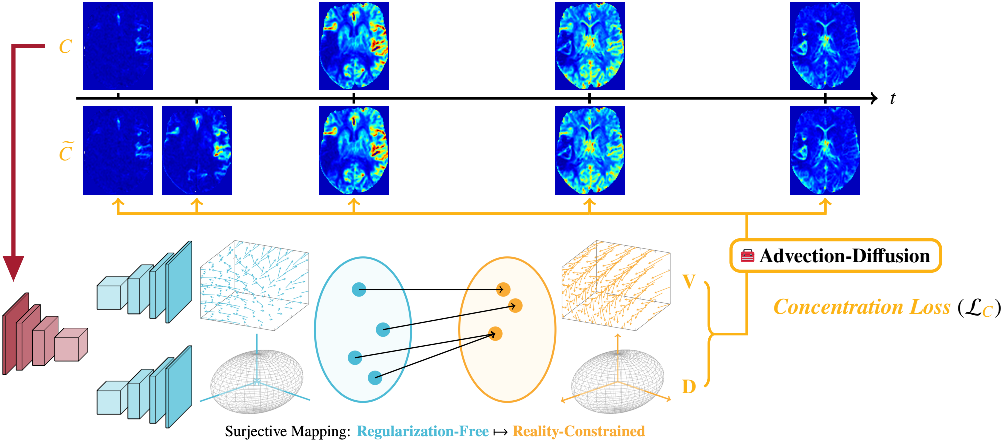
F. Scalzo & D. Liebeskind: Perfusion Angiography in Acute Ischemic Stroke. *Computational and Mathematical Methods in Medicine* (2016)

Perfusion Imaging via *Advection-Diffusion*: *AIF-Free* for the First Time



P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Perfusion Imaging via *Advection-Diffusion*: *AIF-Free* & *Spatiotemporally Continuous*



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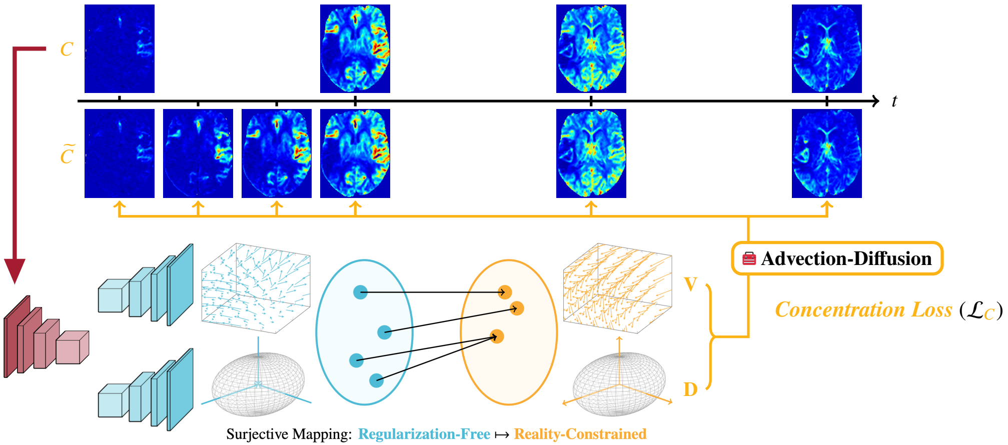

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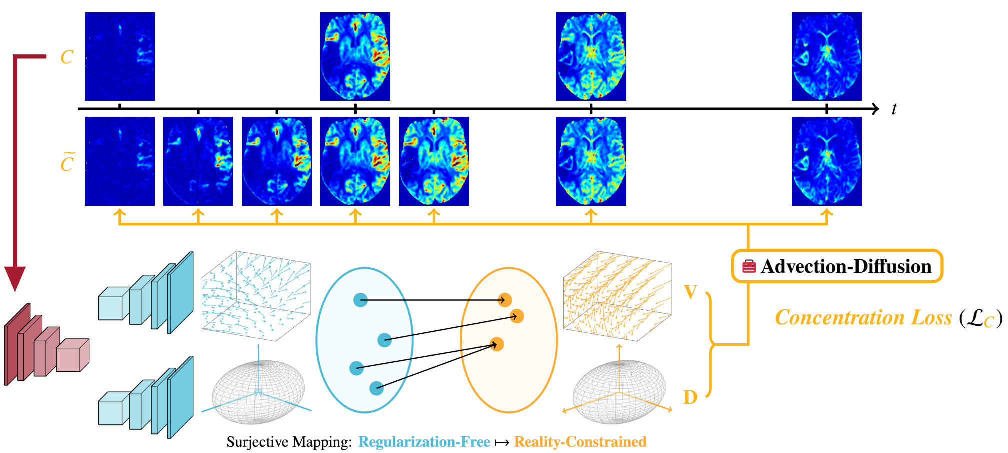

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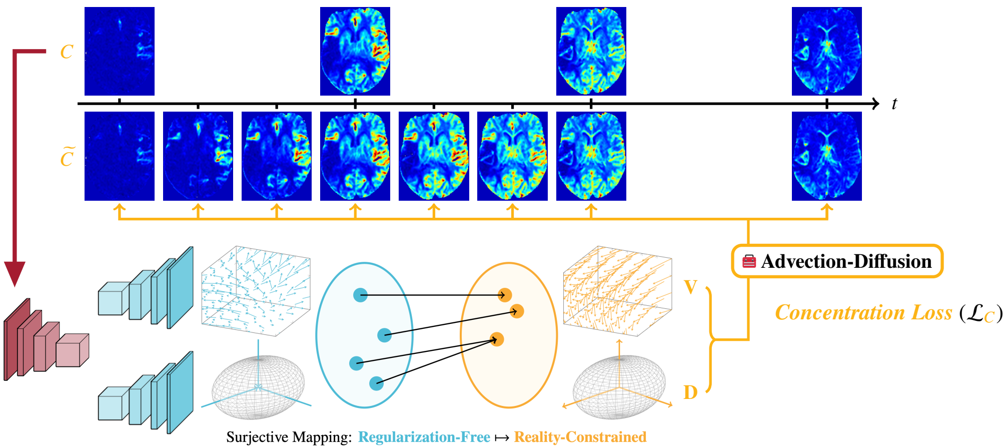

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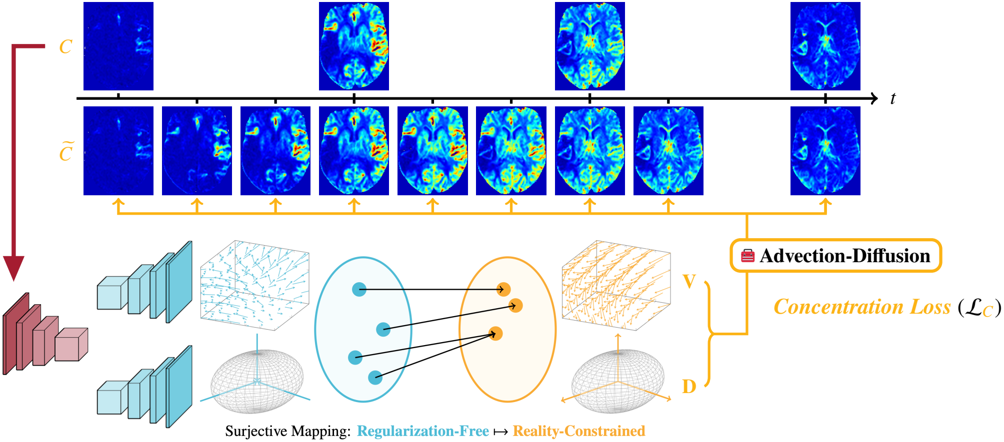

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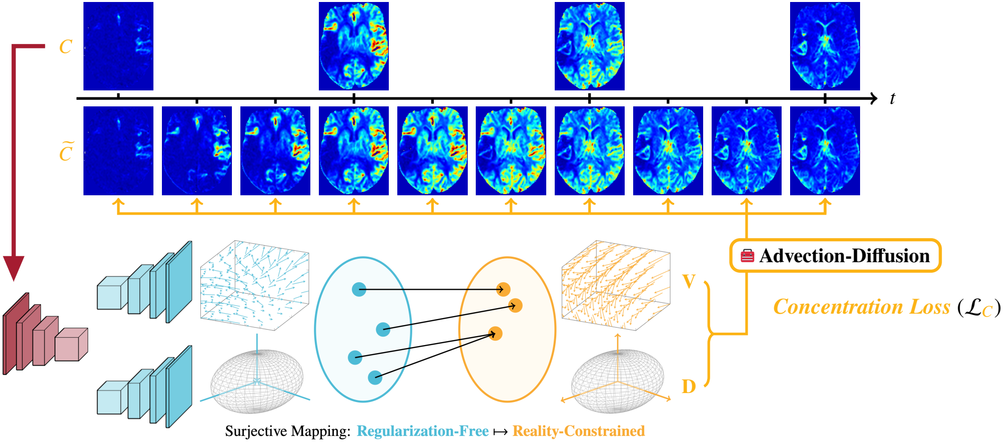
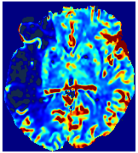
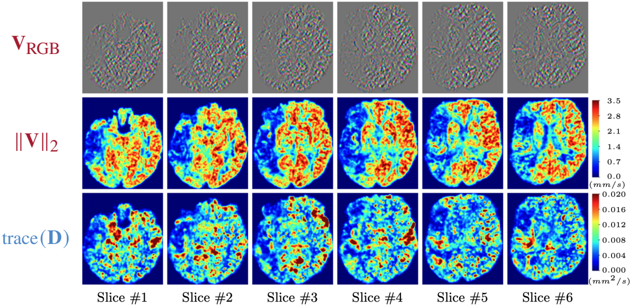


P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

Perfusion Imaging via *Advection-Diffusion* | Qualitative Results



Input $C(t)$
Time-Series



* Gold-Standard Lesion from the ISLES 2017 Stroke Lesion Segmentation Challenge

P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)
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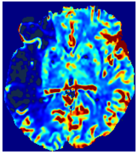
Perfusion Imaging via *Advection-Diffusion* | Qualitative Results



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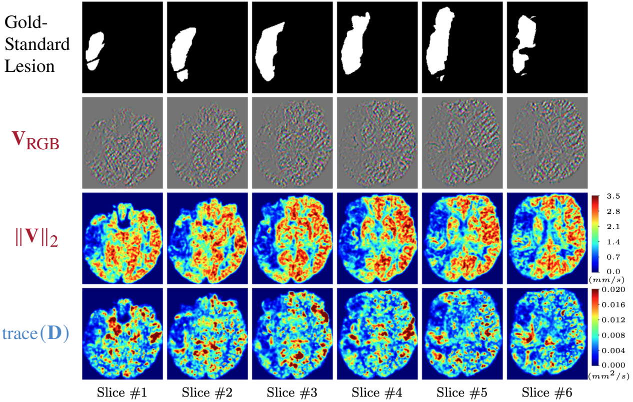

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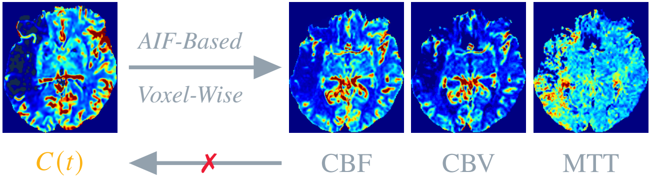
Perfusion Imaging via *Advection-Diffusion* $\bigcup$ Conventional *Voxel-Wise* Approaches

Our Approach
Complements
Conventional Ones



Conventional Perfusion Feature Maps: CBF - Cerebral Blood Flow | CBV - Cerebral Blood Volume | MTT - Mean Transit Time

P. Liu et al.: `PIANO`: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)
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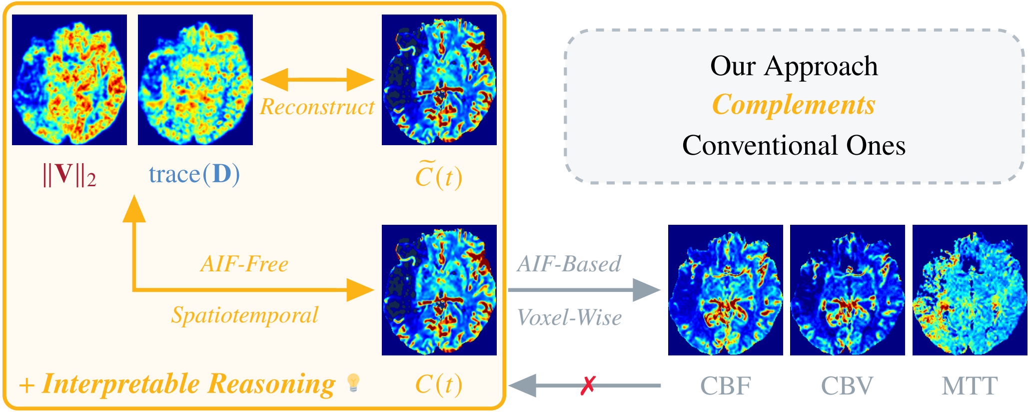

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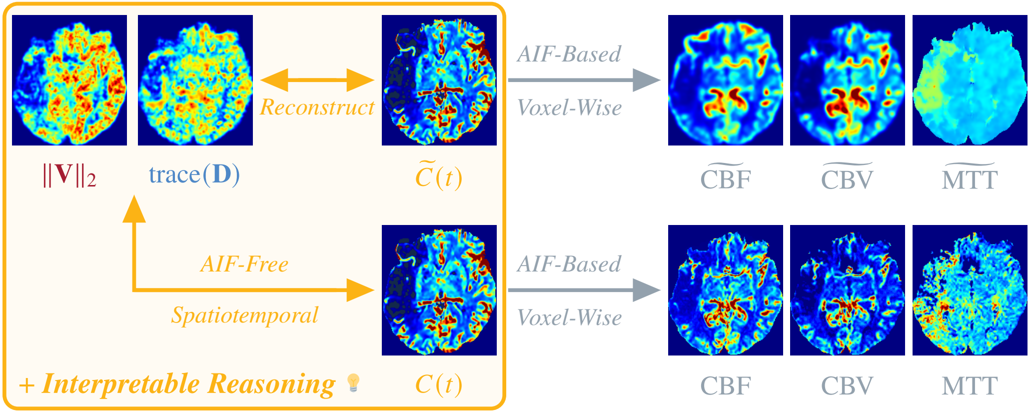

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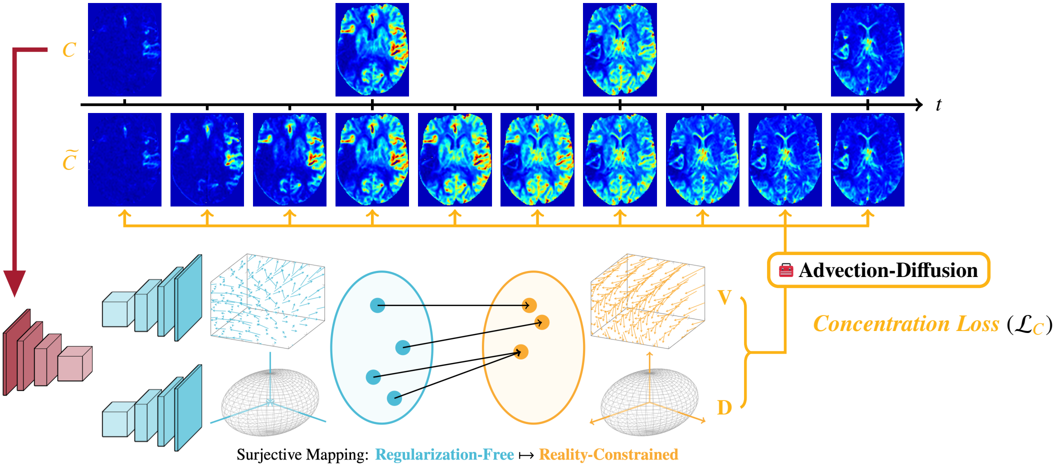
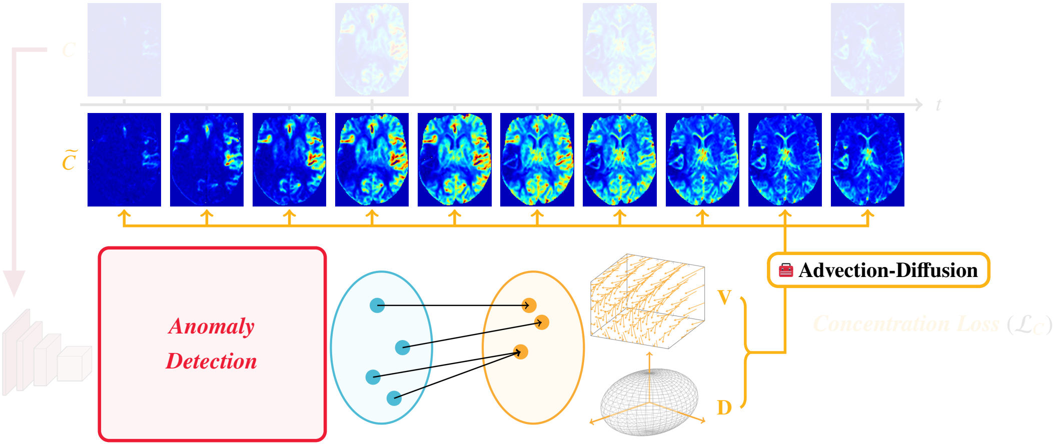
[*Recap*] Perfusion Imaging via *Advection-Diffusion*: *AIF-Free* for the First Time



P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

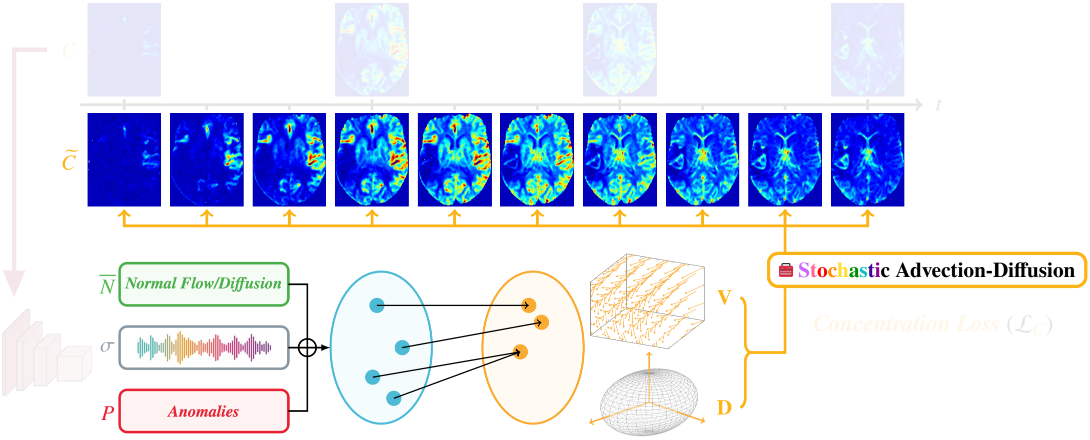
Perfusion Imaging via Advection-Diffusion | *Stroke Diagnosis* & *Lesion Detection*



Surjective Mapping: **Regularization-Free** $\mapsto$ **Reality-Constrained**

P. Liu et al.: Deep Decomposition for Stochastic Normal-Abnormal Transport. ***CVPR*** (2022) (★ *Oral*)
P. Liu et al.: Disentangling Normal and Abnormal Perfusion via Stochastic Advection-Diffusion. *Under Review at **IEEE TPAMI*** (2024)

Disentangling Anomaly within Stochastic Dynamical Systems



Surjective Mapping: Regularization-Free ↦ Reality-Constrained

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P. Liu et al.: Deep Decomposition for Stochastic Normal-Abnormal Transport. ***CVPR*** (2022) (★ *Oral*)
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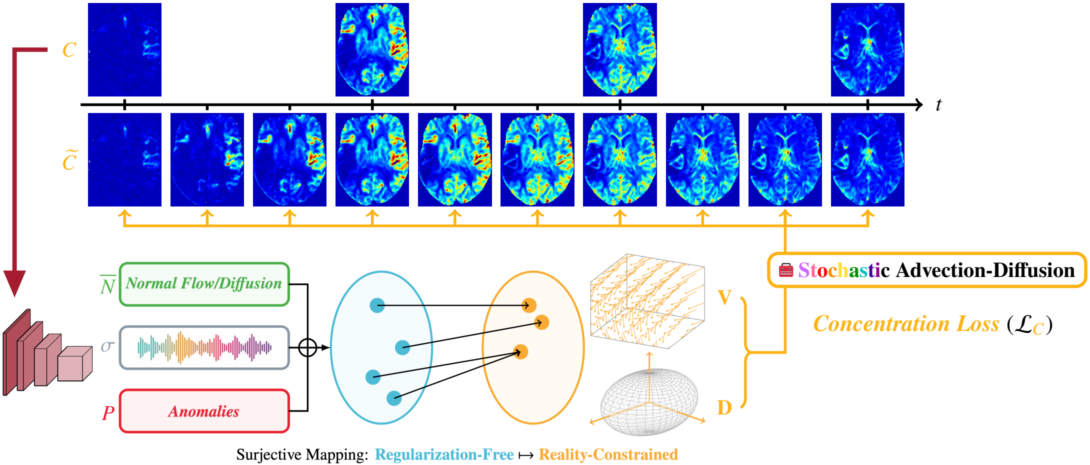
End-to-End & *Interpretable* Stroke Lesion Detection | Framework Overview



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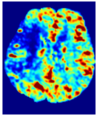
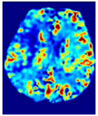
End-to-End & *Interpretable* Stroke Lesion Detection | Qualitative Results

Subject #1

$\|\mathbf{V}\|_2$



$\mathrm{trace}(\mathbf{D})$



✓ *Interpretable* Physics: **V**, **D**

Testing Subjects from the ISLES 2017 Stroke Lesion Segmentation Challenge

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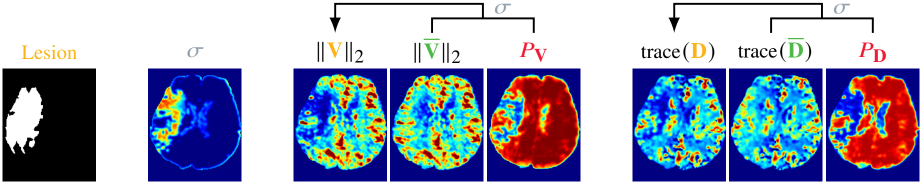
End-to-End & *Interpretable* Stroke Lesion Detection | Qualitative Results



✓ *Interpretable* Physics: $\mathbf{V}$, $\mathbf{D}$

$\Updownarrow$

- ✓ *Normal* Physics: $\overline{\mathbf{V}}$, $\overline{\mathbf{D}}$
- ✓ *Anomaly* Estimation: $\mathbf{P_V}$, $\mathbf{P_D}$
- ✓ *Lesion* Probability: σ

Testing Subjects from the ISLES 2017 Stroke Lesion Segmentation Challenge

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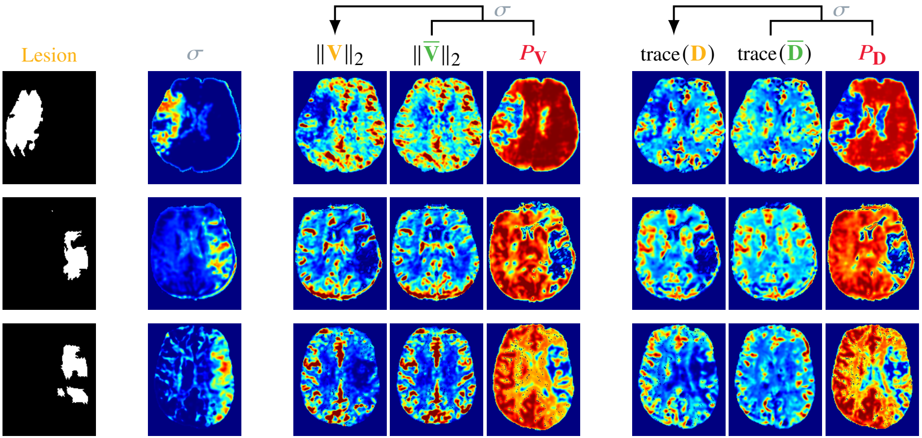
End-to-End & *Interpretable* Stroke Lesion Detection | Qualitative Results



Testing Subjects from the ISLES 2017 Stroke Lesion Segmentation Challenge

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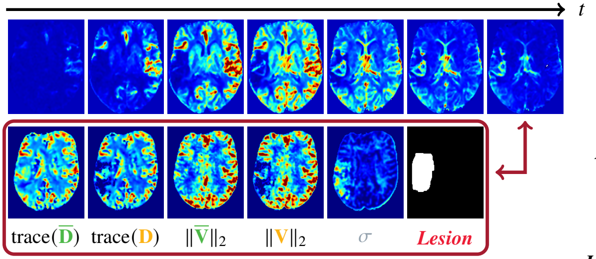
[*Summary*] *End-to-End* & *Interpretable* Stroke Lesion Detection



- ✓ *Interpretable* Physics: $\mathbf{V}$, $\mathbf{D}$
- ✓ *Normal* Physics: $\overline{\mathbf{V}}$, $\overline{\mathbf{D}}$
- ✓ *Lesion* Segmentation

⚑ ***Accuracy***
⚑ ***Speed***

	Conventional	***Ours***
Preprocessing	*AIF Computation Per Subject*	–
Model Type	Voxel-Wise	*Spatiotemporal*
Inference Time	> 1 hour	< ***5 seconds***
Lesion Detection AUC	0.65	***0.79*** (↑ 20%)

(AUC: area under the curve — Higher (↑) = Better)

P. Liu et al.: `PIANO`: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)
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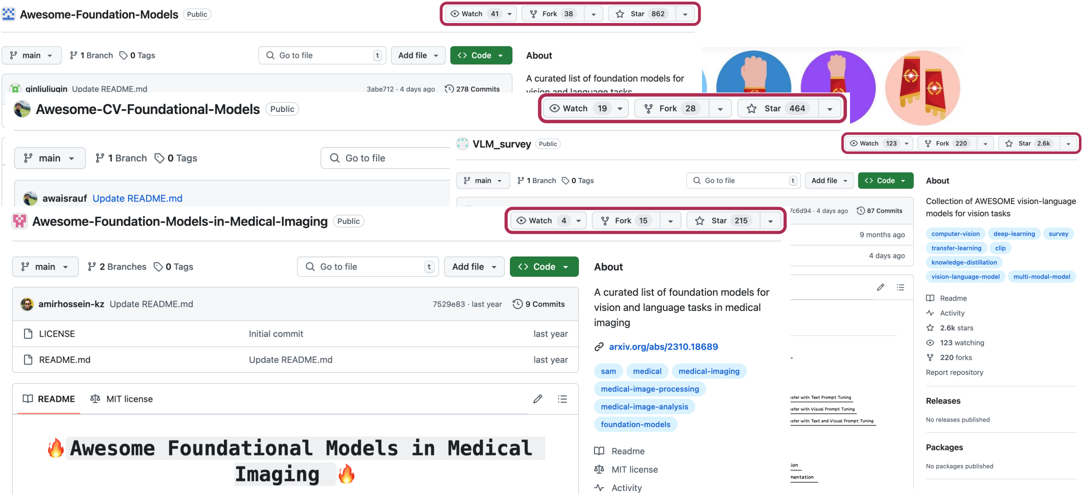
Robust and Interpretable Learning for Modern Healthcare

Towards a "*Superpowered*" Foundation Model for Medical Imaging

Towards a “*Superpowered*” Foundation Model for Medical Imaging



Towards a ***Robust*** & ***Generalized*** Foundation Model for Medical Imaging

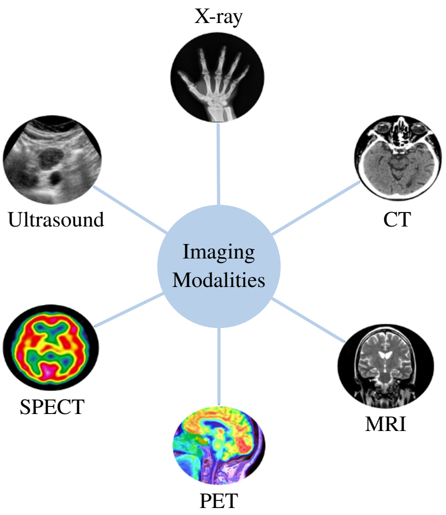
Data Variety
in
Medical Imaging

Accessibility Challenges
in
Modern Healthcare

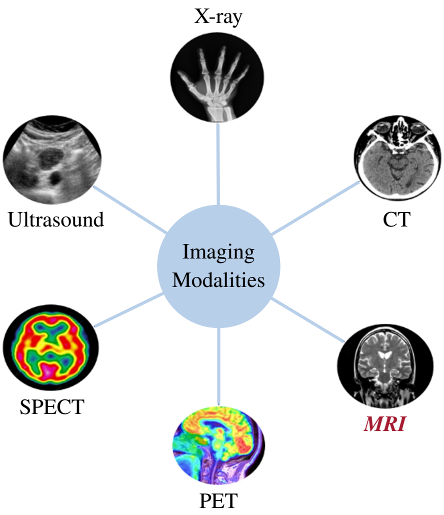
Robustness

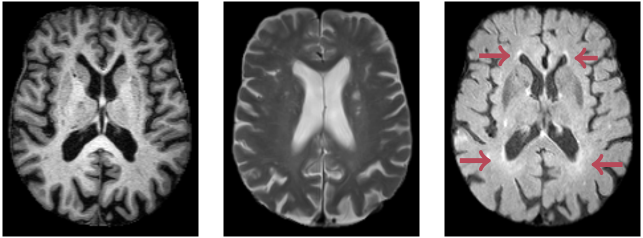
Generalizability

Medical Imaging Modalities | *Variety*



Medical Imaging Modalities | ***Variety*** - The Non-Calibrated MRI

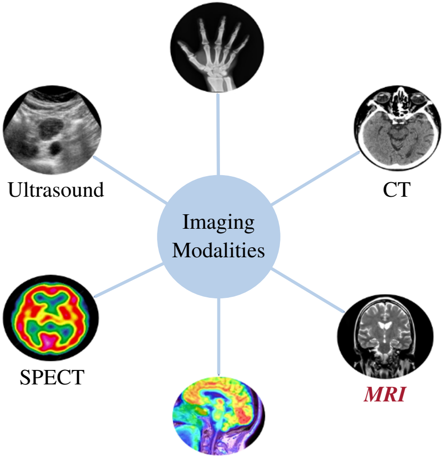




T1-weighted (T1w) *(Grey vs. White Matter)* | T2-weighted (T2w) *(Fluid-Filled Regions)* | FLAIR *(Abnormalities)*

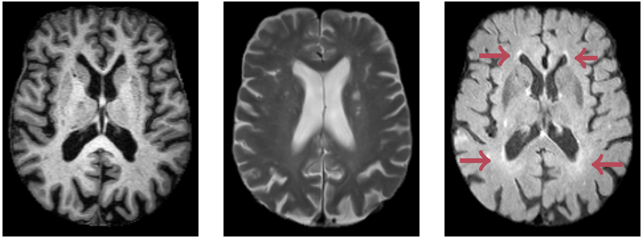
*MRI Scans with Various **Modalities** from the **Same** Subject*

Medical Imaging Modalities | *Variety* - The Non-Calibrated MRI



✓ ***Individual*** *Assessment in Clinical Practice*

✗ ***Data-Driven*** *Quantitative Evaluations*



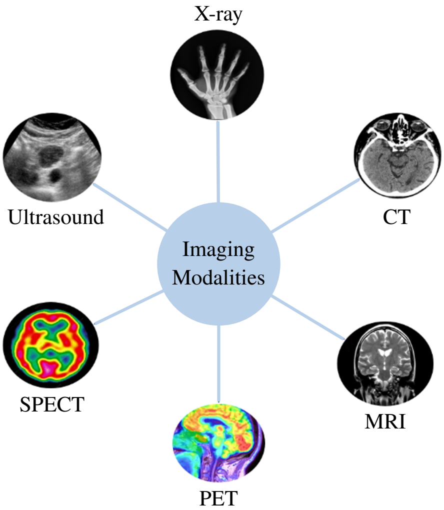
T1-weighted (T1w) *(Grey vs. White Matter)*

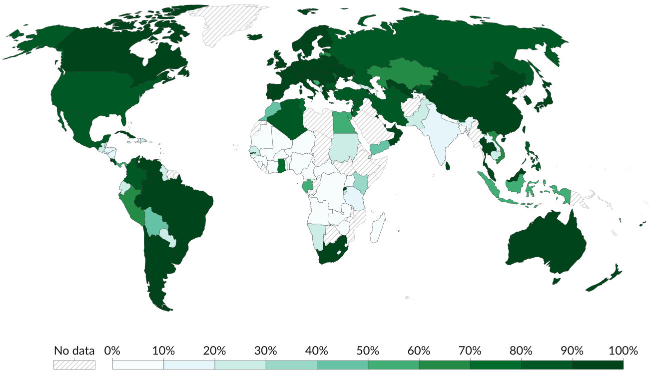
T2-weighted (T2w) *(Fluid-Filled Regions)*

FLAIR *(Abnormalities)*

MRI Scans with Various ***Modalities*** *from the* ***Same*** *Subject*

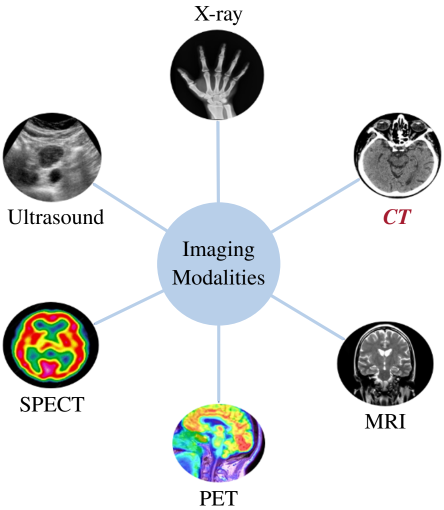
Medical Imaging Modalities | *Variety ≠ Accessibility*

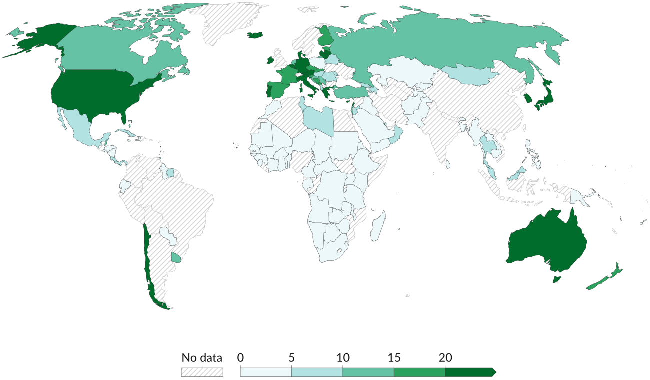




Percentage of Population Covered by ***Health Insurance****, 2017*

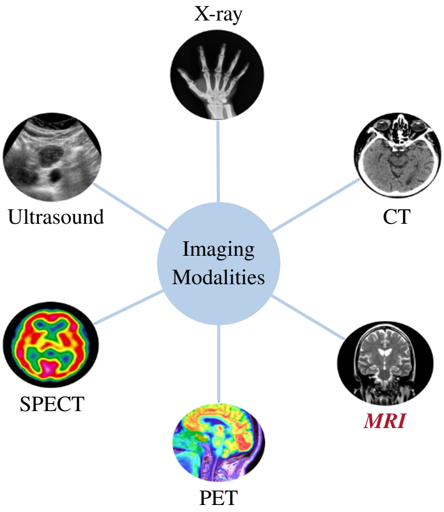
Medical Imaging Modalities | *Variety ≠ Accessibility*

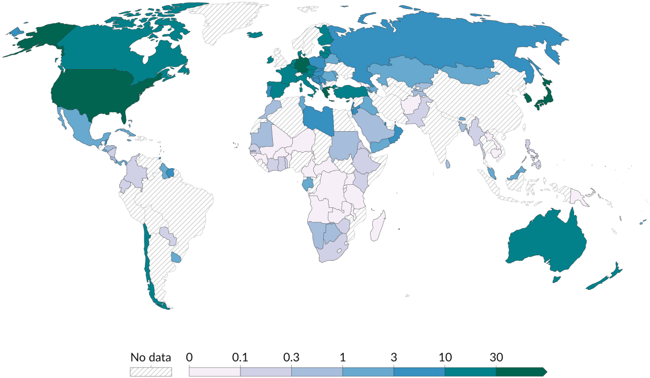




CT Imaging Units Per Million People, 2022

Medical Imaging Modalities | *Variety ≠ Accessibility*



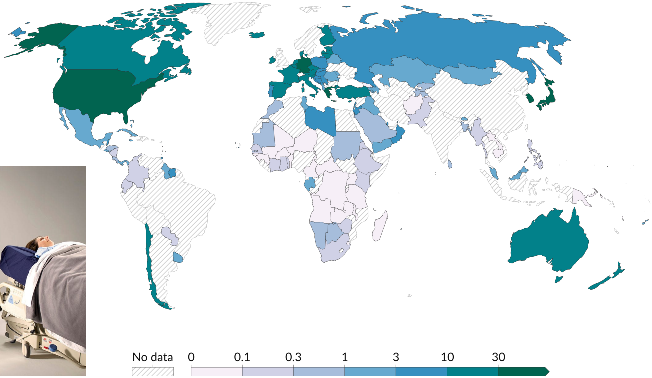


MRI Units Per Million People, 2022

Medical Imaging Modalities | *Variety* & *Accessibility*, *in the Future?*

Field Strength	*Price*
~~1.5 T~~	~~> $1,000,000~~
~~3 T~~	~~> $3,000,000~~
~~7 T~~	~~> $7,000,000~~
0.064 T	**~ $250,000**

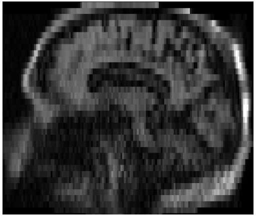
Ultra-Low-Field & *Portable* *MRI Scanner from Hyperfine*



MRI Units Per Million People, 2022

Medical Imaging Modalities | *Variety* & *Accessibility*, *in the Future?*

Field Strength	*Price*	
~~1.5 T~~	~~> $1,000,000~~	
~~3 T~~	~~> $3,000,000~~	
~~7 T~~	~~> $7,000,000~~	
0.064 T	~ **$250,000**	✗ **Low-Quality**



Ultra-Low-Field & ***Portable*** *MRI Scanner from Hyperfine*

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Data Variety
in
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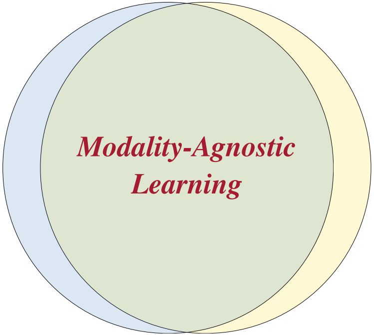
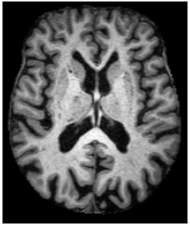
Data Variety
in
Medical Imaging



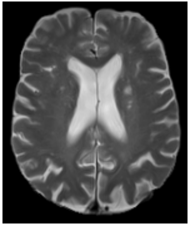
Accessibility Challenges
in
Modern Healthcare

Robust & ***Generalized***

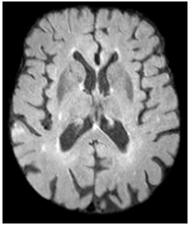
[*Preview*] *Modality-Agnostic* Feature Representation



T1-weighted (T1w)



T2-weighted (T2w)

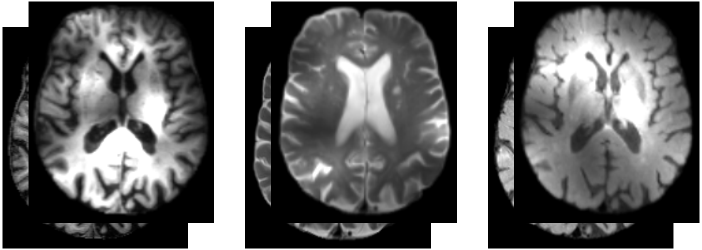


FLAIR

*MRI Scans with Various **Modalities** from the **Same** Subject*

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

[*Preview*] *Modality-Agnostic* Feature Representation



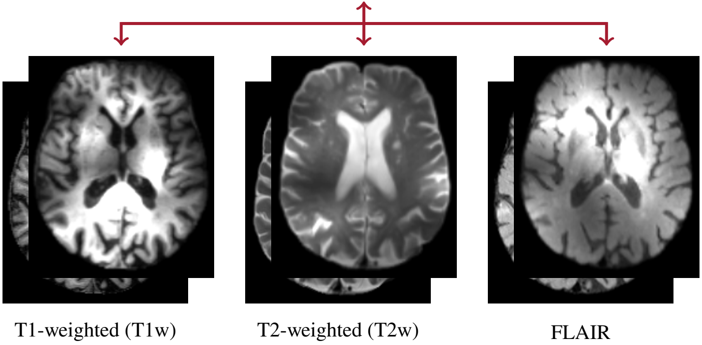
T1-weighted (T1w) T2-weighted (T2w) FLAIR

*MRI Scans with Various **Modalities** & **Qualities** from the **Same** Subject*

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

[*Preview*] *Modality-Agnostic* Feature Representation

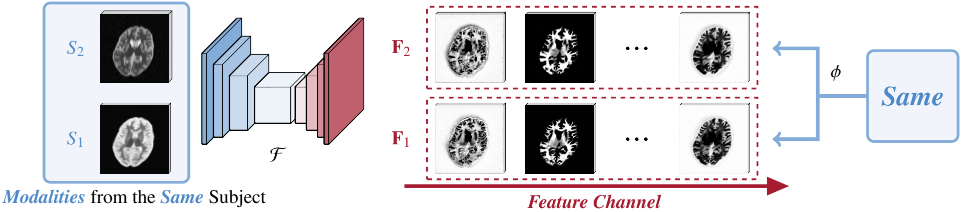
Anatomy-Specific, ***Modality-Agnostic*** Feature Representation



*MRI Scans with Various **Modalities** & **Qualities** from the **Same** Subject*

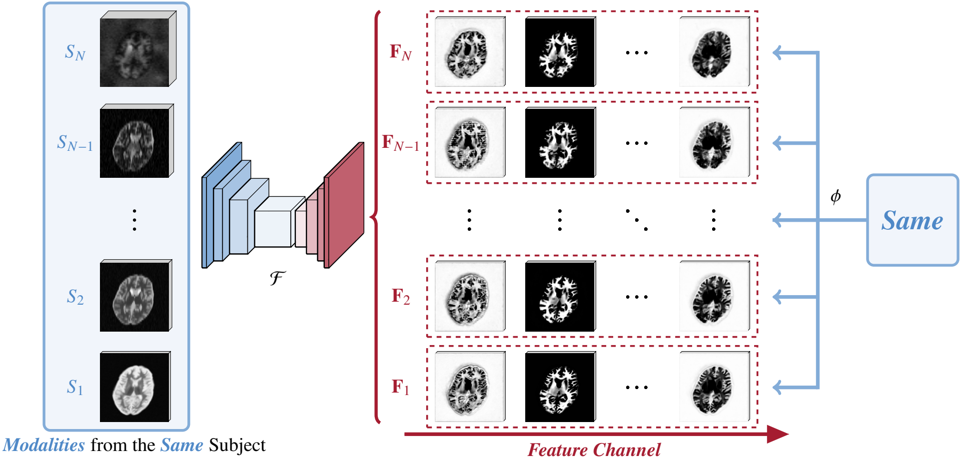
P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

[*Preview*] *Modality-Agnostic* Feature Representation



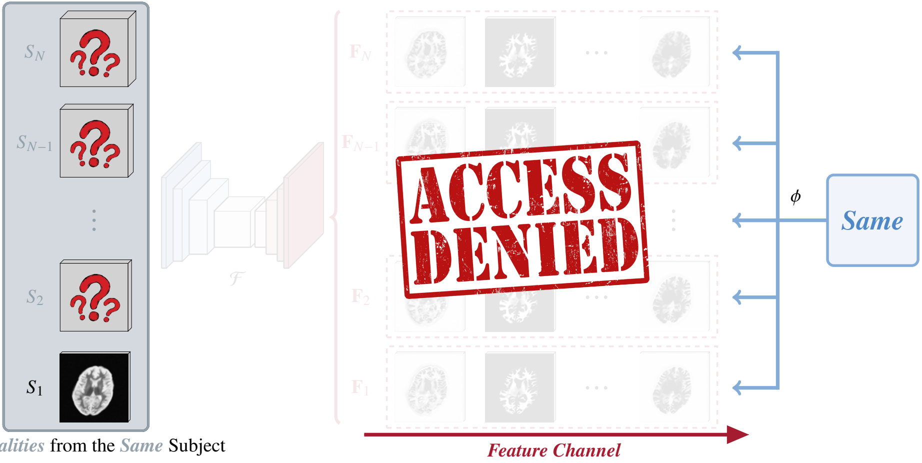
P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

[*Preview*] *Modality-Agnostic* Feature Representation



P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

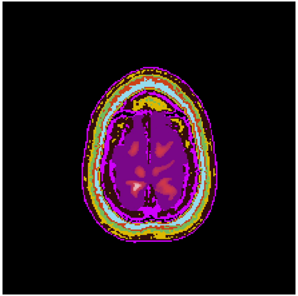
[*Preview*] *Modality-Agnostic* Feature Representation



Modalities from the *Same* Subject

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Image Generation via *Anatomical Domain Randomization*: From Single Anatomy

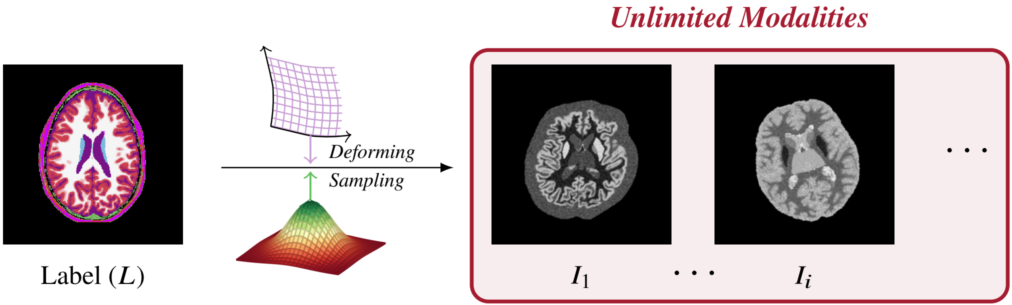


- *Cerebral White Matter*
- *Cerebral Cortex*
- *Lateral Ventricle*
- *Cerebellum White Matter*
- *Cerebellum Cortex*
- *Caudate*
- . . .

Brain *Anatomical* Regions @ FreeSurfer, MGH

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

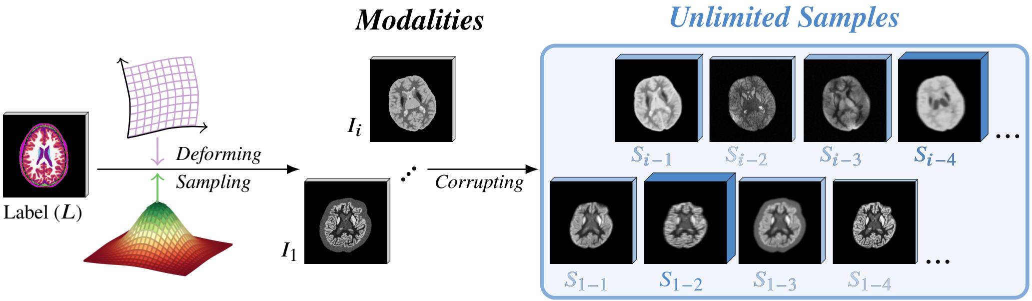
Image Generation via ***Anatomical Domain Randomization*** → Unlimited ***Modalities***



Domain Randomization: Conditioned on ***Anatomical*** Regions

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Image Generation via *Anatomical Domain Randomization* → Unlimited *Samples*



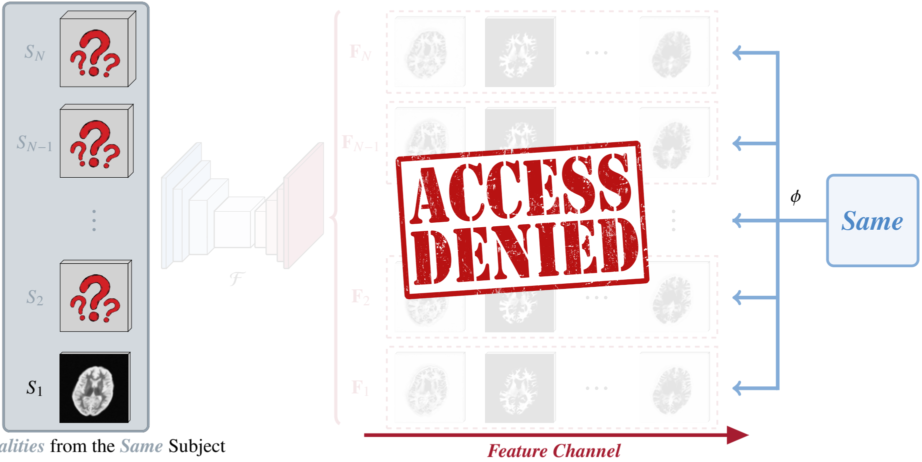
On-the-Fly Corruption Toolbox: **Mild** → **Severe**

Corruption Level

(Resolution, Orientation, Noise, Artifacts, ...)

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

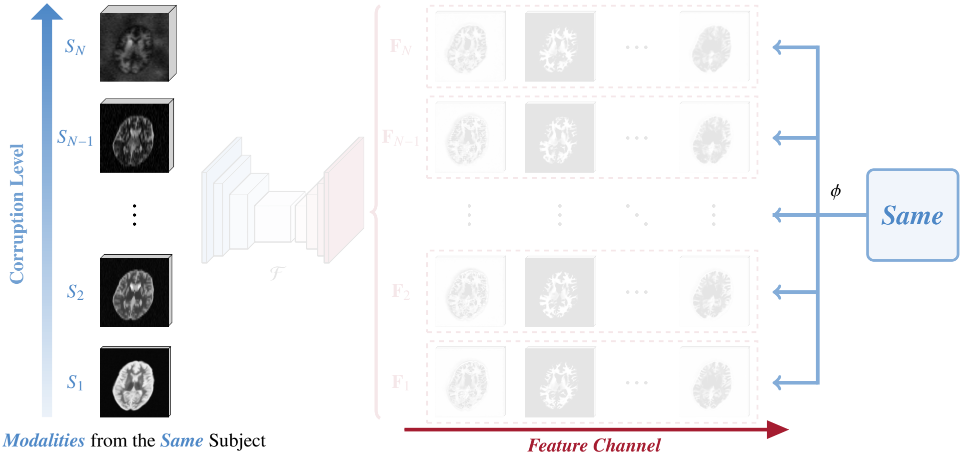
Modality-Agnostic Feature Representation | On-the-Fly *Synthetic* Inputs



Modalities from the *Same* Subject

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

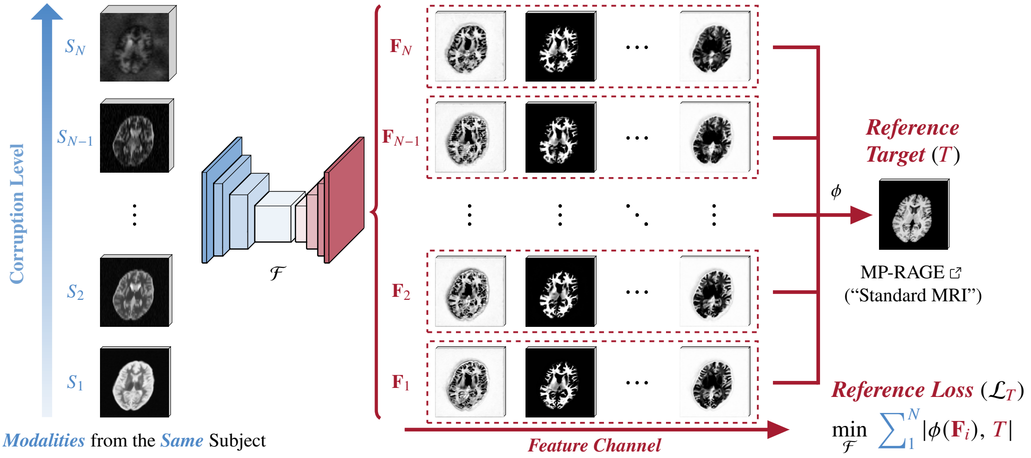
Modality-Agnostic Feature Representation | On-the-Fly *Synthetic* Inputs



Modalities from the *Same* Subject

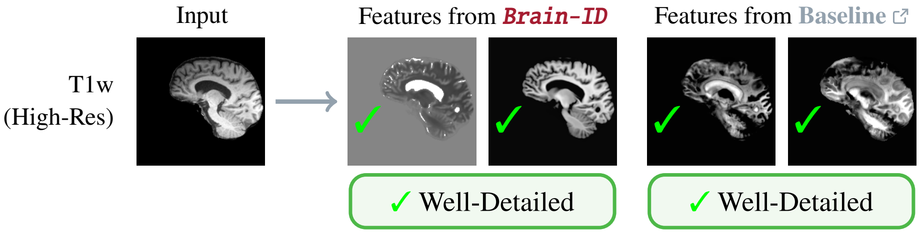
P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Modality-Agnostic Feature Representation | Framework Overview



P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Feature Robustness | Input Image *Quality*

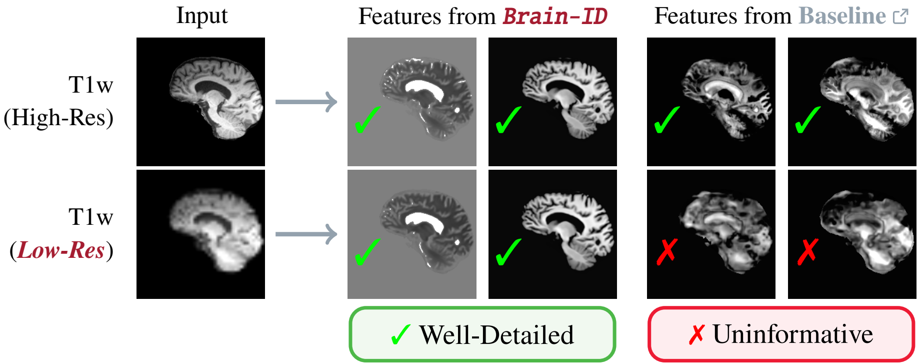


* Feature Maps Selected from the Last Layer of UNet

* Baseline: Trained from Real T1w MRI ($n = 3000$)

P. Liu et al.: ***Brain-ID***: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Feature Robustness | Input Image *Quality*

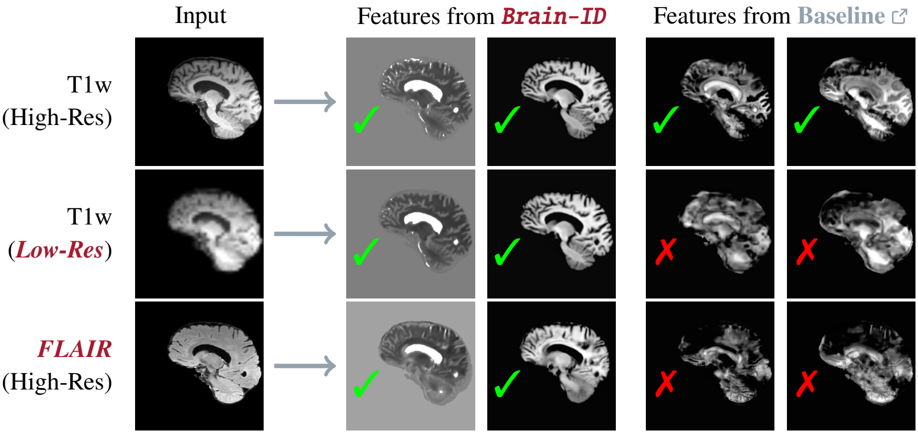


* Feature Maps Selected from the Last Layer of UNet

* Baseline: Trained from Real T1w MRI ($n = 3000$)

P. Liu et al.: **Brain-ID**: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Feature Robustness | Input Image *Quality* & *Modality*

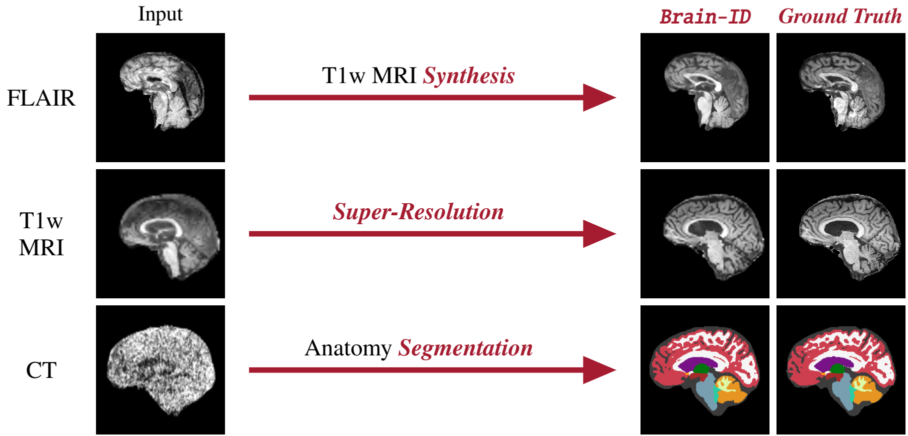


✓ Well-Detailed

✗ Uninformative

P. Liu et al.: ***Brain-ID***: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

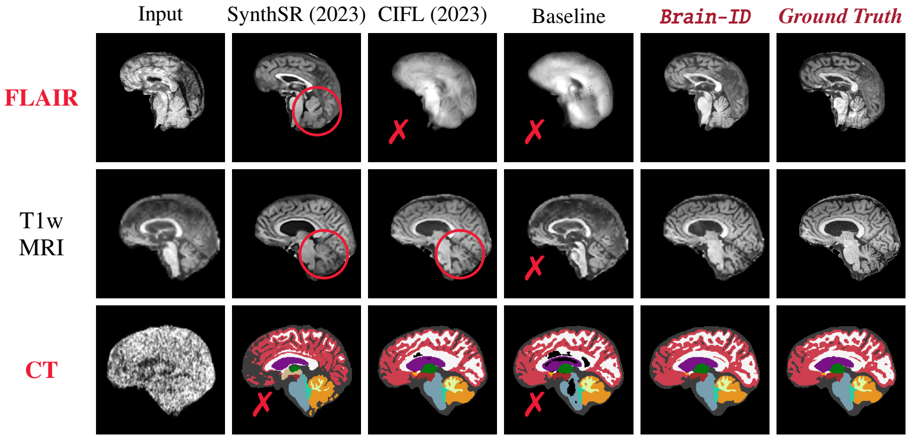
Feature Robustness & *Generalizability* | Downstream Adaptations on *Small* Datasets



Downstream Tasks: Fine-Tuned on **n = 30** samples

P. Liu et al.: ***Brain-ID***: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Feature Robustness & *Generalizability* | Downstream Adaptations on *Small* Datasets

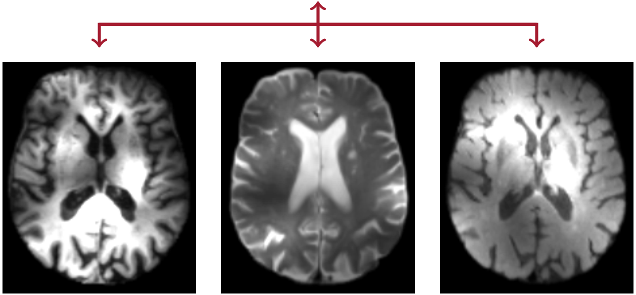


Downstream Tasks: Fine-Tuned on **n = 30** samples

P. Liu et al.: ***Brain-ID***: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

[*Recap*] Brain-ID's *Modality-Agnostic* Learning

Anatomy-Specific, ***Modality-Agnostic*** Feature Representation @ ***Brain-ID***



T1-weighted (T1w) | T2-weighted (T2w) | FLAIR

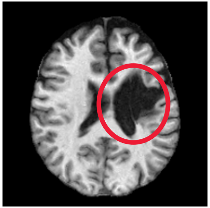
*MRI Scans with Various **Modalities** & **Qualities** from the **Same** Subject*

P. Liu et al.: ***Brain-ID***: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

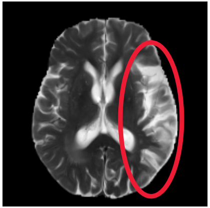
Modality-Agnostic Learning | Tissue *Abnormalities* (*Pathology*)

~~*Anatomy-Specific*, *Modality-Agnostic* Feature Representation @ `Brain-ID`~~

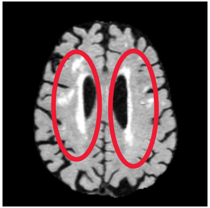
✗ Varying Pathology *Types* & *Shapes*



Stroke @ ATLAS
T1-weighted (T1w)



Tumor @ BraTS
T2-weighted (T2w)



WMH @ ADNI3
FLAIR

*MRI Scans with Various Tissue **Abnormalities** (**Pathology**) across **Different** Datasets*

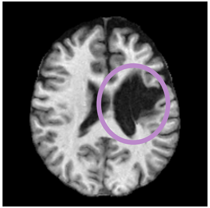
P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Modality-Agnostic Learning | Tissue *Abnormalities* (*Pathology*)

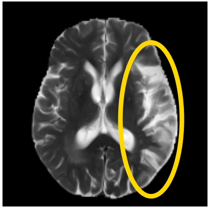
~~*Anatomy-Specific*, *Modality-Agnostic* Feature Representation @ **Brain-ID**~~

✗ Varying Pathology *Types* & *Shapes*

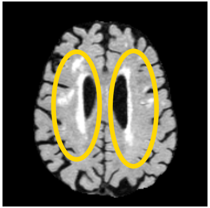
✗ Varying *Appearances* on Modalities



Darker on
T1-weighted (T1w)



Brighter on
T2-weighted (T2w)



Brighter on
FLAIR

*MRI Scans with Various Tissue **Abnormalities** (**Pathology**) across **Different** Datasets*

P. Liu et al.: **Brain-ID**: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

[*Preview*] From `Brain-ID` to `UNA` | Bridging *Diseased* ↦ *Healthy*

Stroke @ ATLAS
T1-weighted (T1w)

Input

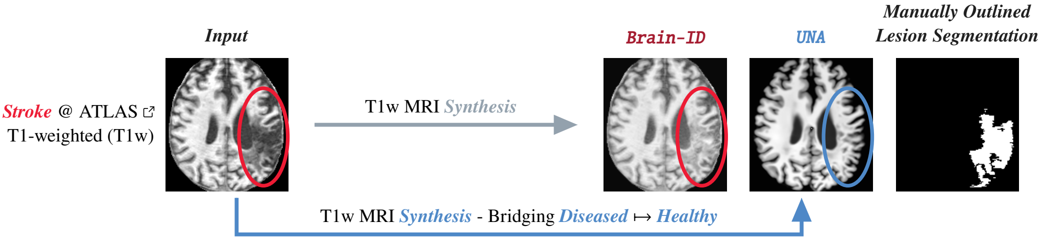
T1w MRI *Synthesis*

`Brain-ID`

Manually Outlined Lesion Segmentation

P. Liu et al.: ***`Brain-ID`***: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)
P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)
P. Liu et al.: ***U***nraveling ***N***ormal ***A***natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

[*Preview*] From Brain-ID to UNA | Bridging *Diseased* ↦ *Healthy*



P. Liu et al.: ***Brain-ID***: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

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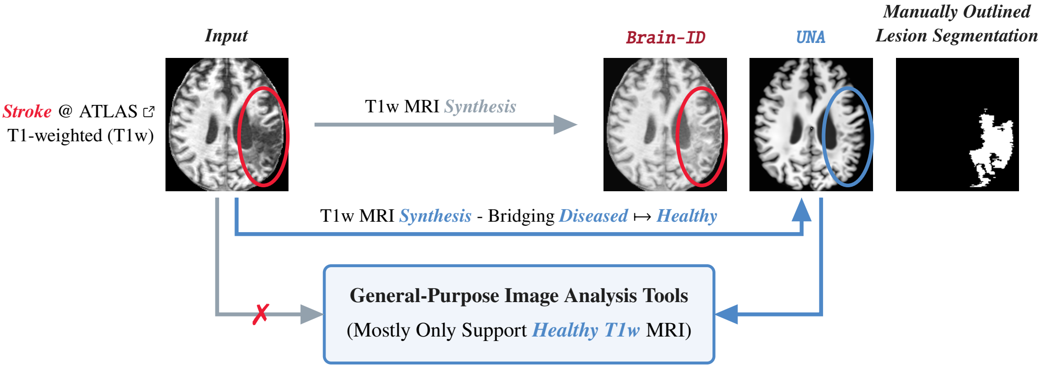
[*Preview*] From Brain-ID to UNA | Bridging *Diseased* ↦ *Healthy*



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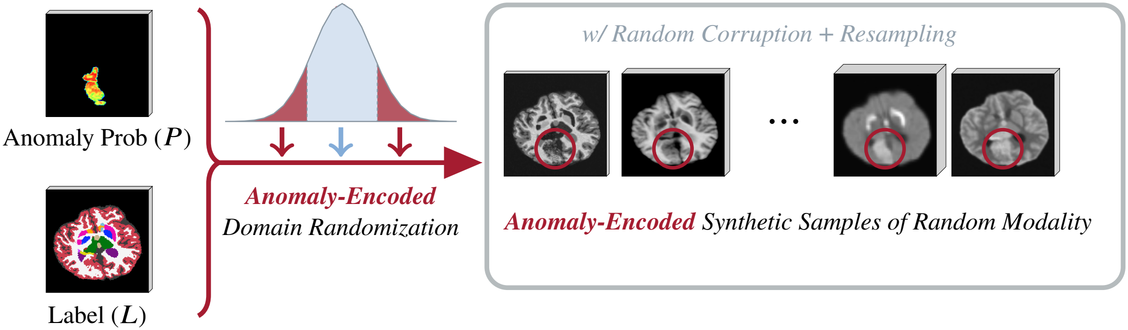
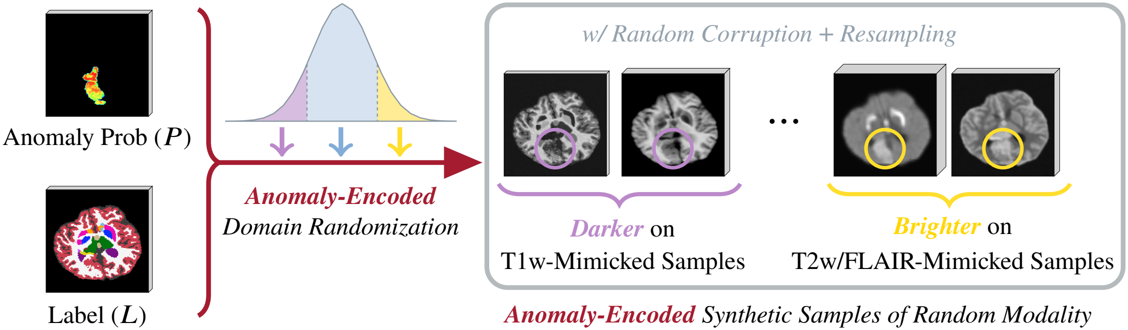
P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Image Generation via *Anomaly-Encoded* Domain Randomization



P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)
P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Image Generation via *Anomaly-Encoded* Domain Randomization

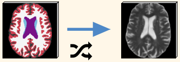


Anomaly-Encoded *Synthetic Samples of Random Modality*

P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)
P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Modality-Agnostic Synthesis | On-the-Fly *Synthetic Healthy* & *Diseased* Inputs

Anatomical Domain Randomization @ ***Brain-ID***



L I_{Healthy}

UNA's Generation is Conditioned on ***Healthy*** Anatomy

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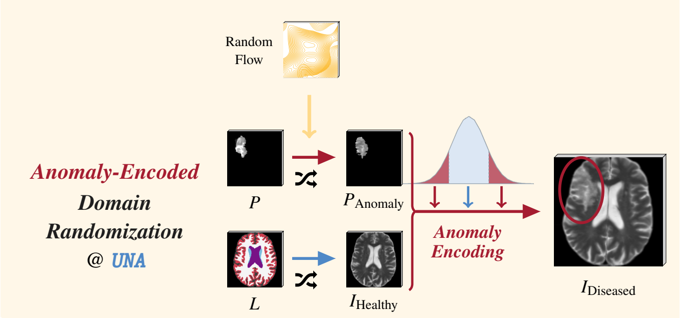
P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)
P. Liu et al.: ***U***nraveling ***N***ormal ***A***natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

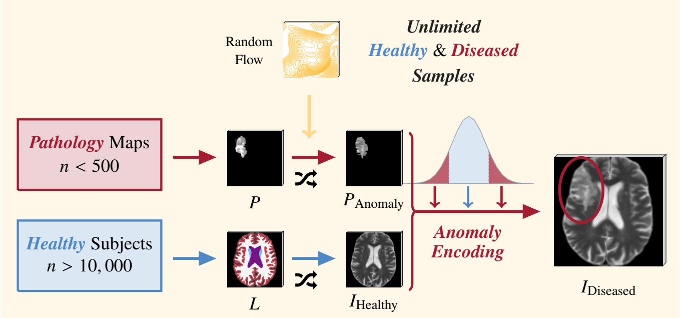
Modality-Agnostic Synthesis | On-the-Fly *Synthetic Healthy* & *Diseased* Inputs



UNA Generates Diseased & Healthy Images ***On-the-Fly***

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)
P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)
P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Modality-Agnostic Synthesis | On-the-Fly *Synthetic Healthy* & *Diseased* Inputs



UNA Generates Diseased & Healthy Images ***On-the-Fly***

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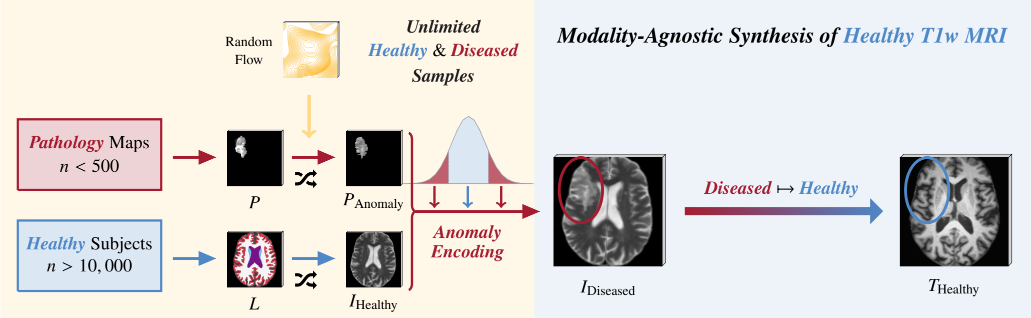
P. Liu et al.: ***U***nraveling ***N***ormal ***A***natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

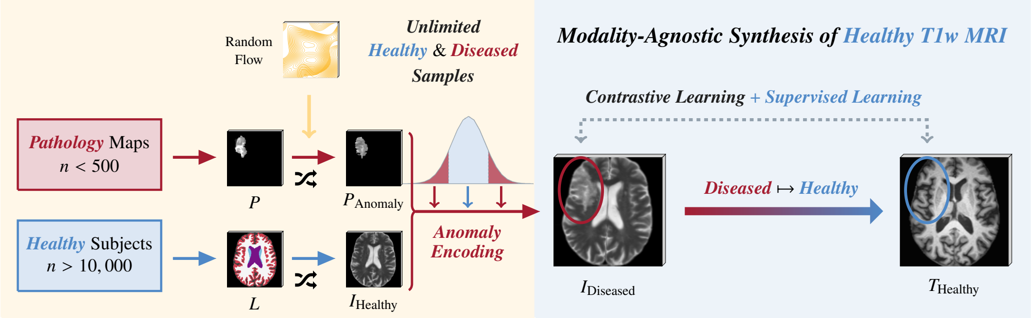
Modality-Agnostic Synthesis | Bridging *Diseased* ↦ *Healthy*



UNA Synthesizes ***Healthy T1w MRI*** from Diseased & Healthy Images of ***Any Modality***

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)
P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)
P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

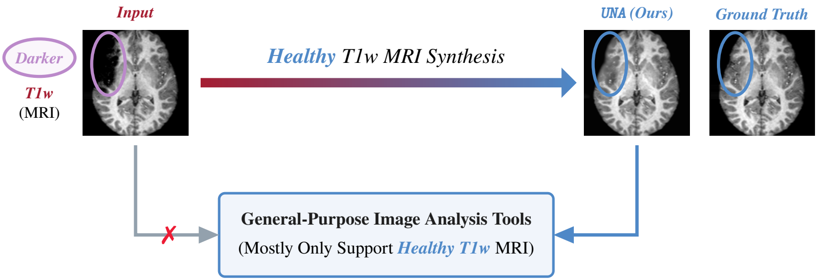
Modality-Agnostic Synthesis | Bridging Diseased ↦ Healthy: *Beyond Annotations*



UNA's Healthy-to-Diseased Generation Naturally Enables ***Supervised Learning***

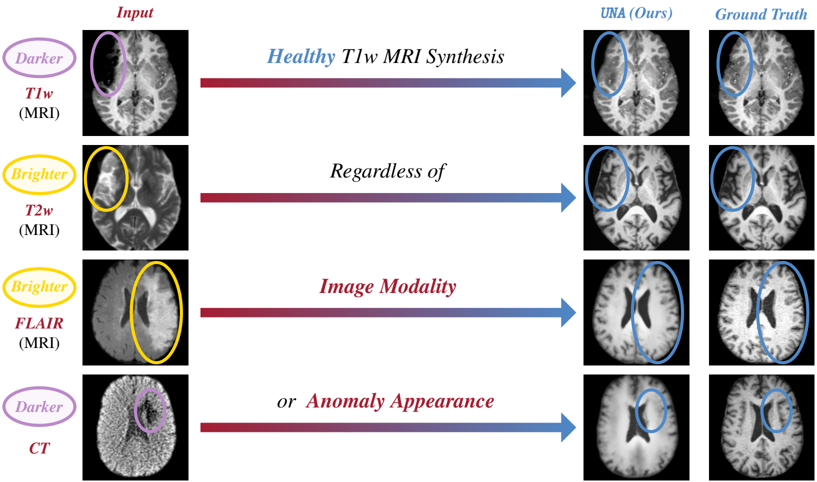
P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)
P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)
P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Robustness & *Generalizability* | Image Modality & Anomaly Appearance (Simulations)



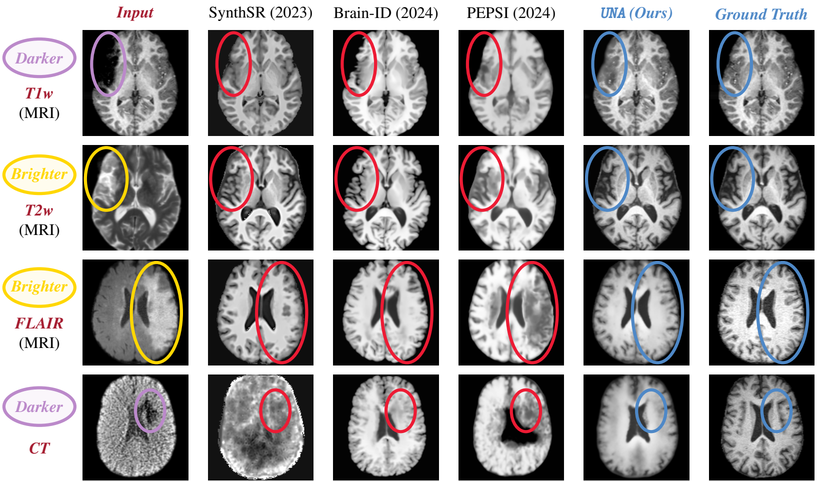
P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Robustness & *Generalizability* | Image Modality & Anomaly Appearance (Simulations)



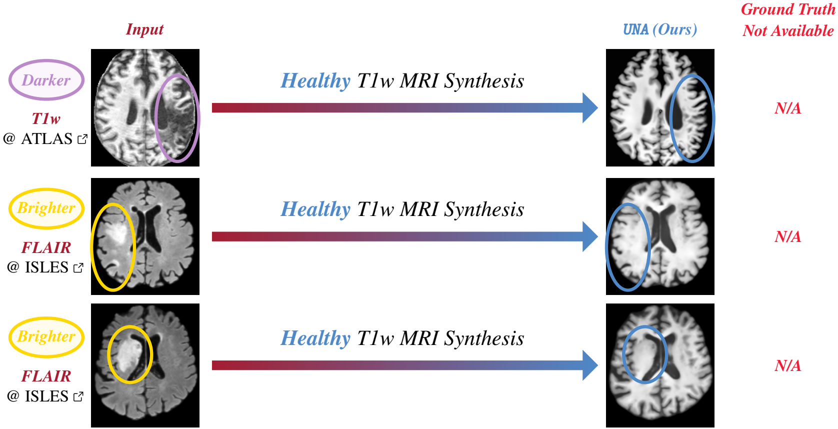
P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Robustness & *Generalizability* | Image Modality & Anomaly Appearance (Simulations)



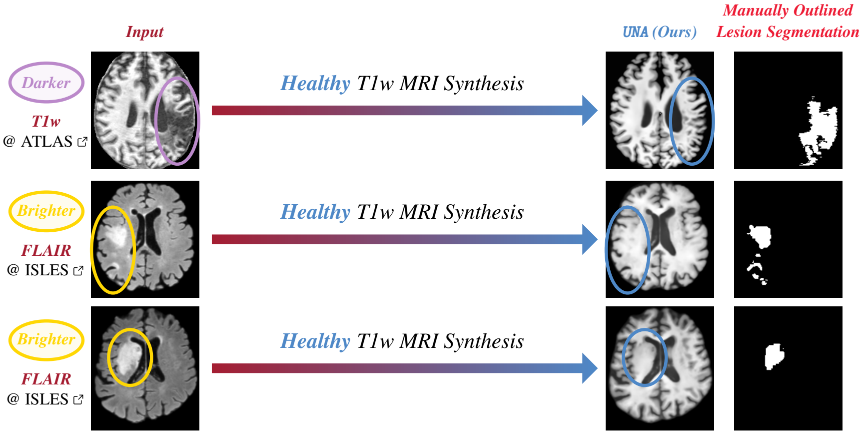
P. Liu et al.: **U**nraveling **N**ormal **A**natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Robustness & ***Generalizability*** | Image Modality & Anomaly Appearance (Stroke)



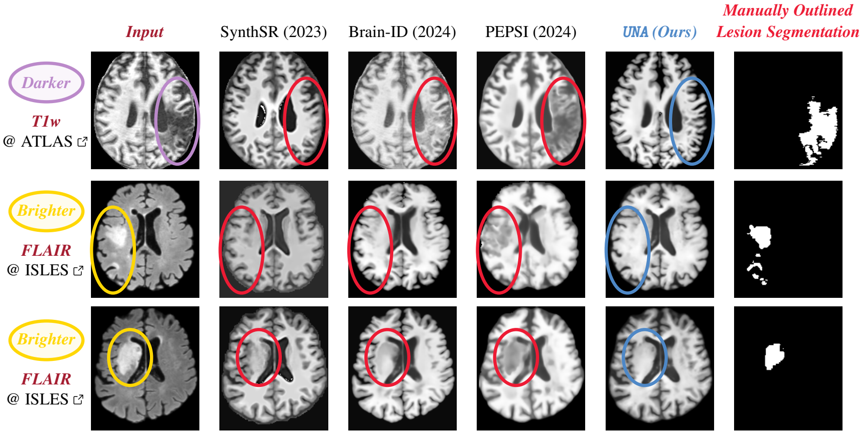
P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Robustness & ***Generalizability*** | Image Modality & Anomaly Appearance (Stroke)



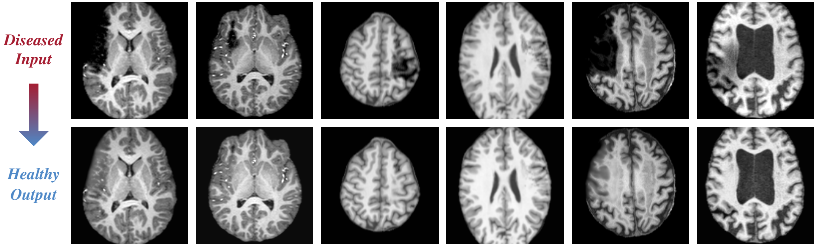
P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Robustness & *Generalizability* | Image Modality & Anomaly Appearance (Stroke)



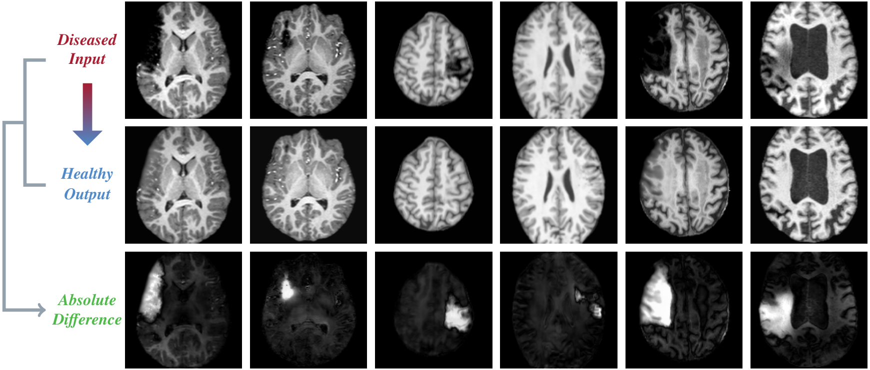
P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Robustness & ***Generalizability*** | Anomaly Detection ***Beyond Annotations***



P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

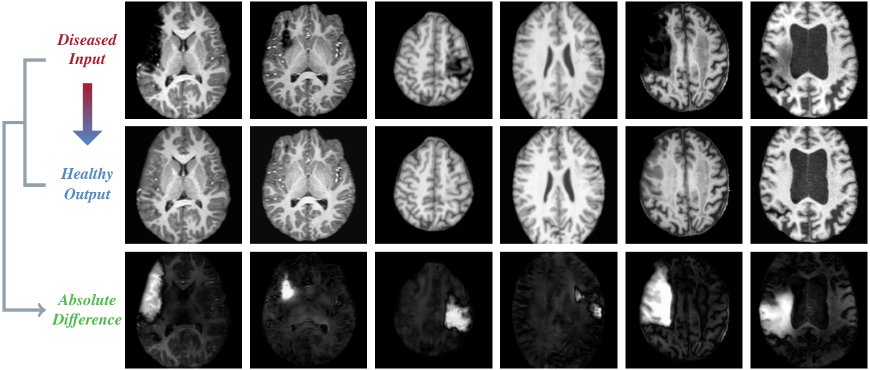
Robustness & *Generalizability* | Anomaly Detection *Beyond Annotations*



✓ Manual Annotations *Unavailable*

P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Robustness & *Generalizability* | Anomaly Detection *Beyond Annotations*

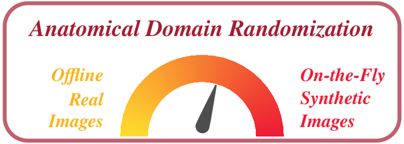


✓ Manual Annotations *Unavailable*

✓ Annotation *Gaps* Across Datasets

P. Liu et al.: **U**nraveling **N**ormal **A**natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

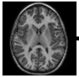
[*Summary*] Modality-Agnostic Foundation Model | ***Ready-to-Use Software @ FreeSurfer***



P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)
P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)
P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)
P. Liu et al.: A Modality-Agnostic Multi-Task Foundation Model for Human Brain Imaging. *Under Review at **IEEE TMI*** (2025)

[*Summary*] Modality-Agnostic Foundation Model | *Ready-to-Use Software @ FreeSurfer*

Inputs



MR / CT / ...

Currently Supported Tasks:

- ✓ ***Image Synthesis*** *(T1w MRI, T2w MRI, FLAIR, CT, ...)*
- ✓ ***Super-Resolution***
- ✓ ***Atlas Registration***
- ✓ ***Surface Extraction***
- ✓ ***Brain Age Estimation***
- ✓ ***Bias Field Correction***
- ✓ ***Anatomy Segmentation***

FreeSurfer

Modality-Agnostic Learning

Anatomical Domain Randomization

Offline Real Images

On-the-Fly Synthetic Images

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

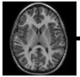
P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)

P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

P. Liu et al.: A Modality-Agnostic Multi-Task Foundation Model for Human Brain Imaging. *Under Review at* ***IEEE TMI*** (2025)

[*Summary*] Modality-Agnostic Foundation Model | *Ready-to-Use Software @ FreeSurfer*

Inputs



MR / CT / ...

Currently Supported Tasks:

- ✓ ***Image Synthesis*** *(T1w MRI, T2w MRI, FLAIR, CT, ...)*
- ✓ ***Super-Resolution***
- ✓ ***Atlas Registration***
- ✓ ***Surface Extraction***
- ✓ ***Brain Age Estimation***
- ✓ ***Bias Field Correction***
- ✓ ***Anatomy Segmentation***

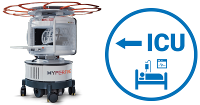
FreeSurfer

Modality-Agnostic Learning

Anatomical Domain Randomization

✓ Out-of-the-Box Usage

✓ Offline Fine-Tuning



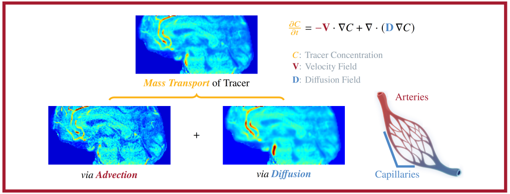
Low-Field & Portable MRI @ Hyperfine

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)
P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)
P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)
P. Liu et al.: A Modality-Agnostic Multi-Task Foundation Model for Human Brain Imaging. *Under Review at* ***IEEE TMI*** (2025)

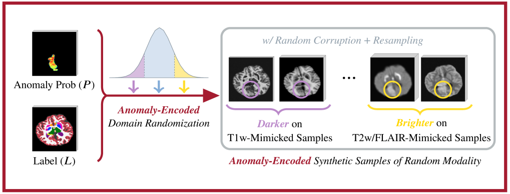
Robust and Interpretable Learning for Modern Healthcare

Research Summary | *Modeling* & *Applications*

Modeling



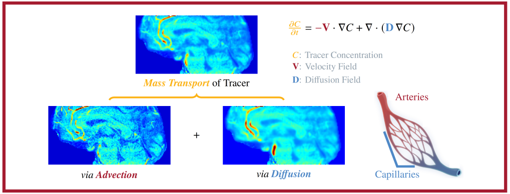
Physics-Driven Learning of Time-Series Dynamics



Domain Randomization & Modality-Agnostic Learning

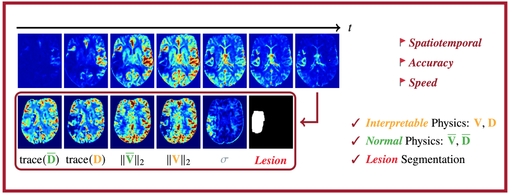
Research Summary | *Modeling* & *Applications*

Modeling

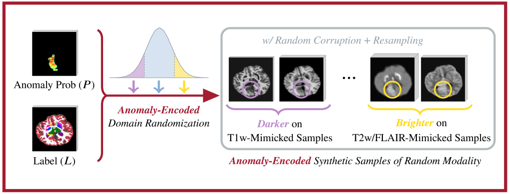


Physics-Driven Learning of Time-Series Dynamics

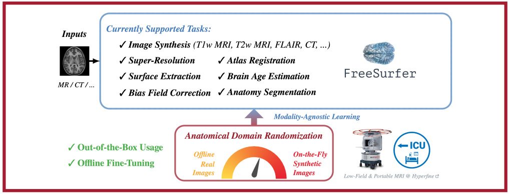
Applications



End-to-End & Interpretable Lesion Detection



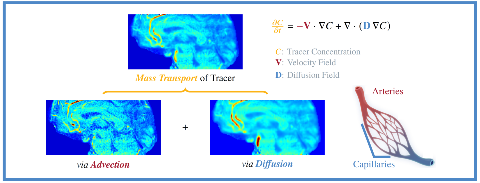
Domain Randomization & Modality-Agnostic Learning



Robust & Generalized Analysis for Medical Imaging

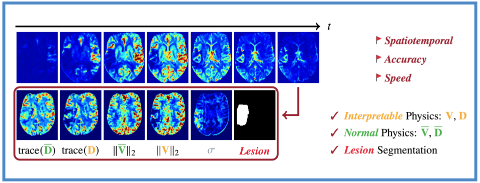
[*Future*] Research Summary | *Modeling* & *Applications*

Modeling



Physics-Driven Learning of Time-Series Dynamics

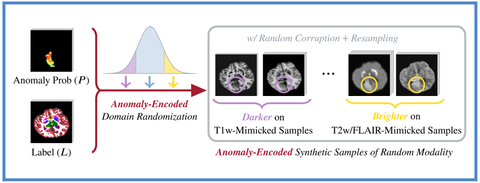
Applications



End-to-End & Interpretable Lesion Detection

Motivate

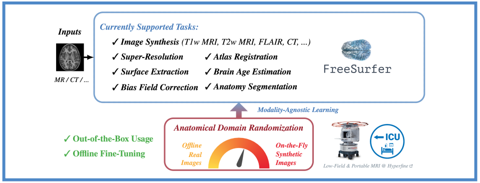
Apply



Domain Randomization & Modality-Agnostic Learning

Motivate

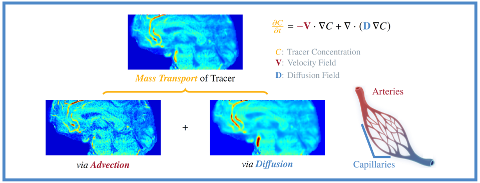
Apply



Robust & Generalized Analysis for Medical Imaging

[*Future*] Research Summary | *Physics-Driven Learning* of Time-Series Dynamics

Modeling

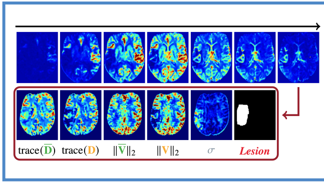


Physics-Driven Learning of Time-Series Dynamics

Motivate

Apply

Applications



- *Spatiotemporal*
- *Accuracy*
- *Speed*

✓ *Interpretable* Physics: $\mathbf{V}$, $\mathbf{D}$
✓ *Normal* Physics: $\bar{\mathbf{V}}$, $\bar{\mathbf{D}}$
✓ *Lesion* Segmentation

End-to-End & Interpretable Lesion Detection

*Interpretable **Physics-Driven** Learning & Prediction*

Detection & Diagnosis ⟷ ***Treatment Outcomes***

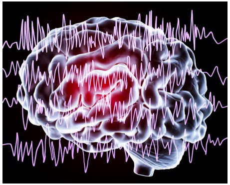
(Inverse Reasoning) *Multimodal Learning* | *Dynamic Modeling* | *Uncertainty Estimation* *(Dynamic Prediction)*

[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Multimodal Learning*

Modeling

- ***Multimodal Learning***
  - Vision + Text/Signal/...
  - Vision + Geometry

Metadata & Medical Reports



Sensor Data, E.g., Electroencephalogram (EEG)

Angiography (MR) for 3D Vascular Modeling

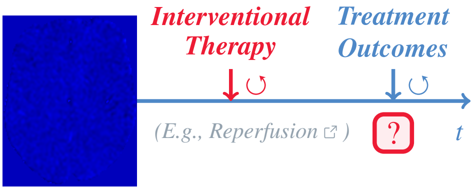
Incorporating Information from ***Multiple Modalities***

S. Çimen et al.: Reconstruction of Coronary Arteries from X-ray Angiography. *Medical Image Analysis* (2016)
K. Singhal et al.: Large Language Models Encode Clinical Knowledge. *Nature* (2023)

[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Dynamic Modeling*

Modeling

- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- *Dynamic Modeling*
  - Prediction & Uncertainty Estimation



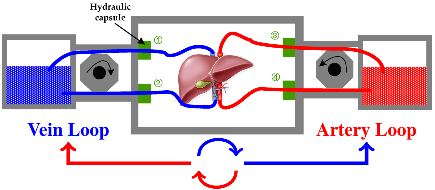
1/2 - From Diagnosis to *Treatment*

E. Antonelo et al.: Physics-Informed Neural Nets for Control of Dynamical Systems. *Neurocomputing* (2024)
X. Hu, K. Gopinath, ***P. Liu*** et al.: Hierarchical Uncertainty Estimation for Learning-Based Registration in Neuroimaging. ***ICLR*** (2025)

[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Dynamic Modeling*

Modeling

- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- ***Dynamic Modeling***
  - Prediction & Uncertainty Estimation



Machine Perfusion in Liver: Vein & Artery Loops

2/2 - From In Vivo to ***Ex Vivo***

S. D. St Peter et al.: Liver and Kidney Preservation by Perfusion. *The Lancet* (2002)
"Liver in a Box" Offers Potential for Providing Liver Transplant to More Patients. *Mayo Clinic News* (2024)

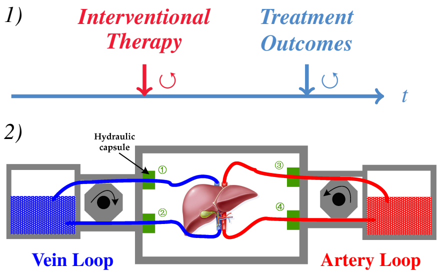
[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Treatment* & *Surgery*

Modeling

- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- Dynamic Modeling
  - Prediction & Uncertainty Estimation

Applications

- *Treatment & Surgery*



1) ***Interventional Therapy*** and *2)* ***Ex Vivo Perfusion***

A. Bagai et al.: Reperfusion Strategies in Acute Coronary Syndromes. *Circulation Research* (2014)
"Liver in a Box" Offers Potential for Providing Liver Transplant to More Patients. *Mayo Clinic News* (2024)

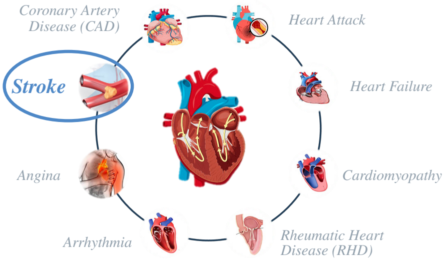
[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Organs* & *Diseases*

Modeling

- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- Dynamic Modeling
  - Prediction & Uncertainty Estimation

Applications

- Treatment & Surgery
- *Organs & Diseases*



Common Type of *Cardiovascular Diseases (CVDs)*

P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)
P. Liu et al.: Deep Decomposition for Stochastic Normal-Abnormal Transport. ***CVPR*** (2022) (★ *Oral*)

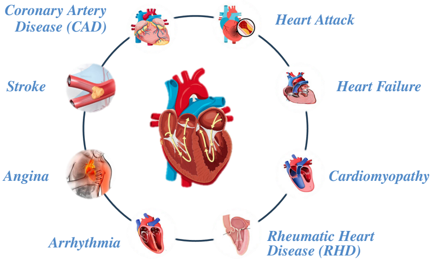
[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Organs* & *Diseases*

Modeling

- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- Dynamic Modeling
  - Prediction & Uncertainty Estimation

Applications

- Treatment & Surgery
- *Organs & Diseases*



Common Type of *Cardiovascular Diseases (CVDs)*

G. Bastarrika et al.: CT of Coronary Artery Disease. *Radiology* (2009)
O. R. Coelho-Filho et al.: MR Myocardial Perfusion Imaging. *Radiology* (2013)

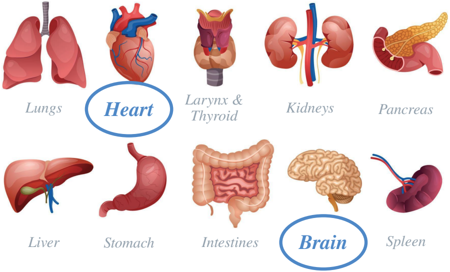
[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Organs* & *Diseases*

Modeling

- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- Dynamic Modeling
  - Prediction & Uncertainty Estimation

Applications

- Treatment & Surgery
- *Organs & Diseases*



Internal Human *Organs*

G. Bastarrika et al.: CT of Coronary Artery Disease. *Radiology* (2009)
O. R. Coelho-Filho et al.: MR Myocardial Perfusion Imaging. *Radiology* (2013)

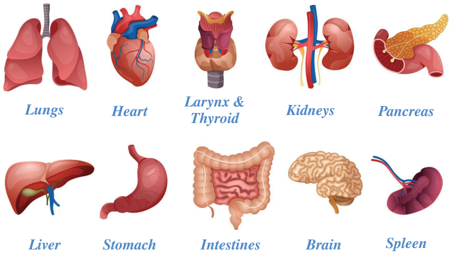
[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Organs* & *Diseases*

Modeling

- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- Dynamic Modeling
  - Prediction & Uncertainty Estimation

Applications

- Treatment & Surgery
- *Organs & Diseases*



Internal Human *Organs*

S. R. Hopkins et al.: Imaging Lung Perfusion. *Journal of Applied Physiology* (2012)
S. H. Kim et al.: CT Perfusion of the Liver: Principles and Applications in Oncology. *Radiology* (2014)

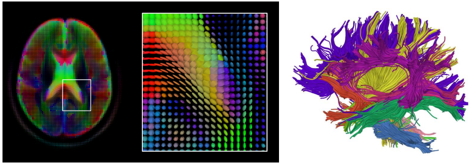
[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Tracking* & *Prediction*

Modeling

- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- Dynamic Modeling
  - Prediction & Uncertainty Estimation

Applications

- Treatment & Surgery
- Organs & Diseases
- ***Tracking & Prediction***
  - Representations: Voxels, Points, Meshes, ...



Diffusion Tensor Imaging (DTI) → *Fiber Tractography (FT)*

1/3 - ***Fiber Tracking*** From Diffusion Tensors

P. Liu et al.: Deep Modeling of Growth Trajectories for Longitudinal Prediction of Missing Infant Cortical Surfaces. ***IPMI*** (2019) (★ *Oral*)

Z. Shen, J. Feydy, ***P. Liu*** et al.: Accurate Point Cloud Registration with Robust Optimal Transport. ***NeurIPS*** (2021)

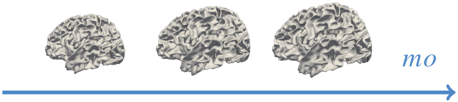
[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Tracking* & *Prediction*

Modeling

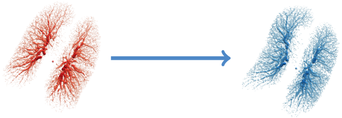
- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- Dynamic Modeling
  - Prediction & Uncertainty Estimation

Applications

- Treatment & Surgery
- Organs & Diseases
- ***Tracking & Prediction***
  - Representations: Voxels, Points, Meshes, ...



Longitudinal Surface Prediction



Point Cloud Registration

2/3 - ***Surface*** and ***Point Cloud*** Representations

P. Liu et al.: Deep Modeling of Growth Trajectories for Longitudinal Prediction of Missing Infant Cortical Surfaces. ***IPMI*** (2019) (★ *Oral*)
Z. Shen, J. Feydy, ***P. Liu*** et al.: Accurate Point Cloud Registration with Robust Optimal Transport. ***NeurIPS*** (2021)

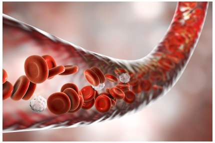
[*Future*] Physics-Driven Learning of Time-Series Dynamics | *Tracking* & *Prediction*

Modeling

- Multimodal Learning
  - Vision + Text/Signal/...
  - Vision + Geometry
- Dynamic Modeling
  - Prediction & Uncertainty Estimation

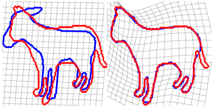
Applications

- Treatment & Surgery
- Organs & Diseases
- ***Tracking & Prediction***
  - Representations: Voxels, Points, Meshes, ...

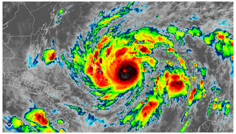


Blood Cells Tracking

Optical Flow for Object Tracking



Non-Rigid Image Registration

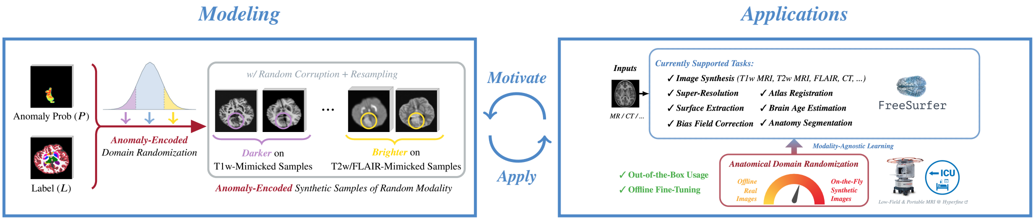


Weather and Climate Forecast

3/3 - ***Fluid-Based*** Modeling and Applications

J. B. Freund: Numerical Simulation of Flowing Blood Cells. *Annual Review of Fluid Mechanics* (2014)
P. Lippe et al.: PDE-Refiner: Achieving Accurate Long Rollouts with Neural PDE Solvers. *NeurIPS* (2023)

[*Future*] Research Summary | *Modality-Agnostic Learning* Towards *Accessible Healthcare*



Domain Randomization & Modality-Agnostic Learning

Robust & Generalized Analysis for Medical Imaging

Modality-Agnostic Learning *via* ***Anomaly-Encoded Data Generation***

Synthetic Data ⟷ ***Clinical Data***

Generative Modeling | ***Domain Adaptation*** | ***Translational Research***

[*Future*] Modality-Agnostic Learning | *Generative Modeling* & *Domain Adaptation*

Data Generation & Modeling

Synthetic → *Generative Modeling* *Domain Adaptation* ← *Real*

N. Charon & L. Younes: Shape Spaces: From Geometry to Biological Plausibility. *Handbook of Math Models and Algorithms in CV and Imaging* (2022)

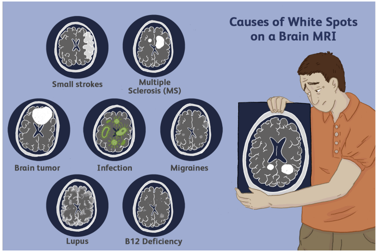
X. Zhao et al.: A Collection of Domain Adaptation Research. *Github Repository Paper List* (2024)

[*Future*] Modality-Agnostic Learning | *Generative Modeling* & *Domain Adaptation*

Data Generation & Modeling

Synthetic → ***Generative Modeling*** / ***Domain Adaptation*** ← *Real*

- *Spatial*



Examples of Lesion ***Types*** & ***Shapes*** on T2w MRIs

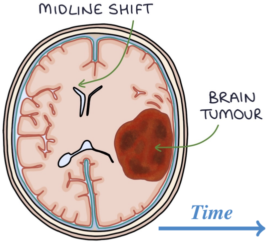
N. Charon & L. Younes: Shape Spaces: From Geometry to Biological Plausibility. *Handbook of Math Models and Algorithms in CV and Imaging* (2022)
X. Zhao et al.: A Collection of Domain Adaptation Research. *Github Repository Paper List* (2024)

[*Future*] Modality-Agnostic Learning | *Generative Modeling* & *Domain Adaptation*

Data Generation & Modeling

Synthetic → ***Generative Modeling*** ***Domain Adaptation*** ← *Real*

- Spatial
- *Spatiotemporal*



1/2 - The *Progression* of Brain Tumors
Pushes & *Displaces* Surrounding Healthy Tissue

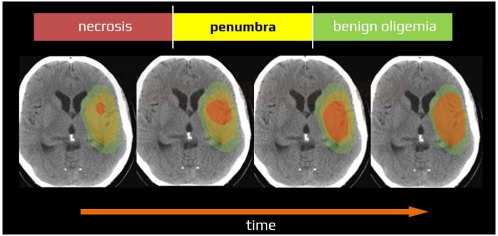
N. Charon & L. Younes: Shape Spaces: From Geometry to Biological Plausibility. *Handbook of Math Models and Algorithms in CV and Imaging* (2022)
Y. Yang et al.: A Survey on Diffusion Models for Time Series, Spatiotemporal Data and Tabular Data. *Github Repository Paper List* (2024)

[*Future*] Modality-Agnostic Learning | *Generative Modeling* & *Domain Adaptation*

Data Generation & Modeling

Synthetic → ***Generative Modeling*** / ***Domain Adaptation*** ← *Real*

- Spatial
- *Spatiotemporal*



2/2 - Lesions ***Worsen*** in Hours/Days after Stroke Onset, Where Penumbra Remains ***Viable for a Limited Time***

H. Saber et al.: Infarct Progression in the Early and Late Phases of Acute Ischemic Stroke. *Neurology* (2021)
Y. Yang et al.: A Survey on Diffusion Models for Time Series, Spatiotemporal Data and Tabular Data. *Github Repository Paper List* (2024)

[*Future*] Modality-Agnostic Learning | *General Analysis* for *Diseased Images*

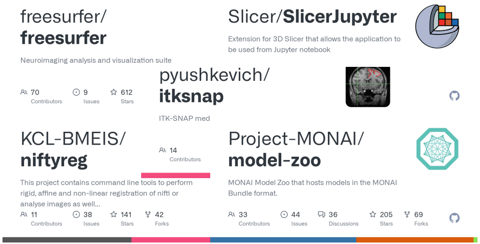
Data Generation & Modeling

Synthetic → Generative Modeling / Domain Adaptation ← *Real*

- ▶ Spatial
- ▶ Spatiotemporal

Broader Applications

- ***General Analysis for Diseased Images***



Most Analysis Tools Suffer from ***Performance Drops***
Given ***Low-Quality*** & ***Diseased*** Images

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)
P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

[*Future*] Modality-Agnostic Learning | *Accessible MRI Diagnosis*

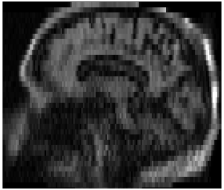
Data Generation & Modeling

Synthetic → Generative Modeling / Domain Adaptation ← *Real*

- ▶ Spatial
- ▶ Spatiotemporal

Broader Applications

- ■ General Analysis for Diseased Images
- ■ ***Accessible MRI Diagnosis***



Low-Field MRI Enables ***Affordable*** & ***Bedside*** Diagnosis, Yet Suffers from ***Less Detailed*** Imaging Quality

N. R. Parasuram et al.: Future of Neurology & Technology: Neuroimaging Made Accessible Using Low-Field, Portable MRI. *Neurology* (2023)
T. C. Arnold et al.: Low-Field MRI: Clinical Promise and Challenges. *Journal of Magnetic Resonance Imaging* (2023)

[*Future*] Modality-Agnostic Learning | *Translational Research* Delivering *Clinical Impact*

Data Generation & Modeling

Synthetic → Generative Modeling / Domain Adaptation ← *Real*

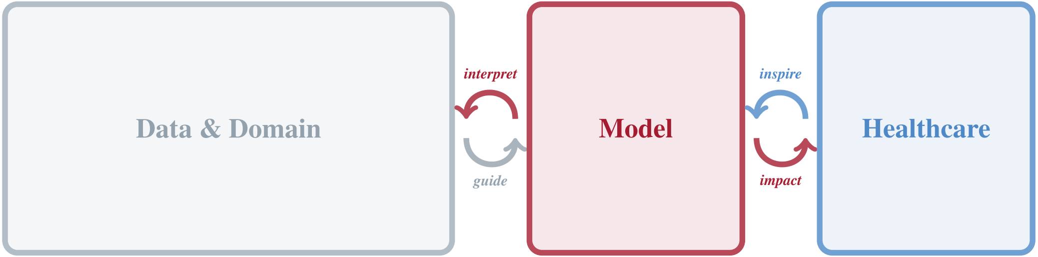
- Spatial
- Spatiotemporal

Broader Applications

- General Analysis for Diseased Images
- *Accessible MRI Diagnosis*
  - *Translational Research*: Assessment, Evaluation, and Analysis of *Clinical Impact*

P. Shah et al.: Artificial Intelligence and Machine Learning in Clinical Development: A Translational Perspective. *NPJ digital medicine* (2019)
C. P. Austin: Opportunities and Challenges in Translational Science. *Clinical and Translational Science* (2021)

[*Future*] *Data* ⇆ Reliable & Generalized *Model* ⇆ Safe & Accessible *Healthcare*



Detection & Diagnosis ⟷ ***Treatment Outcomes***

Interpretable ***Physics-Driven Learning & Prediction***

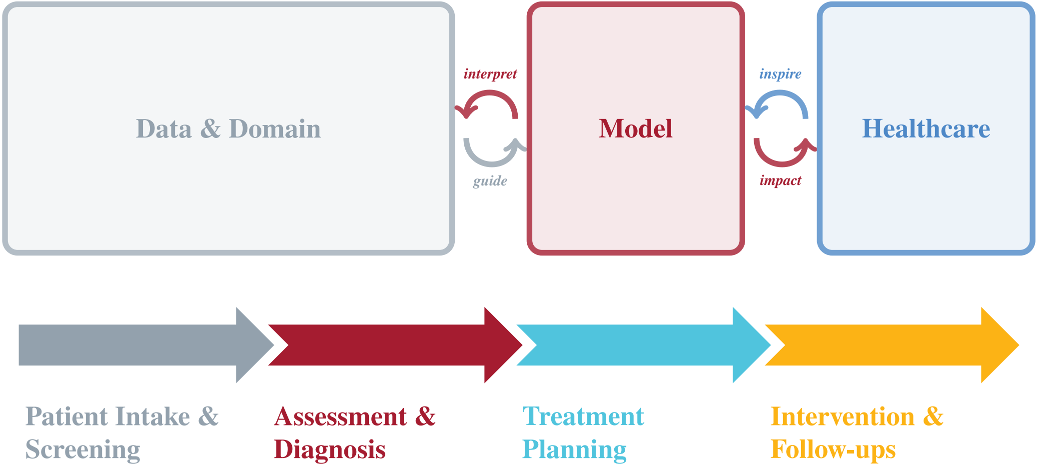
Multimodal Learning | ***Dynamic Modeling*** | ***Uncertainty Estimation***

Synthetic Data ⟷ ***Clinical Data***

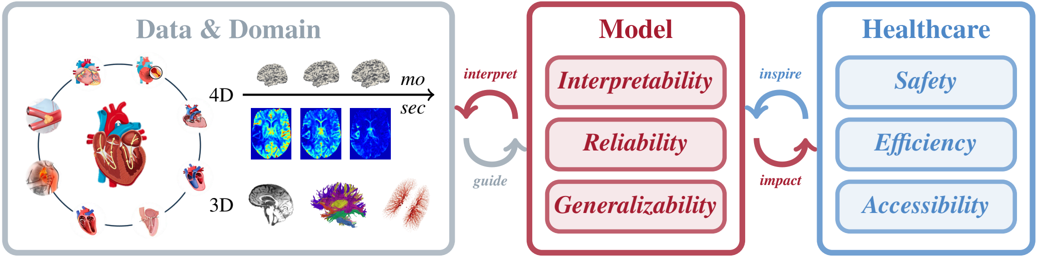
Modality-Agnostic Learning *via* ***Anomaly-Encoded Data Generation***

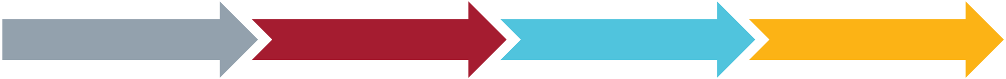
Generative Modeling | ***Domain Adaptation*** | ***Translational Research***

[*Future*] *Data* ⇆ Reliable & Generalized *Model* ⇆ Safe & Accessible *Healthcare*



[*Future*] *External Funding Sources* | Advanced Modeling for Healthcare Applications





Patient Intake & Screening

Assessment & Diagnosis

Treatment Planning

Intervention & Follow-ups

[*Future*] *External Funding Sources* | Advanced Modeling for Healthcare Applications

National & Federal Fundings

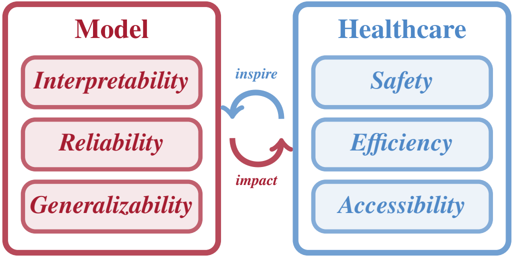
NSF
- *Robust Intelligence (RI)*
- *Smart Health and Biomedical Research in AI and Advanced Data Science (SCH)*, · · ·

American Heart & Stroke Association (AHA & ASA)

Center for Disease Control and Prevention (CDC)

Advanced Scientific Computing Research (ASCR) @ Office of Science, DOE

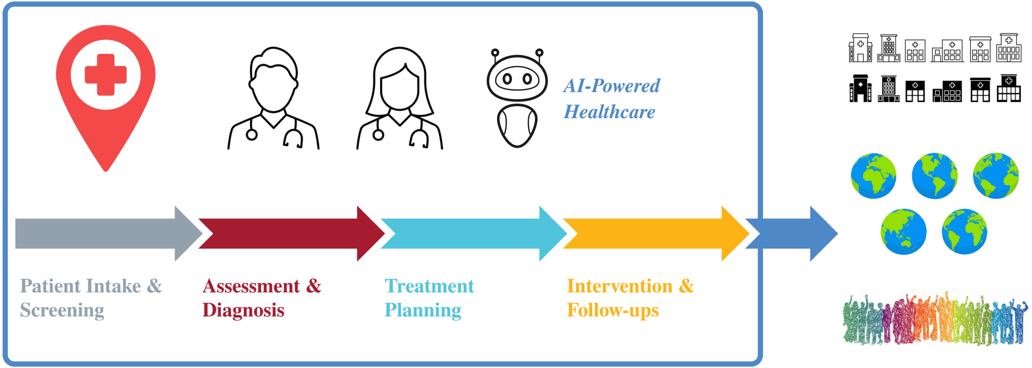
NIH
- *The BRAIN Initiative*
- *National Institute on Aging (NIA)*
- *National Institute of Biomedical Imaging and Bioengineering (NIBIB)*
- *Neurological Disorders and Stroke (NINDS)*
- *National Heart, Lung, and Blood Institute (NHLBI)*
- *National Center for Advancing Translational Sciences (NCATS)*, · · ·



Other Opportunities

Industry & Institutional Awards
- *Meta*
- *Google*
- *Amazon*
- *NVIDIA*
- *Allen Institute*, · · ·

[*Future*] Towards ***Reliable & Accessible Healthcare*** with AI



Thank You !

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MGH 1811

Athinoula A. Martinos Center For Biomedical Imaging

Robust and Interpretable Learning for Modern Healthcare (Appendix)

Mass Transport of Tracer | Governing Equation - *Advection-Diffusion*

$$\frac{\partial C}{\partial t} = \frac{\partial C}{\partial t}\Big|_{Adv} + \frac{\partial C}{\partial t}\Big|_{Diff} \quad s.t. \quad \text{Boundary Conditions (B.C.)}$$

- Advection $:= -\nabla \cdot (\mathbf{V}\, C)$
  - $\mathbf{V} := V(\mathbf{x}) = (V^x(\mathbf{x}), V^y(\mathbf{x}), V^z(\mathbf{x}))^T \in \mathbb{R}^3$
  - Assumption: Incompressible blood flow $\Leftrightarrow \nabla \cdot \mathbf{V} = 0$

$* \; C = C(\mathbf{x}, t)$: Tracer Concentration; $\mathbf{x} = (x, y, z) \in \Omega \subset \mathbb{R}^3$; $t = 0, 1, \ldots, T$

Mass Transport of Tracer | Governing Equation - *Advection-Diffusion*

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \left.\frac{\partial C}{\partial t}\right|_{Diff} \quad s.t. \quad \text{Boundary Conditions (B.C.)}$$

- Advection $:= -\nabla \cdot (\mathbf{V}\, C) \ \big(= -\nabla \cdot \mathbf{V}\, C - \mathbf{V} \cdot \nabla C \big) \Rightarrow -\mathbf{V} \cdot \nabla C$
  - $\mathbf{V} := V(\mathbf{x}) = (V^x(\mathbf{x}), V^y(\mathbf{x}), V^z(\mathbf{x}))^T \in \mathbb{R}^3$
  - Assumption: Incompressible blood flow $\Leftrightarrow \nabla \cdot \mathbf{V} = 0$

$* \ C = C(\mathbf{x}, t)$: Tracer Concentration; $\mathbf{x} = (x, y, z) \in \Omega \subset \mathbb{R}^3$; $t = 0,\ 1,\ \dots,\ T$

Mass Transport of Tracer | Governing Equation - *Advection-Diffusion*

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (\mathbf{D}\, \nabla C) \quad s.t. \quad \text{Boundary Conditions (B.C.)}$$

- Advection $:= -\nabla \cdot (\mathbf{V}\, C) \;\left(= -\nabla \cdot \mathbf{V}\, C - \mathbf{V} \cdot \nabla C \right) \Rightarrow -\mathbf{V} \cdot \nabla C$
  - $\mathbf{V} := V(\mathbf{x}) = (V^x(\mathbf{x}), V^y(\mathbf{x}), V^z(\mathbf{x}))^T \in \mathbb{R}^3$
  - Assumption: Incompressible blood flow $\Leftrightarrow \nabla \cdot \mathbf{V} = 0$
- Diffusion $:= \nabla \cdot (\mathbf{D}\, \nabla C)$
  - $\mathbf{D} := D(\mathbf{x}) = \begin{bmatrix} D^{xx} & D^{xy} & D^{xz} \\ D^{xy} & D^{yy} & D^{yz} \\ D^{xz} & D^{yz} & D^{zz} \end{bmatrix} \in \mathbb{R}^{3\times 3}$
  - Assumption: $\mathbf{D}$ is symmetric positive semi-definite (PSD)

$* \; C = C(\mathbf{x}, t)$: Tracer Concentration; $\mathbf{x} = (x, y, z) \in \Omega \subset \mathbb{R}^3$; $t = 0,\, 1,\, \ldots,\, T$

Advection-Diffusion Solvers Toolbox in PyTorch | ***First-Order Upwind*** Scheme in 3D

Given $C = \left(C_{i,j,k}\right)_{N_x \times N_y \times N_z}$ with uniformly distributed mesh sizes Δx, Δy, Δz:

Advection-Diffusion Solvers Toolbox in PyTorch | ***First-Order Upwind*** Scheme in 3D

Given $C = \left(C_{i,j,k}\right)_{N_x \times N_y \times N_z}$ with uniformly distributed mesh sizes Δx, Δy, Δz:

$$x \text{ direction:} \quad \left.\frac{\partial C}{\partial x}\right|_{i,j,k} = \begin{cases} \frac{C_{i,j,k} - C_{i-1,j,k}}{\Delta x}, & V^x_{i,j,k} \geq 0 \\ \frac{C_{i+1,j,k} - C_{i,j,k}}{\Delta x}, & V^x_{i,j,k} < 0 \end{cases}$$

Advection-Diffusion Solvers Toolbox in PyTorch | *First-Order Upwind* Scheme in 3D

Given $C = \left(C_{i,j,k}\right)_{N_x \times N_y \times N_z}$ with uniformly distributed mesh sizes Δx, Δy, Δz:

$$x \text{ direction:} \quad \left.\frac{\partial C}{\partial x}\right|_{i,j,k} = \begin{cases} \frac{C_{i,j,k} - C_{i-1,j,k}}{\Delta x}, & V^x_{i,j,k} \geq 0 \\ \frac{C_{i+1,j,k} - C_{i,j,k}}{\Delta x}, & V^x_{i,j,k} < 0 \end{cases}$$

$$y \text{ direction:} \quad \left.\frac{\partial C}{\partial y}\right|_{i,j,k} = \begin{cases} \frac{C_{i,j,k} - C_{i,j-1,k}}{\Delta y}, & V^y_{i,j,k} \geq 0 \\ \frac{C_{i,j+1,k} - C_{i,j,k}}{\Delta y}, & V^y_{i,j,k} < 0 \end{cases}$$

Advection-Diffusion Solvers Toolbox in PyTorch | *First-Order Upwind* Scheme in 3D

Given $C = \left(C_{i,j,k}\right)_{N_x \times N_y \times N_z}$ with uniformly distributed mesh sizes Δx, Δy, Δz:

$$x \text{ direction:} \quad \left.\frac{\partial C}{\partial x}\right|_{i,j,k} = \begin{cases} \frac{C_{i,j,k} - C_{i-1,j,k}}{\Delta x}, & V^x_{i,j,k} \geq 0 \\ \frac{C_{i+1,j,k} - C_{i,j,k}}{\Delta x}, & V^x_{i,j,k} < 0 \end{cases}$$

$$y \text{ direction:} \quad \left.\frac{\partial C}{\partial y}\right|_{i,j,k} = \begin{cases} \frac{C_{i,j,k} - C_{i,j-1,k}}{\Delta y}, & V^y_{i,j,k} \geq 0 \\ \frac{C_{i,j+1,k} - C_{i,j,k}}{\Delta y}, & V^y_{i,j,k} < 0 \end{cases}$$

$$z \text{ direction:} \quad \left.\frac{\partial C}{\partial z}\right|_{i,j,k} = \begin{cases} \frac{C_{i,j,k} - C_{i,j,k-1}}{\Delta z}, & V^z_{i,j,k} \geq 0 \\ \frac{C_{i,j,k+1} - C_{i,j,k}}{\Delta z}, & V^z_{i,j,k} < 0 \end{cases}$$

Advection-Diffusion Solvers Toolbox in PyTorch | *Nested Forward/Backward* Difference

$$(df(db)) = (db(df)) = (ddc)$$

Proof.

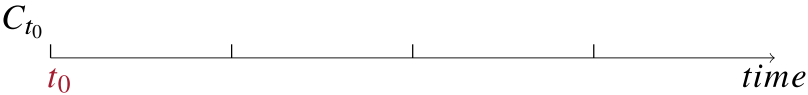
For $X = [X_1, X_2, ..., X_n]$, Let:

$$ddX := (df(db)) \cdot X$$

For $i = 1, \ldots, n$:

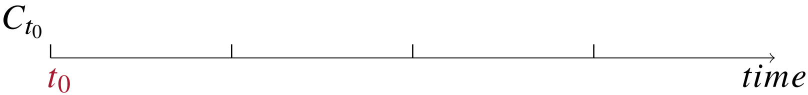
$$\begin{aligned} ddX_i &= X'_{i+1} - X'_i \\ &= (X_{i+1} - X_i) - (X_i - X_{i-1}) \quad &\Leftrightarrow \quad (db(df)) \cdot X \\ &= X_{i+1} - 2X_i + X_{i-1} \quad &\Leftrightarrow \quad (ddC) \cdot X \end{aligned}$$

Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *Method of Lines*



Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *Method of Lines*

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (D \, \nabla C) \quad s.t. \quad \frac{\partial C}{\partial \mathbf{n}} = 0$$



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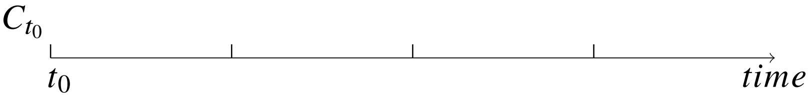
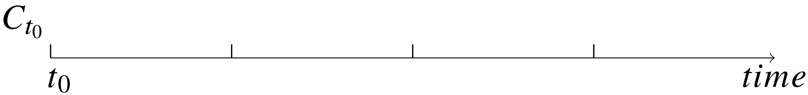


- Discretize in space

Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *Method of Lines*

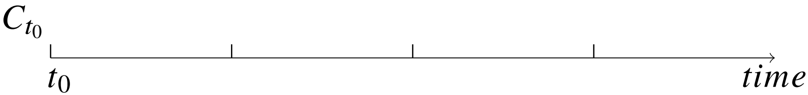
$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (D\, \nabla C) \quad s.t. \quad \frac{\partial C}{\partial \mathbf{n}} = 0$$



- Discretize in space
  - First order upwind scheme for advection $-\mathbf{V} \cdot \nabla C_t$

Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *Method of Lines*

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (D \, \nabla C) \quad s.t. \quad \frac{\partial C}{\partial \mathbf{n}} = 0$$



- Discretize in space
  - First order upwind scheme for advection $-\mathbf{V} \cdot \nabla C_t$
  - Nested forward/backward difference for diffusion $\nabla \cdot (D \, \nabla C_t)$

Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *Method of Lines*

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (D\, \nabla C) \quad s.t. \quad \frac{\partial C}{\partial \mathbf{n}} = 0$$

- Discretize in space
  - First order upwind scheme for advection $-\mathbf{V} \cdot \nabla C_t$
  - Nested forward/backward difference for diffusion $\nabla \cdot (D\, \nabla C_t)$
- March in time

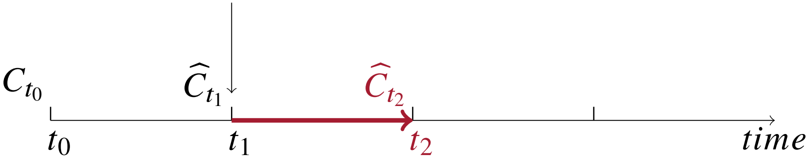
Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *Method of Lines*

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (D\, \nabla C) \quad s.t. \quad \frac{\partial C}{\partial \mathbf{n}} = 0$$

- Discretize in space
  - First order upwind scheme for advection $-\mathbf{V} \cdot \nabla C_t$
  - Nested forward/backward difference for diffusion $\nabla \cdot (D\, \nabla C_t)$
- March in time
  - Runge-Kutta-Fehlberg method (Adaptive time-step control)

Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *Method of Lines*

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (D \, \nabla C) \quad s.t. \quad \frac{\partial C}{\partial \mathbf{n}} = 0$$



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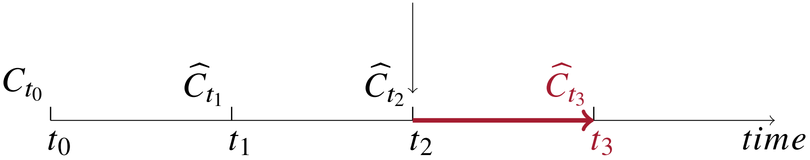
Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *Method of Lines*

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (D\, \nabla C) \quad s.t. \quad \frac{\partial C}{\partial \mathbf{n}} = 0$$



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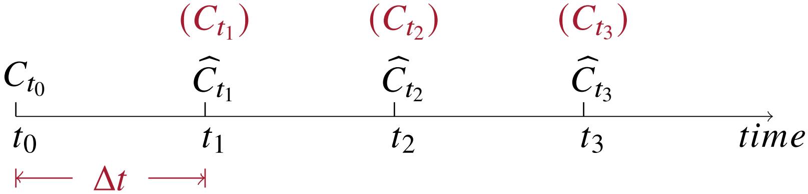
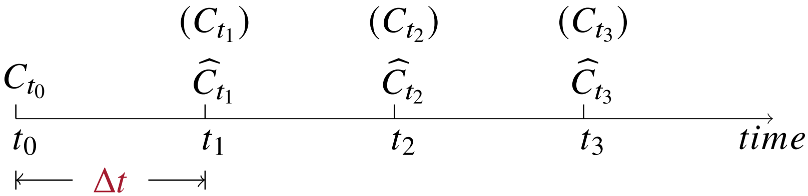
- March in time
  - Runge-Kutta-Fehlberg method (Adaptive time-step control)

Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *CFL* Condition



[1] S. Gottlieb et al.: Strong Stability Preserving Properties of Runge–Kutta Time Discretization Methods for Linear Constant Coefficient Operators (2003)

Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *CFL* Condition

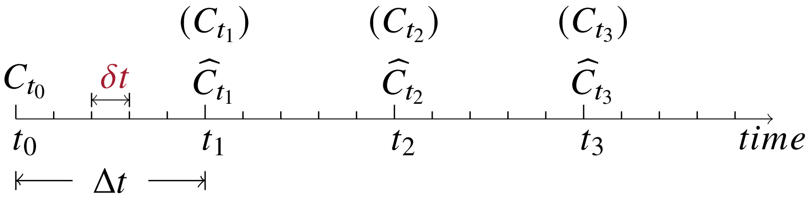


Courant-Friedrichs-Lewy (CFL) condition:

$$c = \sum_{ax \in \{x,y,z\}} \frac{V^{ax}\,\Delta t}{\Delta ax} \leq c_{\max} \quad (\approx 1 \text{ for explicit method})$$

[1]S. Gottlieb et al.: Strong Stability Preserving Properties of Runge–Kutta Time Discretization Methods for Linear Constant Coefficient Operators (2003)

Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *CFL* Condition



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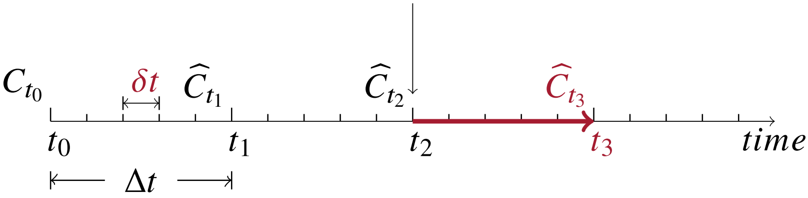
[1] S. Gottlieb et al.: Strong Stability Preserving Properties of Runge–Kutta Time Discretization Methods for Linear Constant Coefficient Operators (2003)

Advection-Diffusion Solvers Toolbox in PyTorch | Numerical Flow - *Method of Lines*

$$\frac{\partial C}{\partial t} = -\mathbf{V} \cdot \nabla C + \nabla \cdot (D\, \nabla C) \quad s.t. \quad \frac{\partial C}{\partial \mathbf{n}} = 0$$



- Discretize in space
  - First order upwind scheme for advection $-\mathbf{V} \cdot \nabla C_t$
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- March in time
  - Runge-Kutta-Fehlberg method (Adaptive time-step control)

Advection-Diffusion Solvers Toolbox in PyTorch (1D, 2D, 3D)

$$\frac{\partial C}{\partial t} = \text{advection and/or diffusion } s.t. \text{ Boundary Condition(s)}$$

C^{t_0}

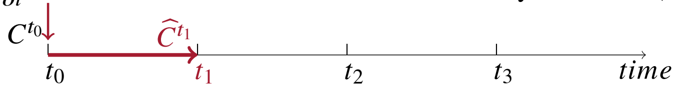
t_0 t_1 t_2 t_3 $time$

Advection-Diffusion

PDEs Toolbox

Advection-Diffusion Solvers Toolbox in PyTorch (1D, 2D, 3D)

$$\frac{\partial C}{\partial t} = \text{advection and/or diffusion } s.t. \text{ Boundary Condition(s)}$$

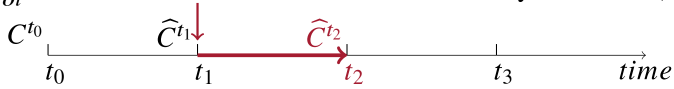


Advection-Diffusion

PDEs Toolbox

Advection-Diffusion Solvers Toolbox in PyTorch (1D, 2D, 3D)

$$\frac{\partial C}{\partial t} = \text{advection and/or diffusion } s.t. \text{ Boundary Condition(s)}$$

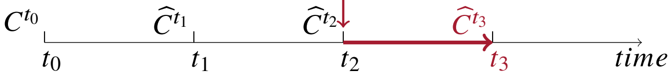


Advection-Diffusion

PDEs Toolbox

Advection-Diffusion Solvers Toolbox in PyTorch (1D, 2D, 3D)

$$\frac{\partial C}{\partial t} = \text{advection and/or diffusion } s.t. \text{ Boundary Condition(s)}$$

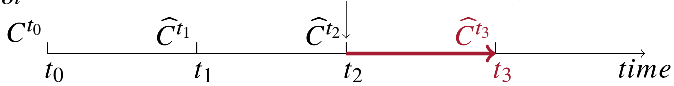


Advection-Diffusion

PDEs Toolbox

Advection-Diffusion Solvers Toolbox in PyTorch (1D, 2D, 3D)

$\frac{\partial C}{\partial t}$ = advection and/or diffusion $s.t.$ Boundary Condition(s)



$$\text{PDEs} \begin{cases} \text{Advection PDE: } -\nabla(\mathbf{V}\, C) \\ \text{Diffusion PDE: } \nabla \cdot (\mathbf{D}\, \nabla \mathbf{C}) \end{cases}$$

Advection-Diffusion

PDEs Toolbox

Advection-Diffusion Solvers Toolbox in PyTorch (1D, 2D, 3D)

$$\frac{\partial C}{\partial t} = \text{advection and/or diffusion } s.t. \text{ Boundary Condition(s)}$$

C^{t_0} $\widehat{C}^{t_1}$ $\widehat{C}^{t_2}$ $\widehat{C}^{t_3}$

t_0 t_1 t_2 t_3 $time$

$$\text{PDEs} \begin{cases} \text{Advection PDE: } -\nabla(\mathbf{V}\, C) \\ \text{Diffusion PDE: } \nabla \cdot (\mathbf{D}\, \nabla \mathbf{C}) \end{cases}$$

$$\text{B.C.} \begin{cases} \text{Neumann, Dirichlet} \\ \text{Cauchy, Robin} \end{cases}$$

Advection-Diffusion

PDEs Toolbox

Advection-Diffusion Solvers Toolbox in PyTorch (1D, 2D, 3D)

$$\frac{\partial C}{\partial t} = \text{advection and/or diffusion } s.t. \text{ Boundary Condition(s)}$$

C^{t_0} $\widehat{C}^{t_1}$ $\widehat{C}^{t_2}$ $\widehat{C}^{t_3}$

t_0 t_1 t_2 t_3 $time$

PDEs $\begin{cases} \text{Advection PDE: } -\nabla(\mathbf{V}\, C) \\ \text{Diffusion PDE: } \nabla \cdot (\mathbf{D}\, \nabla \mathbf{C}) \end{cases}$

B.C. $\begin{cases} \text{Neumann, Dirichlet} \\ \text{Cauchy, Robin} \end{cases}$

$\mathbf{V}$: constant, scalar, vector, divergence-free vector $\begin{cases} \text{Stream} \\ \text{Clebsch} \end{cases}$

Advection-Diffusion

PDEs Toolbox

Advection-Diffusion Solvers Toolbox in PyTorch (1D, 2D, 3D)

$$\frac{\partial C}{\partial t} = \text{advection and/or diffusion } s.t. \text{ Boundary Condition(s)}$$

C^{t_0} $\widehat{C}^{t_1}$ $\widehat{C}^{t_2}$ $\widehat{C}^{t_3}$

t_0 t_1 t_2 t_3 $time$

PDEs $\begin{cases} \text{Advection PDE: } -\nabla(\mathbf{V}\, C) \\ \text{Diffusion PDE: } \nabla \cdot (\mathbf{D}\, \nabla \mathbf{C}) \end{cases}$

B.C. $\begin{cases} \text{Neumann, Dirichlet} \\ \text{Cauchy, Robin} \end{cases}$

V: constant, scalar, vector, divergence-free vector $\begin{cases} \text{Stream} \\ \text{Clebsch} \end{cases}$

D: constant, scalar, symmetric PSD tensor $\begin{cases} \text{Cholesky} \\ \text{Spectral} \\ \text{Dual basis} \end{cases}$

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Differential operators $\begin{cases} 1^{st}: \text{ upwind, forward, backward, central} \\ 2^{nd}: \text{ nested forward-backward-central} \end{cases}$

Advection-Diffusion Solvers Toolbox in PyTorch (1D, 2D, 3D)

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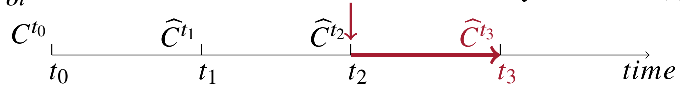

PDEs $\begin{cases} \text{Advection PDE: } -\nabla(\mathbf{V}\,C) \\ \text{Diffusion PDE: } \nabla \cdot (\mathbf{D}\,\nabla \mathbf{C}) \end{cases}$

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Differential operators $\begin{cases} 1^{st}\text{: upwind, forward, backward, central} \\ 2^{nd}\text{: nested forward-backward-central} \end{cases}$

Integrators (Neural Ordinary Differential Equations (NeurIPS'2018))

Robust and Interpretable Learning for Modern Healthcare (Appendix)

Brain Advection-Diffusion Synthesis | *Dataset* (Link to Simulation & Pre-Training)

`IXI` brain dataset[1]:

- Total: 200 patients
- T1-/T2-weighted images, MR angiography (MRA) image
  $\Rightarrow$ Velocity vector fields simulation
- Diffusion weighted images (DWI) with 15 directions
  $\Rightarrow$ Diffusion tensor fields simulation
- Brain advection-diffusion time-series: length $N_T = 40$, time interval $\Delta t = 0.1\ s$

[1] Dataset available for download at `http://brain-development.org/ixi-dataset/`

Brain Advection-Diffusion Synthesis | *Velocity* (Link to Simulation & Pre-Training)

MRA

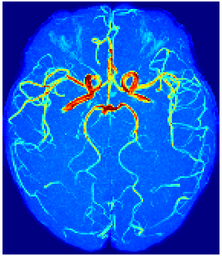


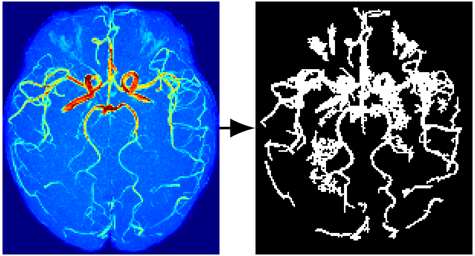
Figure: Velocity simulation workflow (images shown in maximum intensity projection (MIP)), the last two vector fields are displayed in RGB maps (red - sagittal; green - coronal; blue - axial).

---

[1]Code in `https://github.com/InsightSoftwareConsortium/ITKTubeTK/tree/master/examples/MRA-Head`

[2]A. F. Frangi et al.: Multiscale Vessel Enhancement Filtering. *MICCAI* (1998)

Brain Advection-Diffusion Synthesis | *Velocity* (Link to Simulation & Pre-Training)



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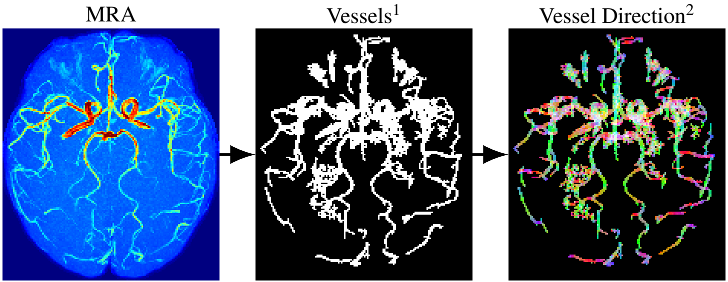
Brain Advection-Diffusion Synthesis | *Velocity* (Link to Simulation & Pre-Training)



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Brain Advection-Diffusion Synthesis | *Velocity* (Link to Simulation & Pre-Training)

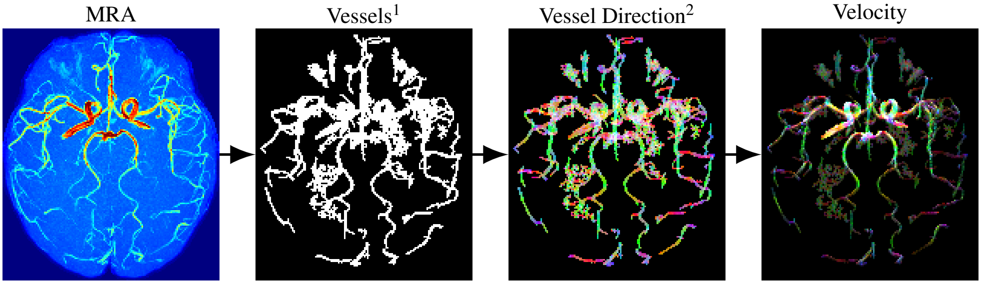

Figure: Velocity simulation workflow (images shown in maximum intensity projection (MIP)), the last two vector fields are displayed in RGB maps (red - sagittal; green - coronal; blue - axial).

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[2] A. F. Frangi et al.: Multiscale Vessel Enhancement Filtering. *MICCAI* (1998)

Brain Advection-Diffusion Synthesis | *Diffusion* (Link to Simulation & Pre-Training)

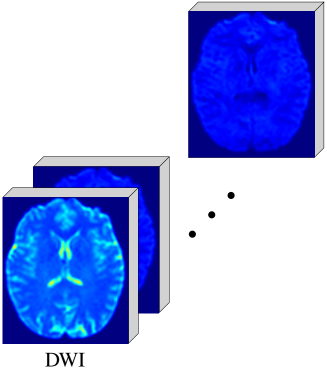

Figure: Diffusion simulation workflow.

[1] Dipy: python library for MR diffusion imaging analysis (Code in https://github.com/dipy/dipy)

Brain Advection-Diffusion Synthesis | *Diffusion* (Link to Simulation & Pre-Training)

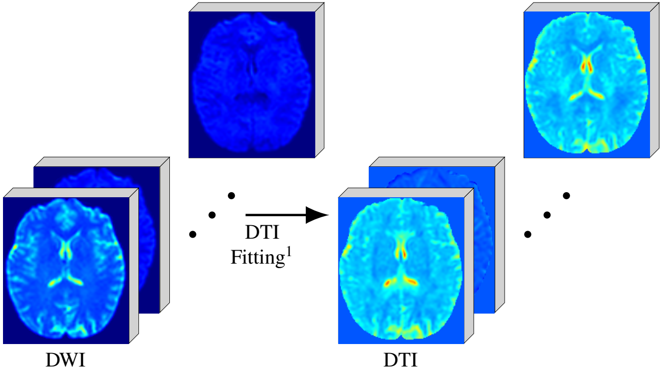

Figure: Diffusion simulation workflow.

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Brain Advection-Diffusion Synthesis | *Diffusion* (Link to Simulation & Pre-Training)

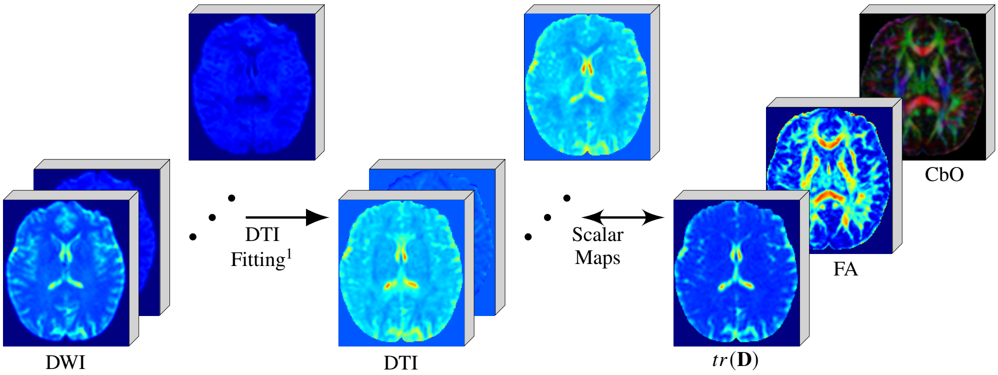
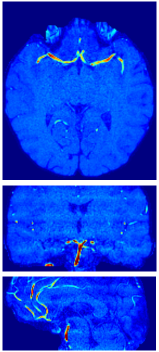


Figure: Diffusion simulation workflow.

[1] Dipy: python library for MR diffusion imaging analysis (Code in https://github.com/dipy/dipy)

Brain Advection-Diffusion Synthesis | *Time Series* (Link to Simulation & Pre-Training)



$t = 1$

Figure: Example brain advection-diffusion time series. Top: axial slice; Middle: coronal slice; Bottom: sagittal slice.

Brain Advection-Diffusion Synthesis | *Time Series* (Link to Pre-Training)

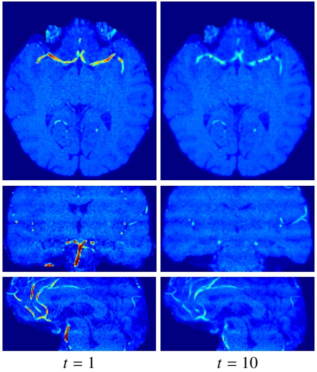


Figure: Example brain advection-diffusion time series. Top: axial slice; Middle: coronal slice; Bottom: sagittal slice.

Brain Advection-Diffusion Synthesis | *Time Series* (Link to Pre-Training)

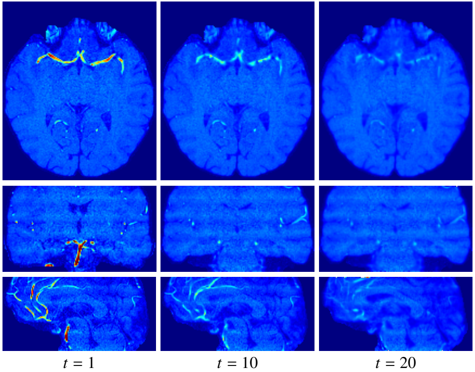
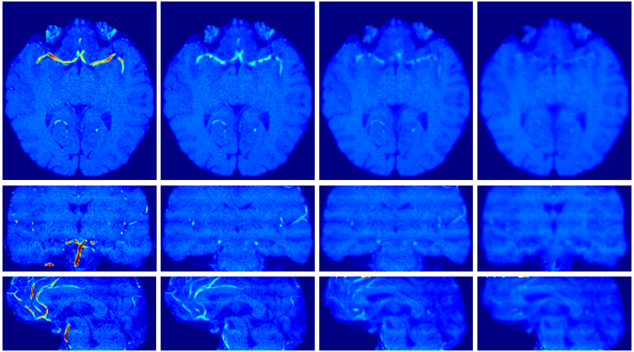


Figure: Example brain advection-diffusion time series. Top: axial slice; Middle: coronal slice; Bottom: sagittal slice.

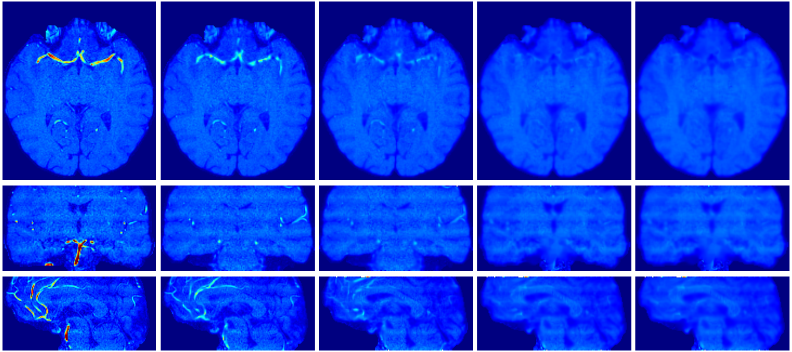
Brain Advection-Diffusion Synthesis | *Time Series* (Link to Pre-Training)



$t = 1$ $t = 10$ $t = 20$ $t = 30$

Figure: Example brain advection-diffusion time series. Top: axial slice; Middle: coronal slice; Bottom: sagittal slice.

Brain Advection-Diffusion Synthesis | *Time Series* (Link to Pre-Training)

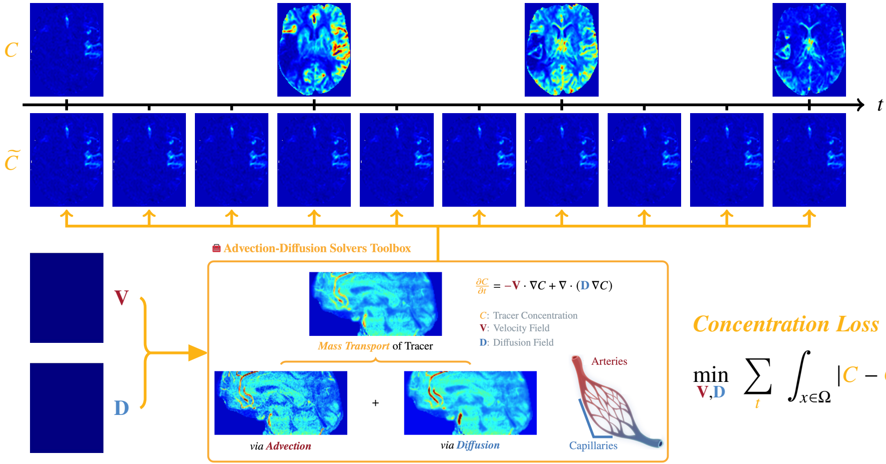


$t = 1$ $t = 10$ $t = 20$ $t = 30$ $t = 40$

Figure: Example brain advection-diffusion time series. Top: axial slice; Middle: coronal slice; Bottom: sagittal slice.

Robust and Interpretable Learning for Modern Healthcare (Appendix)

Perfusion Imaging via *Advection-Diffusion*: For the First Time (Link to Results)

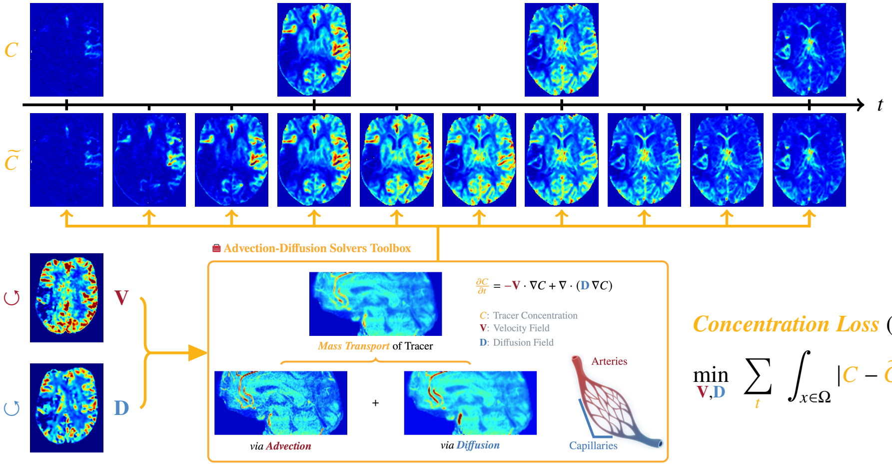


Concentration Loss ($\mathcal{L}_C$)

$$\min_{\mathbf{V},\mathbf{D}} \sum_t \int_{x\in\Omega} |C - \widetilde{C}|\, dx$$

P. Liu et al.: `PIANO`: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)
P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

Perfusion Imaging via *Advection-Diffusion*: For the First Time (Link to Results)



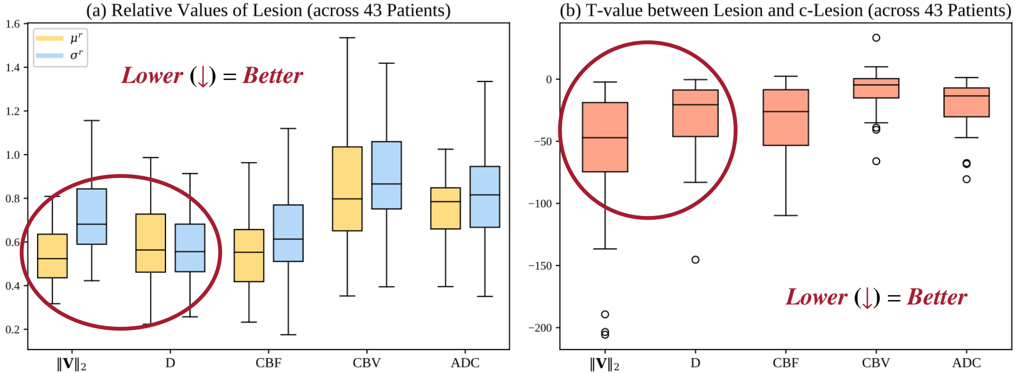
Concentration Loss ($\mathcal{L}_C$)

$$\min_{\mathbf{V},\mathbf{D}} \sum_t \int_{x\in\Omega} |C - \widetilde{C}|\, dx$$

P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)

P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

Perfusion Imaging via *Advection-Diffusion* | Quantitative Comparisons



Box plots of relative mean values (μ^r), relative standard deviation (σ^r) and t-values of perfusion feature maps.

c-Lesion: contralateral region of the lesion | CBF, CBV, ADC: conventional voxel-wise perfusion feature maps

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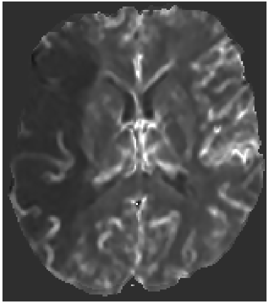
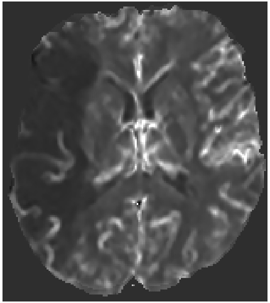
P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)
P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)
P. Liu et al.: Discovering Hidden Physics Behind Transport Dynamics. ***CVPR*** (2021) (★ *Oral*)

ISLES2017-MRP: PIANO-Estimated Concentration Time-Series (Link to Framework)

C_t



$\widehat{C}_t$



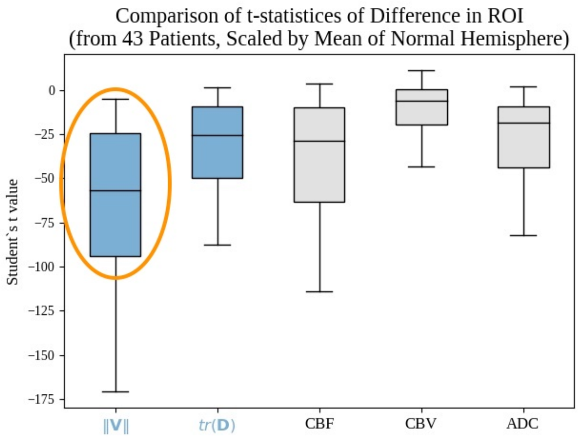
C_t: Concentration map computed from acquired MR perfusion images

$\widehat{C}_t$: Predicted concentration map from estimated parameters $\mathbf{V}$ and D

P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)

P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

ISLES2017-MRP: Quantitative Comparison (Box Plots) (Link to Framework & Metrics)

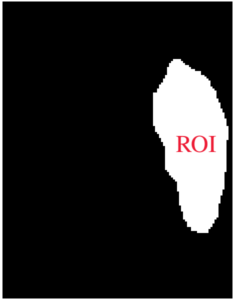


P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)

P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

Comparison Metrics | *Contralateral* (Link to Table, Box Plots in Main & Appendix)

ROI: lesion area



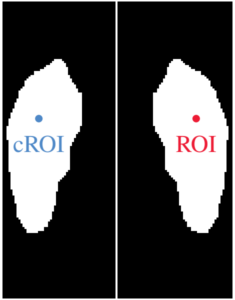
P. Liu et al.: `PIANO`: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)

P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

Comparison Metrics | *Contralateral* (Link to Table, Box Plots in Main & Appendix)

ROI: lesion area

cROI: corresponding contralateral (midline of the cerebral hemispheres as axis) area of ROI in the unaffected side



P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)

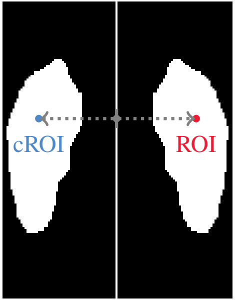
P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

Comparison Metrics | *Contralateral* (Link to Table, Box Plots in Main & Appendix)

ROI: lesion area

cROI: corresponding contralateral (midline of the cerebral hemispheres as axis) area of ROI in the unaffected side

Relative value of ROI ($\text{value}^r_{\text{ROI}}$) = $\text{value}_{\text{ROI}} / \text{value}_{\text{cROI}}$



P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)

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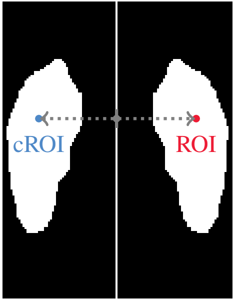

Metrics of feature maps in ROI:

- Relative mean ($\mu^r_{\text{ROI}} \in [0, 1]$):

$$\mu^r_{\text{ROI}} = min\left\{ \frac{\text{mean in ROI}}{\text{mean in cROI}}, \frac{\text{mean in cROI}}{\text{mean in ROI}} \right\}$$

P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)

P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

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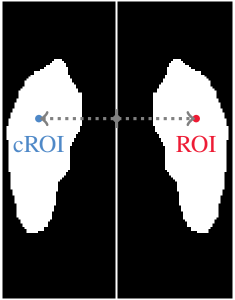

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- Relative mean ($\mu^r_{\text{ROI}} \in [0, 1]$):

$$\mu^r_{\text{ROI}} = min\left\{\frac{\text{mean in ROI}}{\text{mean in cROI}}, \frac{\text{mean in cROI}}{\text{mean in ROI}}\right\}$$

- Absolute t-value between ROI, cROI ($|t|$)

P. Liu et al.: `PIANO`: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)

P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

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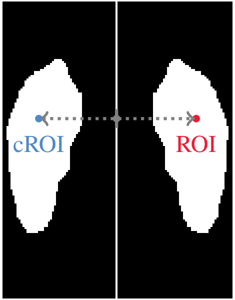


Metrics of feature maps in ROI:

- Relative mean ($\mu^r_{\text{ROI}} \in [0, 1]$):

$$\mu^r_{\text{ROI}} = min\left\{\frac{\text{mean in ROI}}{\text{mean in cROI}}, \frac{\text{mean in cROI}}{\text{mean in ROI}}\right\}$$

- Absolute t-value between ROI, cROI ($|t|$)
- Mean principal diffusion angle deviation ($\angle$):

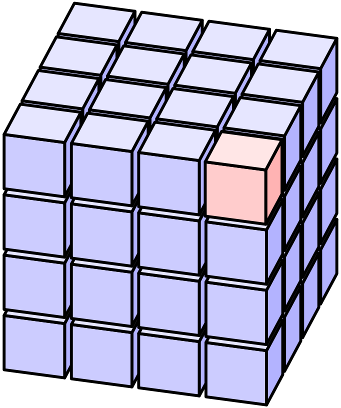
$$\angle = min\left\{\angle(\pm\mathbf{U}_{\text{prin}}(\text{ROI}), \mathbf{U}^c_{\text{prin}}(\text{cROI}))\right\}$$

(* $\mathbf{U}^c_{\text{prin}}(\text{cROI})$: $\mathbf{U}_{\text{prin}}$ mirrored from cROI)

P. Liu et al.: PIANO: Perfusion Imaging via Advection-Diffusion. ***MICCAI*** (2020) (★ *Oral*)
P. Liu et al.: Perfusion Imaging: An Advection Diffusion Approach. ***IEEE TMI*** (2021)

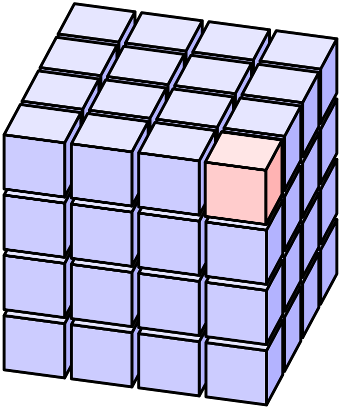
Robust and Interpretable Learning for Modern Healthcare (Appendix)

Mass Transport of Tracer | ***Patch-Based*** Advection-Diffusion (Link to Full Equation)



$$\frac{\partial C(\mathbf{x},t)}{\partial t} = \frac{\partial C(\mathbf{x},t)}{\partial t}\bigg|_{Adv} + \frac{\partial C(\mathbf{x},t)}{\partial t}\bigg|_{Diff}$$

Mass Transport of Tracer | ***Patch-Based*** Advection-Diffusion (Link to Full Equation)

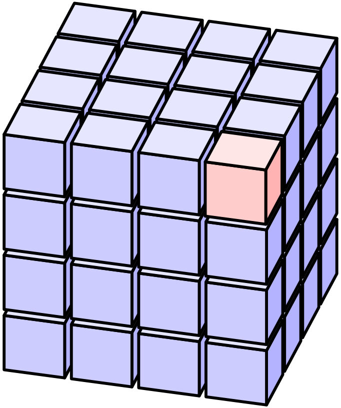


$$\frac{\partial C(\mathbf{x},t)}{\partial t} = \left.\frac{\partial C(\mathbf{x},t)}{\partial t}\right|_{Adv} + \left.\frac{\partial C(\mathbf{x},t)}{\partial t}\right|_{Diff}$$

- Advection $:= -\nabla \cdot (\mathbf{V}\, C)$
  - $\mathbf{V} := (V^x, V^y, V^z)^T \in \mathbb{R}^3$
    ($\mathbf{V}$: incompressible fluid flow)

$*\ C(\mathbf{x},t)$: CAs concentration $\left(\forall \mathbf{x} = (x,y,z)^T \in \Omega \subset \mathbb{R}^3,\ \forall t \in \{t_0, t_1, \ldots, t_{nT}\}\right)$

Mass Transport of Tracer | ***Patch-Based*** Advection-Diffusion (Link to Full Equation)

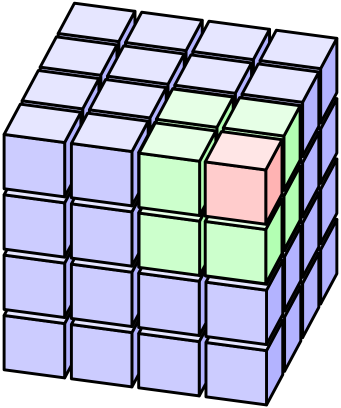


$$\frac{\partial C(\mathbf{x},t)}{\partial t} = \frac{\partial C(\mathbf{x},t)}{\partial t}\Big|_{Adv} + \frac{\partial C(\mathbf{x},t)}{\partial t}\Big|_{Diff}$$

- Advection $:= -\nabla \cdot (\mathbf{V}\, C)$
  - $\mathbf{V} := (V^x, V^y, V^z)^T \in \mathbb{R}^3$
    ($\mathbf{V}$: incompressible fluid flow)
- Diffusion $:= \nabla \cdot (\mathbf{D}\, \nabla C)$
  - $\mathbf{D} := \begin{bmatrix} D^{xx} & D^{xy} & D^{xz} \\ D^{yx} & D^{yy} & D^{yz} \\ D^{zx} & D^{zy} & D^{zz} \end{bmatrix} \in \mathbb{R}^{3\times 3}$
    ($\mathbf{D}$: positive semi-definite (PSD))

$*\ C(\mathbf{x},t)$: CAs concentration $\left(\forall \mathbf{x} = (x,y,z)^T \in \Omega \subset \mathbb{R}^3,\ \forall t \in \{t_0, t_1, \ldots, t_{nT}\}\right)$

Mass Transport of Tracer | *Patch-Based* Advection-Diffusion (Link to Full Equation)



$$\frac{\partial C(\mathbf{x},t)}{\partial t} = \frac{\partial C(\mathbf{x},t)}{\partial t}\bigg|_{Adv} + \frac{\partial C(\mathbf{x},t)}{\partial t}\bigg|_{Diff}$$

- Advection := $-\nabla \cdot (\mathbf{V}\, C)$
  - $\mathbf{V} := (V^x, V^y, V^z)^T \in \mathbb{R}^3$
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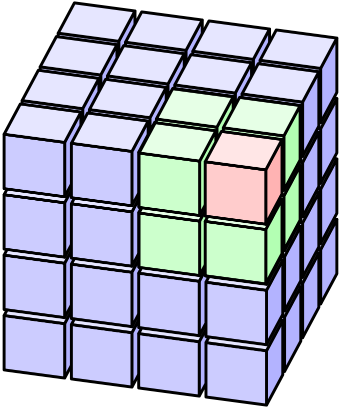
  - $\mathbf{D} := \begin{bmatrix} D^{xx} & D^{xy} & D^{xz} \\ D^{yx} & D^{yy} & D^{yz} \\ D^{zx} & D^{zy} & D^{zz} \end{bmatrix} \in \mathbb{R}^{3\times 3}$
    ($\mathbf{D}$: positive semi-definite (PSD))
- s.t. *Patch-Based* Cauchy B.C.

$*\ C(\mathbf{x},t)$: CAs concentration $\left(\forall \mathbf{x} = (x,y,z)^T \in \Omega \subset \mathbb{R}^3,\ \forall t \in \{t_0, t_1, \dots, t_{nT}\}\right)$

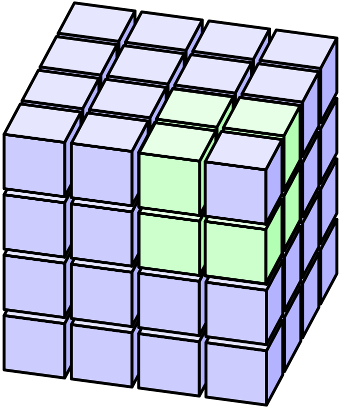
Mass Transport of Tracer | *Patch-Based* Boundary Conditions (Link to Full Equation)



- Cauchy boundary conditions (B.C.)
  - Dirichlet B.C.
  - Zero-Neumann B.C. (Example)

$*$ $\partial\Omega_p$: boundaries of patch Ω_p; $\widehat{C}_p^{t_i}$: predicted concentration at $t_i (i = 1, \ldots, T_{\text{pd}})$

Mass Transport of Tracer | *Patch-Based* Boundary Conditions (Link to Full Equation)



- Cauchy boundary conditions (B.C.)
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$$\widehat{C}_p^{t_i}\big|_{\partial\Omega_p} := C_p^{t_i}\big|_{\partial\Omega_p}$$

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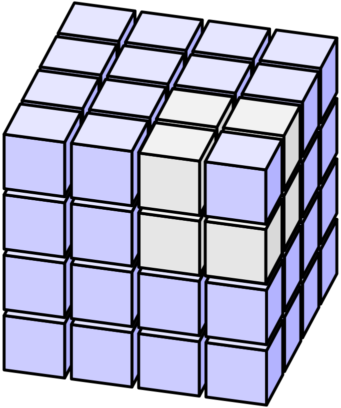
Mass Transport of Tracer | ***Patch-Based*** Boundary Conditions (Link to Full Equation)



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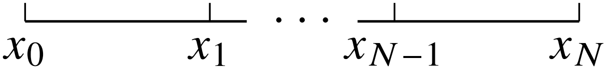
  - Zero-Neumann B.C. (Example)

$$\frac{\partial \widehat{C}_p^{t_i}}{\partial \mathbf{n}}\bigg|_{\partial\Omega_p} := 0$$

$*$ $\partial\Omega_p$: boundaries of patch Ω_p; $\widehat{C}_p^{t_i}$: predicted concentration at $t_i\,(i = 1, \ldots, T_{\text{pd}})$

Zero-Neumann Boundary Condition: 1D Example (Link to Full Equation & B.C.)



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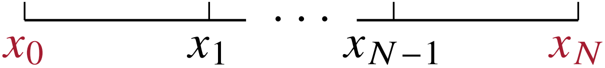
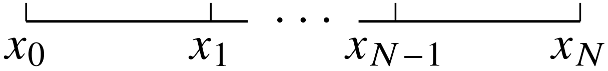


Zero-neumann boundary condition: $\left.\frac{\partial f}{\partial x}\right|_{\{x_0,\, x_N\}} = 0$

Zero-Neumann Boundary Condition: 1D Example (Link to Full Equation & B.C.)



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Approx. of 1^{st} order differential operator $\frac{\partial}{\partial x} \cdot$:

$$\left.\frac{\partial f}{\partial x}\right|_{x_i} \approx \frac{f(x_{i+1}) - f(x_{i-1})}{2\,\Delta x} \quad \text{(Central difference)}$$

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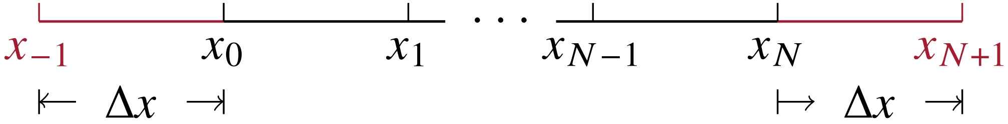

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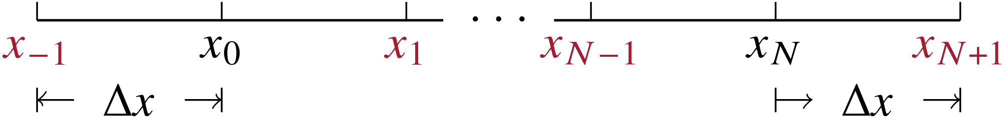

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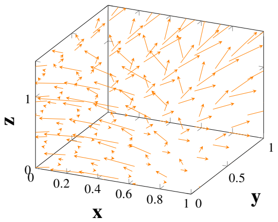
Set values on ghost cells: $\begin{cases} f(x_{-1}) := f(x_1) \\ f(x_{N+1}) := f(x_{N-1}) \end{cases}$

Divergence-Free Vector Representation (Link to Framework in Main & Appendix)

Goal: Surjective Mapping

(a) *By definition*, the predicted velocity fields $\mathbf{V} \in \mathcal{H}_{\text{div}}(\Omega)$;

(b) The representation covers the *entire* $\mathcal{H}_{\text{div}}(\Omega)$.



$\mathbf{V} := \langle a,\, b,\, c \rangle$

Figure: A random vector field ($\mathbf{V}$)

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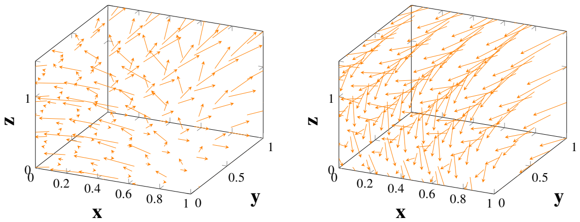


$\mathbf{\Psi} = \langle xy,\ yz,\ xz \rangle$ $\qquad$ $\mathbf{V} := \nabla \times \mathbf{\Psi} = \langle -y,\ -z,\ -x \rangle \quad (\nabla \cdot \mathbf{V} = 0)$

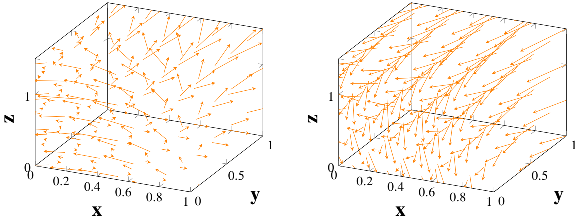
Figure: Represent a divergence-free vector field ($\mathbf{V}$) by the ***curl of vector potentials*** ($\mathbf{\Psi}$)

Divergence-Free Vector Representation (Link to Framework in Main & Appendix)

Theorem: Divergence-Free Vector via the Curl of Potentials

If $\nabla \cdot \mathbf{V} = 0$ for $\mathbf{V} \in L^p(\Omega)^d$ on $\Omega \subset \mathbb{R}^d$ with smooth boundary $\partial\Omega$, $\exists \boldsymbol{\Psi} \in L^p(\Omega)^\alpha$ ($\alpha = 1(3)$ when $d = 2(3)$):

$$\mathbf{V} = \nabla \times \boldsymbol{\Psi}, \quad \boldsymbol{\Psi} \cdot \mathbf{n}\big|_{\partial\Omega} = 0, \; \boldsymbol{\Psi} \in L^p(\Omega)^\alpha .$$



$\boldsymbol{\Psi} = \langle xy,\; yz,\; xz\rangle$ $\quad$ $\mathbf{V} := \nabla \times \boldsymbol{\Psi} = \langle -y,\; -z,\; -x\rangle \quad (\nabla \cdot \mathbf{V} = 0)$

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Conversely, for $\forall \mathbf{\Psi} \in L^p(\Omega)^\alpha$: $\nabla \cdot \mathbf{V} = \nabla \cdot (\nabla \times \mathbf{\Psi}) = 0$.

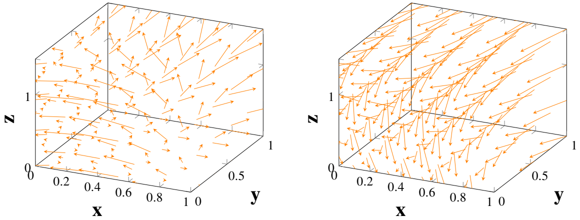

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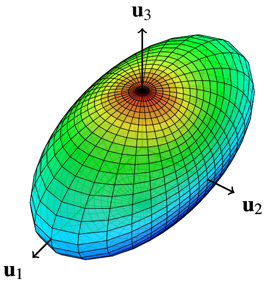
Figure: Represent a divergence-free vector field ($\mathbf{V}$) by the ***curl of vector potentials*** ($\mathbf{\Psi}$)

Symmetric PSD Tensor Representation (Link to Framework in Main & Appendix)

Goal: Represent & learn a PSD tensor via its eigenvalues and eigenvectors:

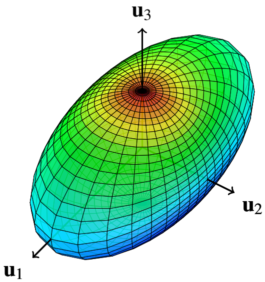
$$\mathbf{D} = \begin{bmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 \end{bmatrix}}_{eigenvectors} \underbrace{\begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3 \end{bmatrix}}_{eigenvalues} \begin{bmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \mathbf{u}_3^T \end{bmatrix} \quad (\lambda_i \geq 0)$$



Symmetric PSD Tensor Representation (Link to Framework in Main & Appendix)

How to represent & learn a set of mutually orthogonal eigenvectors ?

$$\mathbf{D} = \begin{bmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{bmatrix} = \underbrace{\begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 \end{bmatrix}}_{eigenvectors} \underbrace{\begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3 \end{bmatrix}}_{eigenvalues} \begin{bmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \mathbf{u}_3^T \end{bmatrix} \quad (\lambda_i \geq 0)$$



Symmetric PSD Tensor Representation (Link to Framework in Main & Appendix)

Theorem

For $\forall$ tensor $\mathbf{D} \in PSD(n)$, there $\exists\, \mathbf{B} \in \mathbb{R}^{\frac{n(n-1)}{2}}$, and $\mathbf{\Lambda} \in SD(n)$:

$$\mathbf{D} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^T, \quad \mathbf{U} = exp(\mathbf{B} - \mathbf{B}^T) \in SO(n).$$

- $\mathbb{R}^{\frac{n(n-1)}{2}}$: group of upper triangular matrix with zero diagonal entries
- $SD(n)$: group of real diagonal matrices with non-negative entries
- $SO(n)$: group of real orthogonal matrices

[1] M. Lezcano-Casado: Trivializations for Gradient-Based Optimization on Manifolds. *NeurIPS* (2019)

[2] M. Lezcano-Casado: Cheap Orthogonal Constraints in Neural Networks. *ICML* (2019)

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Conversely, for $\forall\, \mathbf{B} \in \mathbb{R}^{\frac{n(n-1)}{2}}$, $\forall\, \mathbf{\Lambda} \in SD(n) \rightarrow \mathbf{D} \in PSD(n)$.

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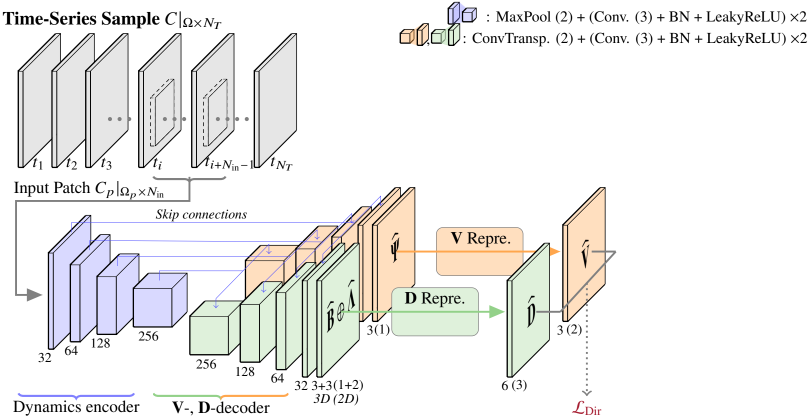
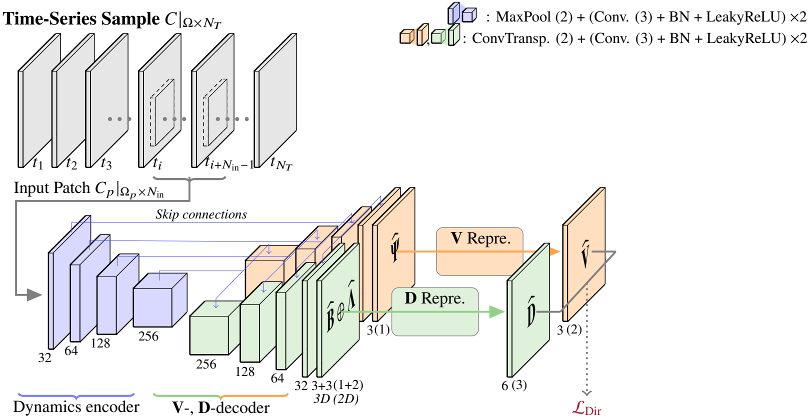
YETI | *Pre-Training* on Synthetic Data (Link to Simulation & Comparisons)



$\mathcal{L}_{\text{Dir}} = \mathcal{L}_{\mathbf{VD}}$

$$\left\{ \mathcal{L}_{\mathbf{VD}} = \frac{1}{|\Omega_p|} \int_{\Omega_p} \left\| \mathbf{V} - \widehat{\mathbf{V}} \right\|_2 + \left\| \mathbf{D} - \widehat{\mathbf{D}} \right\|_F \, d\mathbf{x} \right.$$

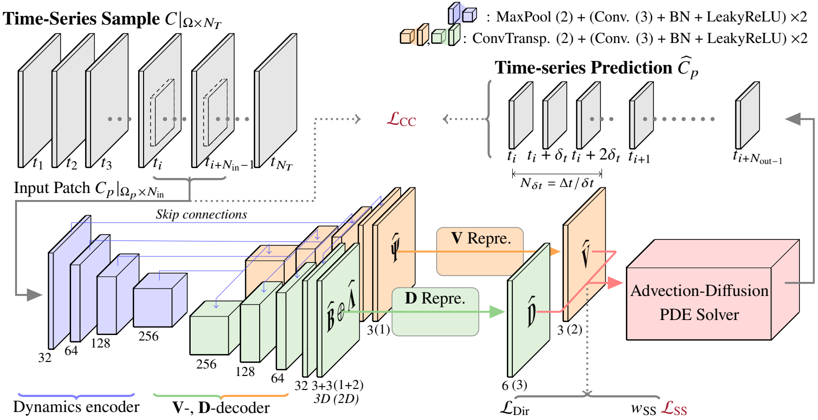
YETI | *Pre-Training* on Synthetic Data (Link to Simulation & Comparisons)



$$\mathcal{L}_{\text{Dir}} = \mathcal{L}_{\mathbf{VD}} + w_{\mathbf{U\Lambda}}\,\mathcal{L}_{\mathbf{U\Lambda}} \quad \begin{cases} \mathcal{L}_{\mathbf{VD}} = \frac{1}{|\Omega_p|}\int_{\Omega_p} \left\|\mathbf{V} - \widehat{\mathbf{V}}\right\|_2 + \left\|\mathbf{D} - \widehat{\mathbf{D}}\right\|_F \, d\mathbf{x} \\ \mathcal{L}_{\mathbf{U\Lambda}} = \frac{1}{|\Omega_p|}\int_{\Omega_p} \sum_{i=1}^{3(2)} min\{\left\|\mathbf{u}_i \pm \hat{\mathbf{u}}_i\right\|_2\} + \left\|\mathbf{\Lambda} - \widehat{\mathbf{\Lambda}}\right\|_F \, d\mathbf{x} \end{cases}$$

(tensor-structure-informed)

YETI | ***Fine-Tuning*** on Real Data (Link to Comparisons)



$$\mathcal{L}_{\text{Lat}} = \mathcal{L}_{\text{CC}} + w_{\text{SS}}\,\mathcal{L}_{\text{SS}}$$

$$\mathcal{L}_{\text{CC}} = \frac{1}{N_{\text{out}}}\sum_{j=i}^{i+N_{\text{out}}-1}\int_{\Omega_p} \frac{\left|C_p^{t_j} - \widehat{C}_p^{t_j}\right|^2 + w_\nabla \left\|\nabla C_p^{t_j} - \nabla \widehat{C}_p^{t_j}\right\|_2^2}{|\Omega_p|}\, d\mathbf{x} \quad \textit{(concentration at collocation)}$$

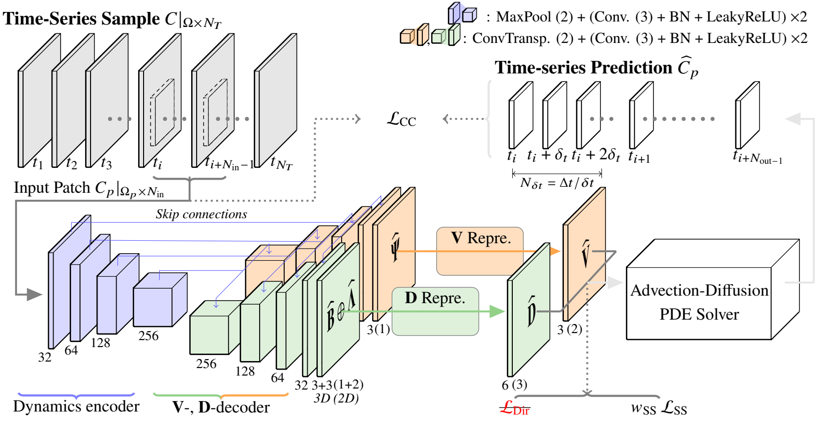
$$\mathcal{L}_{\text{SS}} = \frac{1}{|\Omega_p|}\int_{\Omega_p} \left(\sum_{i=1}^{3(2)} \|\nabla \widehat{\mathbf{V}}_i\|_2^2 + \sum_{i=1}^{9(4)} \|\nabla \widehat{\mathbf{D}}_i\|_2^2\right) d\mathbf{x} \quad \textit{(spatial smoothness)}$$

YETI | *Comparisons* on Pre-Training & Tensor Structure (Link to Framework in Appendix)

Experimental settings:

- "Dynamics-supervised" YETI
  - w/o pre-training
- "**VD**-supervised" YETI
- "Structure-informed" YETI

Experimental Setting: "Dynamics-supervised" YETI (Link to Framework in Appendix)

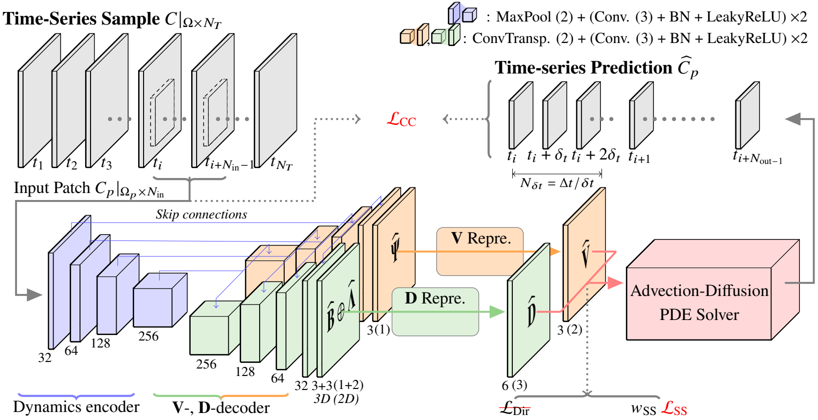


$$\cancel{\mathcal{L}_{\text{Dir}} = \mathcal{L}_{\text{VD}} + w_{\text{UA}}\,\mathcal{L}_{\text{UA}}}$$

$$\cancel{\mathcal{L}_{\text{VD}} = \frac{1}{|\Omega_p|} \int_{\Omega_p} \left\|\mathbf{V} - \widehat{\mathbf{V}}\right\|_2 + \left\|\mathbf{D} - \widehat{\mathbf{D}}\right\|_F dx}$$

$$\cancel{\mathcal{L}_{\text{UA}} = \frac{1}{|\Omega_p|} \int_{\Omega_p} \sum_{i=1}^{3(2)} min\{\left\|\mathbf{u}_i \pm \widehat{\mathbf{u}}_i\right\|_2\} + \left\|\mathbf{\Lambda} - \widehat{\mathbf{\Lambda}}\right\|_F dx \quad \textit{(tensor-structure-informed)}}$$

Experimental Setting: “Dynamics-supervised” YETI (Link to Framework in Appendix)



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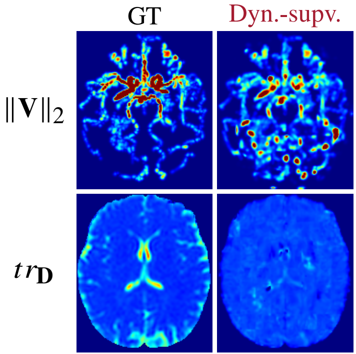
YETI | *Comparisons* on Pre-Training & Tensor Structure (Link to Framework in Appendix)



- $\|\mathbf{V}\|_2$: 2-norm map of velocity vector field $\mathbf{V}$
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  - w/ pre-training, w/o structure-informed supervision
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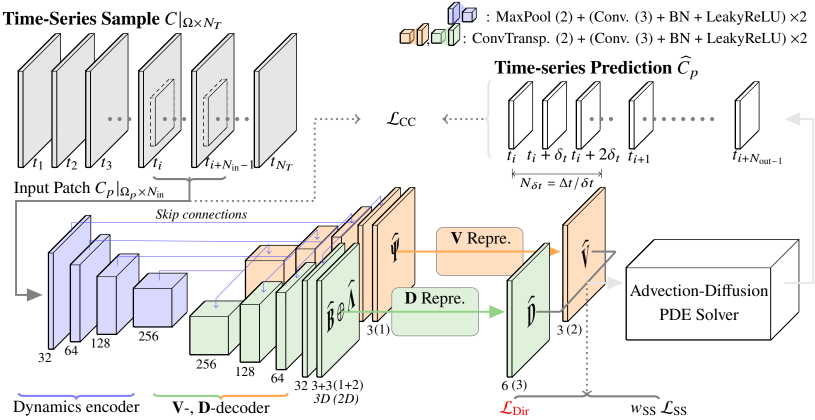
Experimental Setting: "VD-supervised" YETI (Link to Framework in Appendix)



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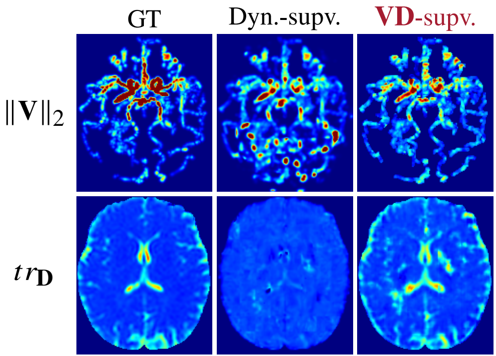
YETI | *Comparisons* on Pre-Training & Tensor Structure (Link to Framework in Appendix)



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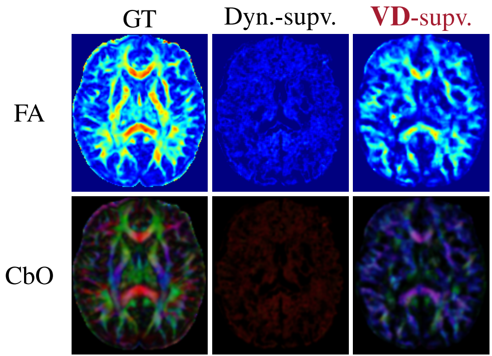
YETI | *Comparisons* on Pre-Training & Tensor Structure (Link to Framework in Appendix)



- FA: fractional anisotropy $\left(\mathrm{FA} = \sqrt{\frac{1}{2}} \sqrt{\frac{(\lambda_1-\lambda_2)^2+(\lambda_2-\lambda_3)^2+(\lambda_3-\lambda_1)^2}{\lambda_1^2+\lambda_2^2+\lambda_3^2}} \right)$
- CbO: colored FA map by the principal eigenvector ($\mathbf{U}_{\mathrm{prin}}$) of $\mathbf{D}$ (Red $= \mathrm{FA} \cdot u^x_{\mathrm{prin}}$; Green $= \mathrm{FA} \cdot u^y_{\mathrm{prin}}$; Blue $= \mathrm{FA} \cdot u^z_{\mathrm{prin}}$)

YETI | *Comparisons* on Pre-Training & Tensor Structure (Link to Framework in Appendix)

Experimental settings:

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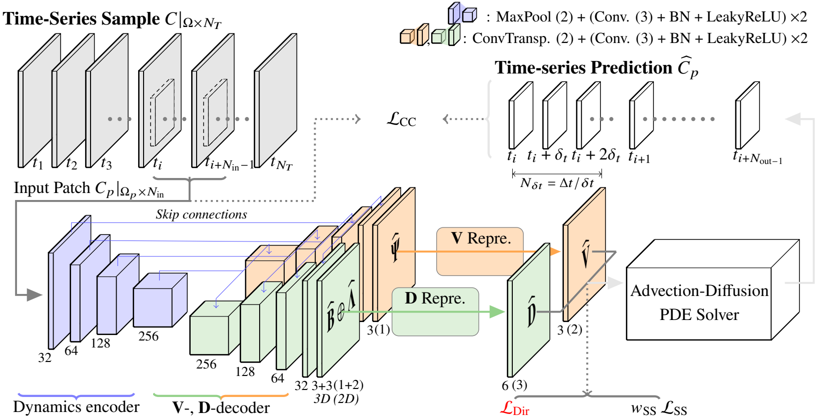
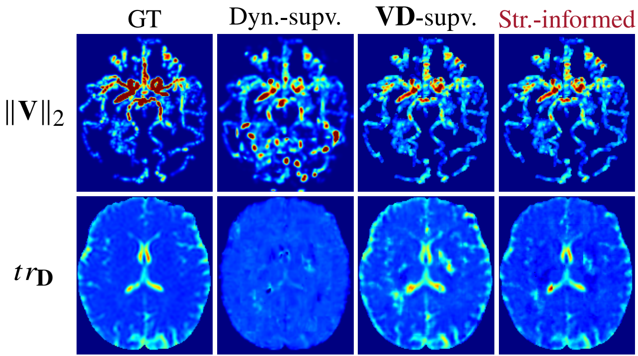
  - w/ pre-training, w/o structure-informed supervision
- "Structure-informed" YETI
  - w/ pre-training, w/ structure-informed supervision

Experimental Setting: “Structure-informed” YETI (Link to Framework in Appendix)



$$\mathcal{L}_{\text{Dir}} = \mathcal{L}_{\textbf{VD}} + w_{\text{U}\Lambda}\,\mathcal{L}_{\text{U}\Lambda} \quad \begin{cases} \mathcal{L}_{\textbf{VD}} = \frac{1}{|\Omega_p|}\int_{\Omega_p} \left\|\mathbf{V}-\widehat{\mathbf{V}}\right\|_2 + \left\|\mathbf{D}-\widehat{\mathbf{D}}\right\|_F \, d\mathbf{x} \\ \mathcal{L}_{\text{U}\Lambda} = \frac{1}{|\Omega_p|}\int_{\Omega_p} \Sigma_{i=1}^{3(2)}\, min\{\left\|\mathbf{u}_i \pm \widehat{\mathbf{u}}_i\right\|_2\} + \left\|\mathbf{\Lambda}-\widehat{\mathbf{\Lambda}}\right\|_F \, d\mathbf{x} \quad \textit{(tensor-structure-informed)} \end{cases}$$

YETI | *Comparisons* on Pre-Training & Tensor Structure (Link to Framework in Appendix)



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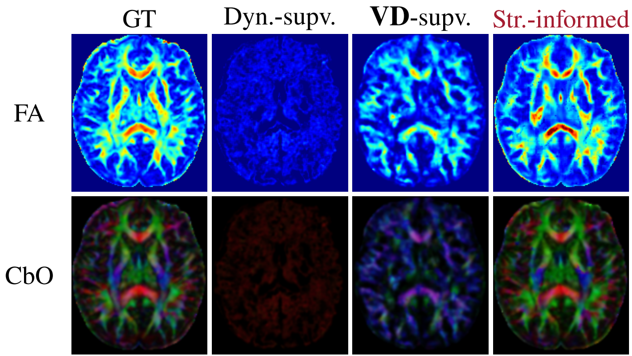
YETI | *Comparisons* on Pre-Training & Tensor Structure (Link to Framework in Appendix)



- FA: fractional anisotropy $\left(\mathrm{FA} = \sqrt{\frac{1}{2}}\sqrt{\frac{(\lambda_1-\lambda_2)^2+(\lambda_2-\lambda_3)^2+(\lambda_3-\lambda_1)^2}{\lambda_1^2+\lambda_2^2+\lambda_3^2}}\right)$
- CbO: colored FA map by the principal eigenvector ($\mathbf{U}_{\text{prin}}$) of **D** (Red $= \mathrm{FA} \cdot u^x_{\text{prin}}$; Green $= \mathrm{FA} \cdot u^y_{\text{prin}}$; Blue $= \mathrm{FA} \cdot u^z_{\text{prin}}$)

YETI | *Comparisons* on Tensor Structure (Link to Framework in Appendix)

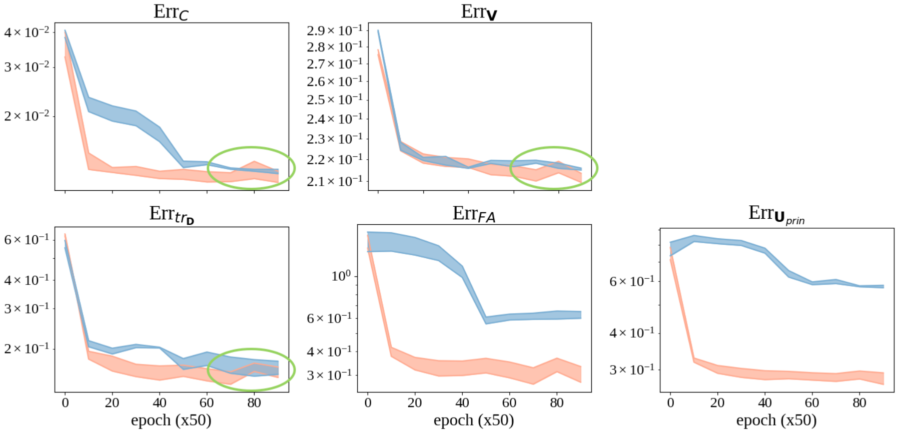


Figure: Mean relative absolute error (RAE) of "VD-supervised" YETI and "Structure-informed" YETI. Horizontal: training epoch; Vertical: RAE in log scale. Banded curves: the 25% & 75% percentile of the errors among 40 test samples.

YETI | *Comparisons* on Tensor Structure (Link to Framework in Appendix)

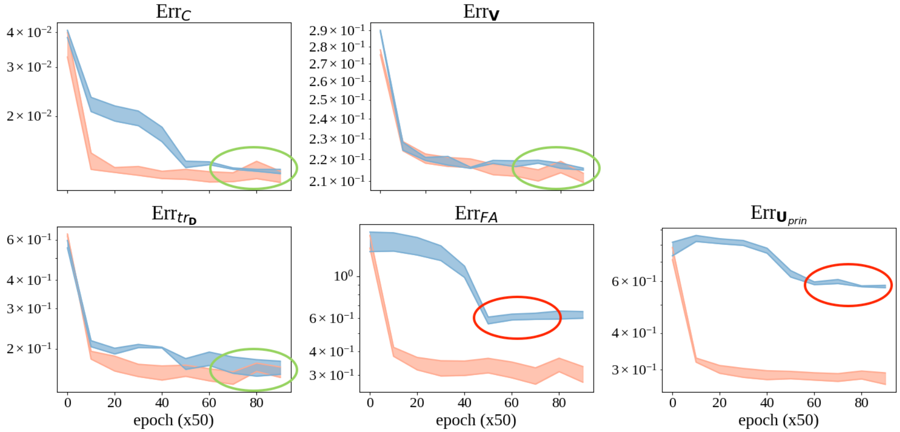


Figure: Mean relative absolute error (RAE) of "VD-supervised" YETI and "Structure-informed" YETI. Horizontal: training epoch; Vertical: RAE in log scale. Banded curves: the 25% & 75% percentile of the errors among 40 test samples.

Robust and Interpretable Learning for Modern Healthcare (Appendix)

[*Recap*] YETI - Governing Equation

$$\frac{\partial C}{\partial t} = - \mathbf{V} \cdot \nabla C + \nabla \cdot (\mathbf{D} \nabla C) \quad s.t. \quad \text{B.C.}$$

- Advection := $-\mathbf{V} \cdot \nabla C$
  - Incompressible fluid flow $\Leftrightarrow \nabla \cdot \mathbf{V} = 0$
- Diffusion := $\nabla \cdot (\mathbf{D} \nabla C)$
  - Symmetric positive semi-definite (PSD) diffusion

$* \, C = C(\mathbf{x}, t)$

[*SONATA*] Stochastic Mass Transport of Tracer - Governing Equation

$$\frac{\partial C}{\partial t} = -(P \diamond \overline{\mathbf{V}}) \cdot \nabla C + \nabla \cdot \left((P \circ \overline{\mathbf{D}}) \, \nabla C \right) + \sigma \partial W \quad s.t. \quad \text{B.C.}$$

- Advection $:= -\mathbf{V} \cdot \nabla C$
  - Incompressible fluid flow $\Leftrightarrow \nabla \cdot \mathbf{V} = 0$
  - $\overline{\mathbf{V}}$: "Anomaly-free" velocity vector field
- Diffusion $:= \nabla \cdot (\mathbf{D} \, \nabla C)$
  - Symmetric positive semi-definite (PSD) diffusion
  - $\overline{\mathbf{D}}$: "Anomaly-free" diffusion tensor field
- $P := P(\mathbf{x}) \in \mathbb{R}_{(0,\,1]}$: Anomaly probability
- $\sigma := \sigma(\mathbf{x}) \in \mathbb{R}_{(0,\,\infty)}$: Model uncertainty ($\propto$ Anomaly probability)

$*$ $C = C(\mathbf{x}, t)$, $W = W(\mathbf{x}, t)$: Brownian motion

Anomaly-Decomposed Divergence-Free Vector Representation

Requirements:

(a) *By construction*, learned velocity field $\mathbf{V}$ is divergence-free;

(b) *Any* divergence-free $\mathbf{V}$ can be represented;

(c) $\mathbf{V}$ can be decomposed into:

- P: anomaly probability field;
- $\overline{\mathbf{V}}$: corresponding "anomaly-free" velocity field.

Anomaly-Decomposed Divergence-Free Vector Representation

Theorem: Anomaly-decomposed Divergence-free Vector

For $\forall$ vector field $\mathbf{V} \in \mathbb{R}(\Omega)^d$ and scalar field P in $\mathbb{R}_{(0,1]}(\Omega)$ on a bounded domain $\Omega \subset \mathbb{R}^d$ with smooth boundary $\partial\Omega$. If $\mathbf{V}$ satisfies $\nabla \cdot \mathbf{V} = 0$, $\exists$ a potential $\boldsymbol{\Psi}$ in $\mathbb{R}(\Omega)^\alpha$:

$$\mathbf{V} = \nabla \times (P\,\boldsymbol{\Psi}), \quad (P\,\boldsymbol{\Psi}) \cdot \mathbf{n}\big|_{\partial\Omega} = 0.$$

Definition: "Anomaly-free" Velocity and Operation

Denote "anomaly-free" operator $\diamond$ for velocity fields:

$$\mathbf{V} = P \diamond \overline{\mathbf{V}} = \nabla P \times \Psi + P\,\overline{\mathbf{V}},$$

where $\overline{\mathbf{V}} = \nabla \times \Psi$.

$*\ \alpha = 1(3)$ when $d = 2(3)$

Anomaly-Decomposed Divergence-Free Vector Representation

Theorem: Anomaly-decomposed Divergence-free Vector

For $\forall$ vector field $\mathbf{V} \in \mathbb{R}(\Omega)^d$ and scalar field P in $\mathbb{R}_{(0,1]}(\Omega)$ on a bounded domain $\Omega \subset \mathbb{R}^d$ with smooth boundary $\partial\Omega$. If $\mathbf{V}$ satisfies $\nabla \cdot \mathbf{V} = 0$, $\exists$ a potential $\mathbf{\Psi}$ in $\mathbb{R}(\Omega)^\alpha$:

$$\mathbf{V} = \nabla \times (P\,\mathbf{\Psi}), \quad (P\,\mathbf{\Psi}) \cdot \mathbf{n}\big|_{\partial\Omega} = 0.$$

Conversely, for $\forall$ $P \in \mathbb{R}_{(0,1]}(\Omega)$, $\mathbf{\Psi} \in \mathbb{R}(\Omega)^\alpha$, $\nabla \cdot \mathbf{V} = \nabla \cdot (\nabla \times (P\,\mathbf{\Psi})) = 0$.

Definition: "Anomaly-free" Velocity and Operation

Denote "anomaly-free" operator $\diamond$ for velocity fields:

$$\mathbf{V} = P \diamond \overline{\mathbf{V}} = \nabla P \times \Psi + P\,\overline{\mathbf{V}},$$

where $\overline{\mathbf{V}} = \nabla \times \Psi$.

$*\ \alpha = 1(3)$ when $d = 2(3)$

Anomaly-Decomposed Symmetric PSD Tensor Representation

Definition: $n \times n$ Symmetric PSD Tensor Group

$$PSD(n) \equiv \{\mathbf{D} \in \mathbb{R}^{n\times n} \,\big|\, \forall \mathbf{x} \in \mathbb{R}^n : \mathbf{x}^T \mathbf{D} \mathbf{x} \geq 0\}.$$

Requirements:

(a) *By construction*, learned diffusion field **D** is symmetric PSD;

(b) *Any* symmetric PSD tensor field **D** can be represented;

(c) **D** can be decomposed into:

- P: anomaly probability field;
- $\overline{\mathbf{D}}$: corresponding “anomaly-free” diffusion tensor field.

Anomaly-Decomposed Symmetric PSD Tensor Representation

Theorem: Symmetric PSD Tensor via Spectral Decomposition

For $\forall$ $n \times n$ symmetric PSD tensor $\mathbf{D}$ and $P \in \mathbb{R}_{(0,1]}(\Omega)$, $\exists$ an upper triangular matrix with zero diagonal entries, $\mathbf{B} \in \mathbb{R}^{\frac{n(n-1)}{2}}$, and a non-negative diagonal matrix, $\mathbf{\Lambda} \in SD(n)$, satisfying:

$$\mathbf{D} = \mathbf{U}\,(P\,\mathbf{\Lambda})\,\mathbf{U}^T, \quad \mathbf{U} = exp(\mathbf{B} - \mathbf{B}^T) \in SO(n).$$

Definition: "Anomaly-free" Diffusion and Operation

Denote "anomaly-free" operator $\circ$ for diffusion tensor fields:

$$\mathbf{D} = P \circ \overline{\mathbf{D}} = P\,\overline{\mathbf{D}},$$

where $\overline{\mathbf{D}} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^T$.

Anomaly-Decomposed Symmetric PSD Tensor Representation

Theorem: Symmetric PSD Tensor via Spectral Decomposition

For $\forall\ n \times n$ symmetric PSD tensor $\mathbf{D}$ and $P \in \mathbb{R}_{(0,1]}(\Omega)$, $\exists$ an upper triangular matrix with zero diagonal entries, $\mathbf{B} \in \mathbb{R}^{\frac{n(n-1)}{2}}$, and a non-negative diagonal matrix, $\mathbf{\Lambda} \in SD(n)$, satisfying:

$$\mathbf{D} = \mathbf{U}\,(P\,\mathbf{\Lambda})\,\mathbf{U}^T, \quad \mathbf{U} = exp(\mathbf{B} - \mathbf{B}^T) \in SO(n).$$

Conversely, for $\forall P \in \mathbb{R}_{(0,1]}(\Omega)$, $\forall \mathbf{B} \in \mathbb{R}^{\frac{n(n-1)}{2}}$, and any diagonal matrix with non-negative diagonal entries, $\mathbf{\Lambda} \in SD(n)$, the above Eq. results in a symmetric PSD tensor, $\mathbf{D}$.

Definition: "Anomaly-free" Diffusion and Operation

Denote "anomaly-free" operator $\circ$ for diffusion tensor fields:

$$\mathbf{D} = P \circ \overline{\mathbf{D}} = P\,\overline{\mathbf{D}},$$

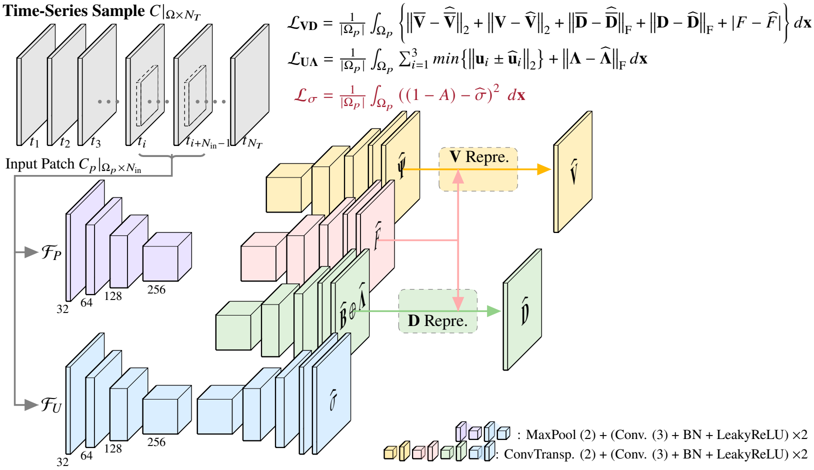
where $\overline{\mathbf{D}} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{U}^T$.

SONATA | *Pre-Training* on Synthetic Data (Link to Simulation)

$$\mathcal{L}_{\mathbf{VD}} = \frac{1}{|\Omega_p|}\int_{\Omega_p}\left\{\left\|\overline{\mathbf{V}}-\widehat{\overline{\mathbf{V}}}\right\|_2+\left\|\mathbf{V}-\widehat{\mathbf{V}}\right\|_2+\left\|\overline{\mathbf{D}}-\widehat{\overline{\mathbf{D}}}\right\|_F+\left\|\mathbf{D}-\widehat{\mathbf{D}}\right\|_F+\left|F-\widehat{F}\right|\right\}d\mathbf{x}$$

$$\mathcal{L}_{\mathbf{U\Lambda}} = \frac{1}{|\Omega_p|}\int_{\Omega_p}\sum_{i=1}^{3} min\left\{\left\|\mathbf{u}_i \pm \widehat{\mathbf{u}}_i\right\|_2\right\}+\left\|\mathbf{\Lambda}-\widehat{\mathbf{\Lambda}}\right\|_F\,d\mathbf{x}$$

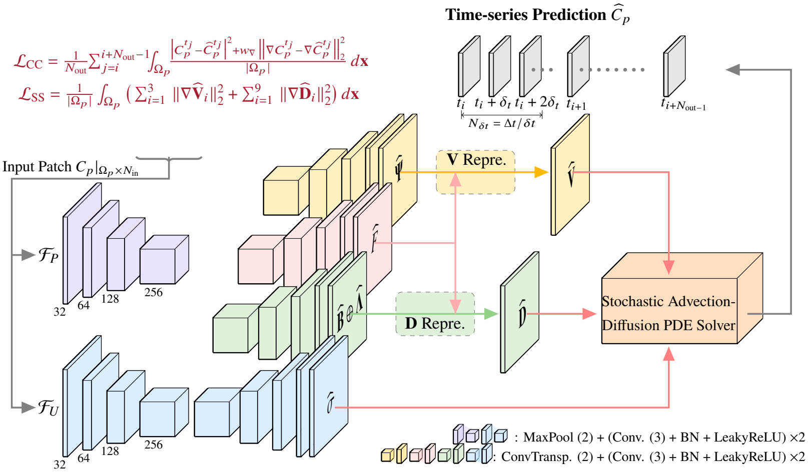
$$\mathcal{L}_{\sigma} = \frac{1}{|\Omega_p|}\int_{\Omega_p}\left((1-A)-\widehat{\sigma}\right)^2\,d\mathbf{x}$$



SONATA | *Fine-Tuning* on Real Data

$$\mathcal{L}_{\mathrm{CC}} = \frac{1}{N_{\mathrm{out}}} \sum_{j=i}^{i+N_{\mathrm{out}}-1} \int_{\Omega_p} \frac{\left|C_p^{t_j} - \widehat{C}_p^{t_j}\right|^2 + w_\nabla \left\|\nabla C_p^{t_j} - \nabla \widehat{C}_p^{t_j}\right\|_2^2}{|\Omega_p|} \, d\mathbf{x}$$

$$\mathcal{L}_{\mathrm{SS}} = \frac{1}{|\Omega_p|} \int_{\Omega_p} \left(\sum_{i=1}^{3} \|\nabla \widehat{\mathbf{V}}_i\|_2^2 + \sum_{i=1}^{9} \|\nabla \widehat{\mathbf{D}}_i\|_2^2 \right) d\mathbf{x}$$



End-to-End & *Interpretable* Stroke Lesion Detection | Quantitative Comparisons (Metrics)

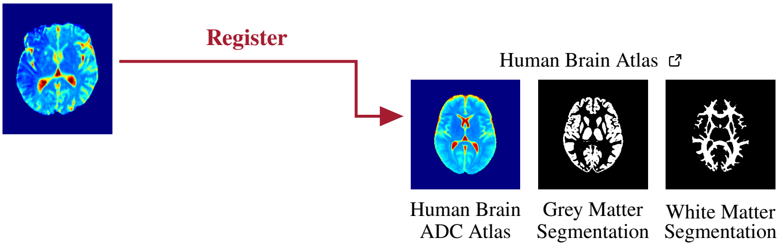
Metrics		$\mathtt{D^2}$-SONATA+			$\mathtt{D^2}$-SONATA			YETI		PIANO		ISLES		
		F	$\lVert\mathbf{V}\rVert_2$	$tr_{\mathbf{D}}$	F	$\lVert\mathbf{V}\rVert_2$	$tr_{\mathbf{D}}$	$\lVert\mathbf{V}\rVert_2$	$tr_{\mathbf{D}}$	$\lVert\mathbf{V}\rVert_2$	D	CBF	CBV	MTT
μ^r (↓)	*Me.*	0.45	**0.27**	0.44	0.47	0.29	0.42	0.30	0.59	0.55	0.58	0.67	0.78	0.57
	Med.	0.47	0.31	0.49	0.49	**0.30**	0.48	0.31	0.59	0.54	0.55	0.59	0.79	0.58
	(*STD*)	(0.13)	(0.15)	(0.14)	(0.13)	(0.17)	(0.15)	(0.11)	(0.19)	(0.15)	(0.16)	(0.12)	(0.23)	(0.13)
$\lvert t\rvert$ (↑)	*Me.*	**289**	167	159	280	165	166	155	49	108	52	34	16	31
	Med.	**292**	169	151	286	164	158	134	42	89	48	28	11	32
	(*STD*)	(51)	(42)	(56)	(58)	(37)	(60)	(62)	(22)	(35)	(26)	(22)	(12)	(37)
AUC (↑)	*Me.*	**0.80**	0.71	0.63	0.79	0.70	0.64	0.73	0.51	0.74	0.68	0.72	0.65	0.65
	Med.	**0.76**	0.72	0.65	0.76	0.71	0.65	0.73	0.50	0.74	0.69	0.73	0.68	0.66
	(*STD*)	(0.06)	(0.04)	(0.08)	(0.05)	(0.04)	(0.07)	(0.06)	(0.03)	(0.04)	(0.03)	(0.07)	(0.06)	(0.06)

* ↓ (↑) indicates the lower (higher) values are better.

Quantitative comparison between $\mathtt{D^2}$-SONATA+, $\mathtt{D^2}$-SONATA, YETI, PIANO and ISLES maps across 10 test subjects from ISLES2017-MRP dataset, using *Mean (Me.)*, *Median (Med.)*, *Standard Deviation (STD)* of relative mean μ^r, absolute ($|t|$), and area under the curve (AUC).

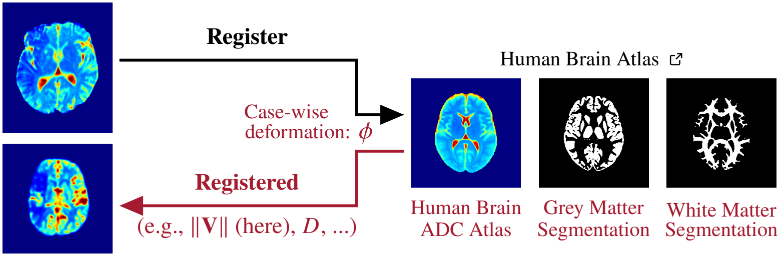
Robust and Interpretable Learning for Modern Healthcare (Appendix)

Building Averaged Perfusion Feature Atlas (Link to Results)



P. Liu et al.: `HARP`: Hemisphere-Normalized Atlas Representing Perfusion. *Under Review at **Stroke*** (2024)

Building Averaged Perfusion Feature Atlas (Link to Results)



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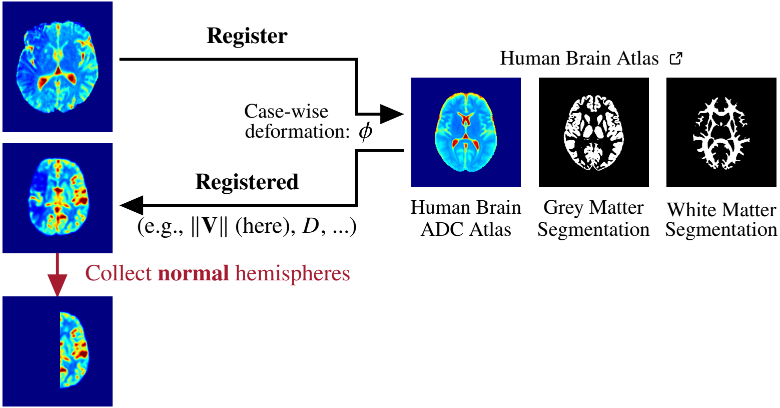

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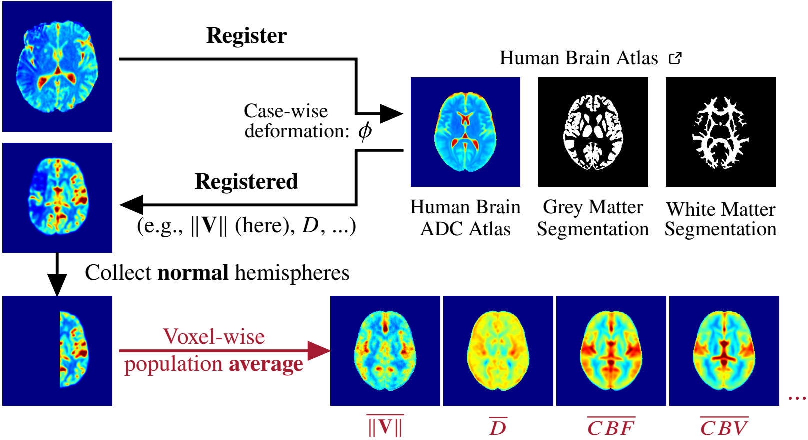
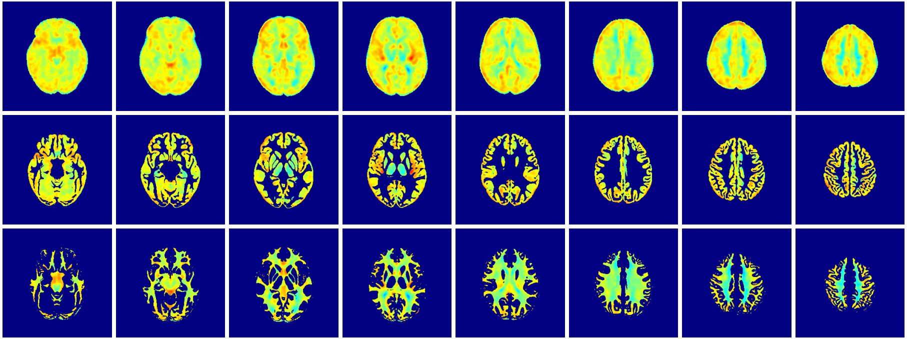


P. Liu et al.: HARP: Hemisphere-Normalized Atlas Representing Perfusion. *Under Review at **Stroke*** (2024)

Diffusion Atlas (D) Maps (Link to Pipeline)

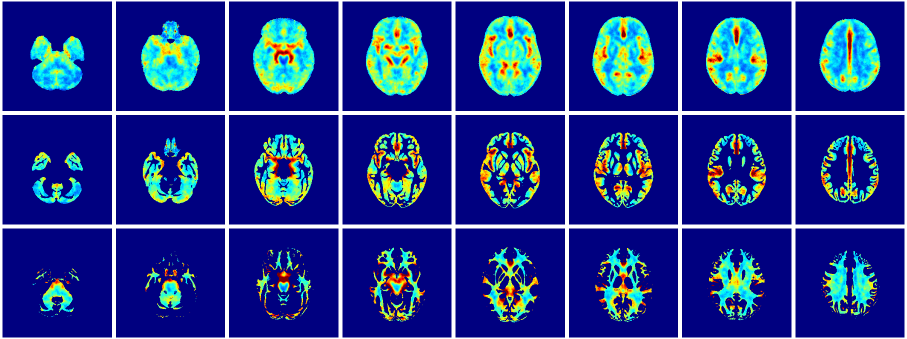


* Top: D atlas averaged from normal hemispheres;

Middle (Bottom): D atlas segmented by gray (white) matter.

P. Liu et al.: HARP: Hemisphere-Normalized Atlas Representing Perfusion. *Under Review at **Stroke*** (2024)

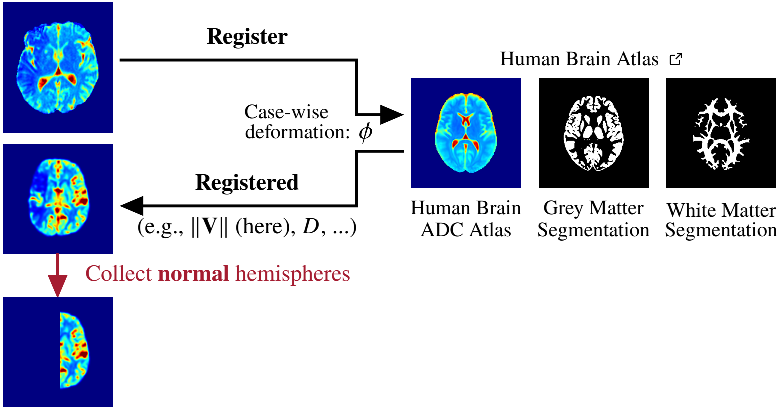
Velocity Atlas (||V||) Maps (Link to Pipeline)



* Top: ||**V**|| atlas averaged from normal hemispheres;
  Middle (Bottom): ||**V**|| atlas segmented by gray (white) matter.

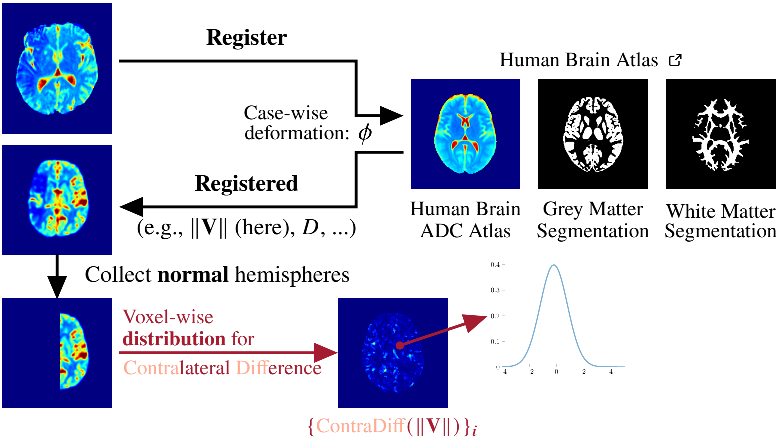
P. Liu et al.: HARP: Hemisphere-Normalized Atlas Representing Perfusion. *Under Review at **Stroke*** (2024)

Building Contralateral Difference Atlas



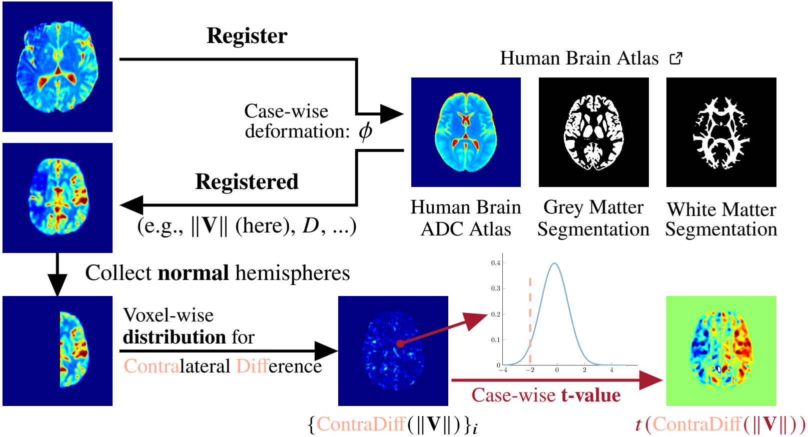
P. Liu et al.: HARP: Hemisphere-Normalized Atlas Representing Perfusion. *Under Review at **Stroke*** (2024)

Building Contralateral Difference Atlas



P. Liu et al.: HARP: Hemisphere-Normalized Atlas Representing Perfusion. *Under Review at **Stroke*** (2024)

Building Contralateral Difference Atlas



P. Liu et al.: HARP: Hemisphere-Normalized Atlas Representing Perfusion. *Under Review at **Stroke*** (2024)

ISLES2017 Brain Perfusion Dataset: Comparison Results (Link to Metrics)

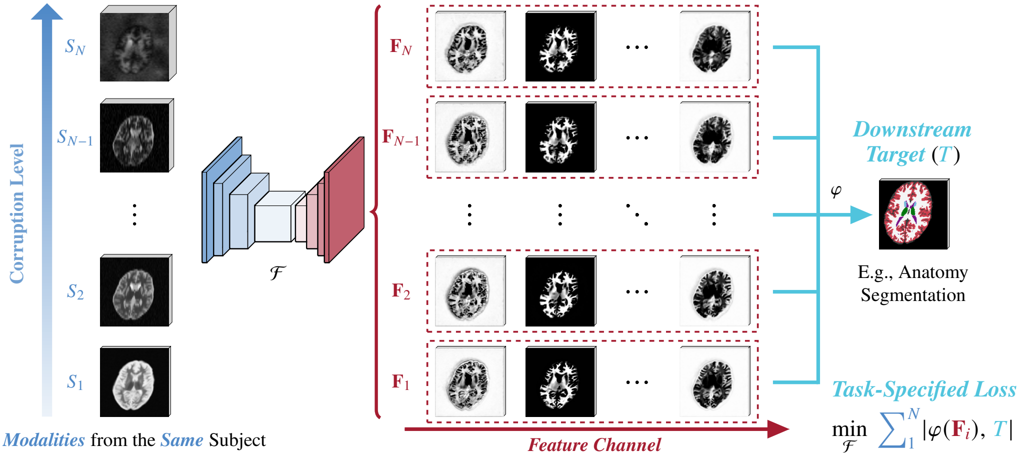
Maps		$\|\mathbf{V}\|_2$	$\|\mathbf{V}\|_2$-T_{CD}	D	D-T_{CD}	ADC	CBF	CBV	MTT	TTP	Tmax
μ^r	*Mean*	0.54	-	0.59	-	0.76	0.57	0.72	0.61	0.69	**0.21**
	Median	0.52	-	0.56	-	0.78	0.56	0.76	0.63	0.68	**0.15**
	STD	**0.12**	-	0.19	-	0.14	0.19	0.15	0.20	0.13	0.16
σ^r	*Mean*	0.69	-	0.55	-	0.75	0.63	0.76	0.56	0.55	**0.35**
	Median	0.66	-	0.55	-	0.78	0.61	0.77	0.55	0.54	**0.29**
	STD	**0.14**	-	0.17	-	0.20	0.18	0.16	0.17	0.19	0.23
$\|t\|$	*Mean*	60.10	**80.56**	29.51	34.20	20.55	32.61	13.53	33.56	44.59	59.86
	Median	47.13	**50.13**	20.58	26.28	13.50	26.08	8.48	18.52	28.87	46.44
	STD	51.83	**67.30**	27.67	38.84	19.53	27.47	14.21	31.70	44.16	50.33
AUC	*Actual*	0.73	**0.81**	0.59	0.63	0.69	0.66	0.57	0.64	0.75	0.78
	Ratio	0.81	**0.84**	0.72	0.73	0.66	0.71	0.57	0.60	0.80	0.78

Quantitative comparison between PIANO feature maps, their ***contra-lateral difference significance*** (T_{CD}), and ISLES2017 summary maps over 43 subjects, using relative mean μ^r, STD ratio σ^r, absolute t-value $|t|$, and area under curve (AUC) of receiver operating characteristic (ROC) curves.

P. Liu et al.: HARP: Hemisphere-Normalized Atlas Representing Perfusion. *Under Review at **Stroke*** (2024)

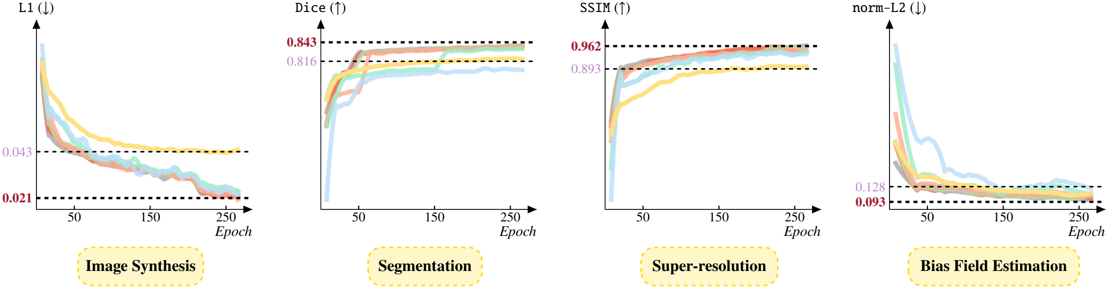
Robust and Interpretable Learning for Modern Healthcare (Appendix)

Modality-Agnostic Feature Representation | Downstream Adaptation



P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

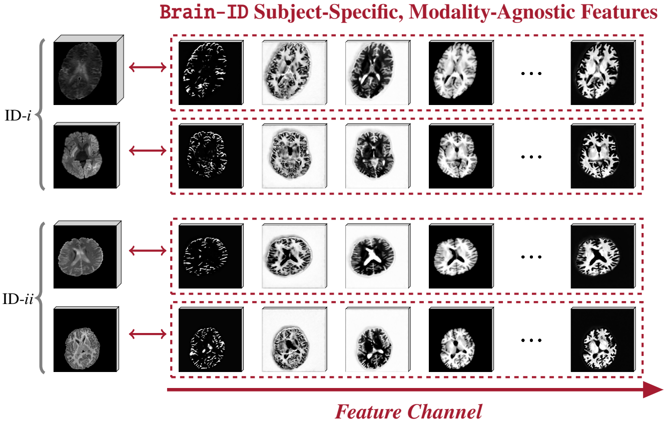
Feature Robustness & *Generalizability* | Downstream Adaptations on *Small* Datasets



# of Training Samples:	300	300	240	180	120	60	30
Model:	w/o Brain-ID	*Brain-ID*	*Brain-ID*	*Brain-ID*	*Brain-ID*	*Brain-ID*	*Brain-ID*
Curve:							

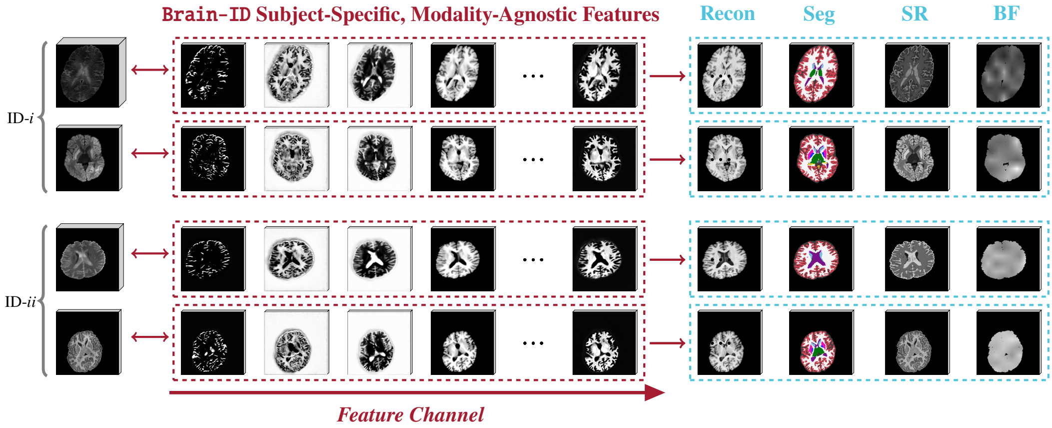
P. Liu et al.: ***Brain-ID***: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Feature Robustness & *Generalizability* | Adapt Features to Downstream Tasks



P. Liu et al.: **Brain-ID**: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

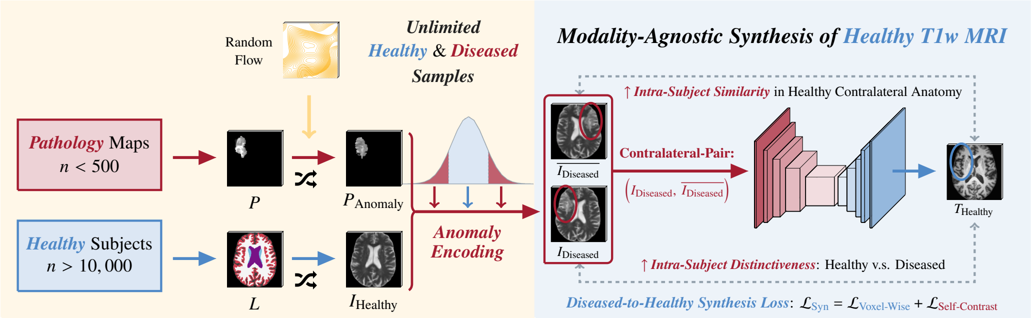
Feature Robustness & *Generalizability* | Adapt Features to Downstream Tasks



P. Liu et al.: ***Brain-ID***: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

Robust and Interpretable Learning for Modern Healthcare (Appendix)

Modality-Agnostic Synthesis | Bridging Diseased ↦ Healthy: *Beyond Annotations*



UNA's Healthy-to-Diseased Generation Naturally Enables ***Supervised Learning***

P. Liu et al.: Brain-ID: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)

P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

Robustness & ***Generalizability*** | Pathology Appearance & Modality - Comparisons

Table: Quantitative comparisons of healthy anatomy reconstruction performance between ***UNA*** and state-of-the-art contrast-agnostic T1w synthesis models, using images with simulated pathology.

Modality	**Method**	**L1 (↓)**			**PSNR (↑)**			**SSIM (↑)**		
		Full	Healthy	Diseased	Full	Healthy	Diseased	Full	Healthy	Diseased
T1w MRI	SynthSR (2023)	0.0285	0.0253	0.0010	20.71	22.90	36.59	0.823	0.879	0.895
	Brain-ID (2024)	0.0231	0.0219	0.0007	22.86	23.71	40.22	0.859	0.890	0.904
	PEPSI (2024)	0.0257	0.0194	N/A	21.78	23.21	N/A	0.831	0.872	N/A
	UNA	**0.0147**	**0.0143**	**0.0003**	**31.98**	**33.25**	**45.61**	**0.981**	**0.992**	**0.998**
T2w MRI	SynthSR (2023)	0.0362	0.0337	0.0016	18.25	20.66	35.47	0.816	0.864	0.880
	Brain-ID (2024)	0.0277	0.0269	0.0008	20.98	22.31	39.62	0.844	0.881	0.892
	PEPSI (2024)	0.0295	0.0279	N/A	19.33	23.18	N/A	0.820	0.845	N/A
	UNA	**0.0184**	**0.0182**	**0.0003**	**25.14**	**26.22**	**45.69**	**0.938**	**0.981**	**0.998**
FLAIR MRI	SynthSR (2023)	0.0327	0.0300	0.0016	19.30	21.04	34.88	0.823	0.869	0.895
	Brain-ID (2024)	0.0285	0.0242	0.0010	19.98	20.32	38.76	0.840	0.879	0.907
	PEPSI (2024)	0.0301	0.0287	N/A	19.82	21.59	N/A	0.842	0.850	N/A
	UNA	**0.0202**	**0.0194**	**0.0007**	**28.34**	**28.93**	**42.91**	**0.921**	**0.982**	**0.996**
CT	SynthSR (2023)	0.0541	0.0536	0.0029	13.97	13.13	28.50	0.712	0.763	0.725
	Brain-ID (2024)	0.0339	0.0357	0.0018	20.15	21.20	32.87	0.811	0.824	0.843
	PEPSI (2024)	0.0473	0.0420	N/A	16.72	16.90	N/A	0.723	0.782	N/A
	UNA	**0.0259**	**0.0266**	**0.0010**	**25.63**	**25.70**	**42.53**	**0.883**	**0.897**	**0.895**

P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

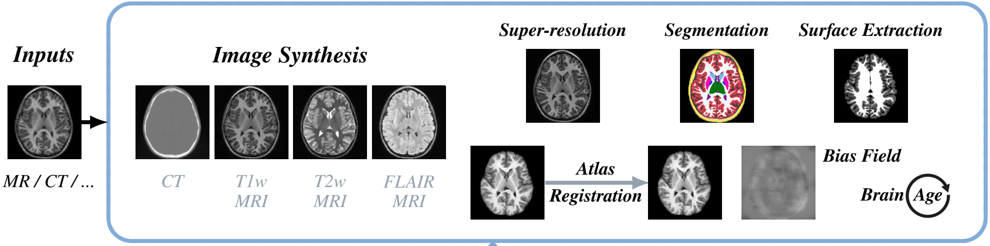
Robustness & *Generalizability* | Anomaly Detection *Beyond Annotations*

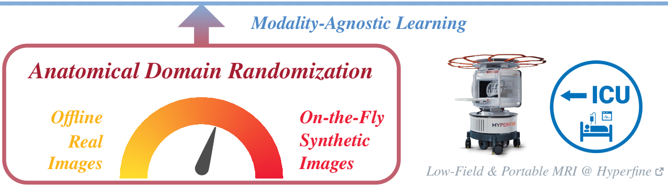
Table: **Dice** scores (↑) of anomaly detection performance based on the voxel-wise absolute differences between the diseased input and the reconstructed anatomy.

Image Source	**Dataset**	SynthSR (2023)	Brain-ID (2024)	VAE (2021)	LDM (2023)	***UNA***
Healthy T1w with Simulated Pathology	ADNI	0.27	0.26	0.18	0.23	**0.36**
	HCP	0.28	0.28	0.13	0.21	**0.33**
	ADHD200	0.23	0.25	0.15	0.23	**0.34**
	ADNI3	0.27	0.28	0.17	0.24	**0.37**
	AIBL	0.25	0.24	0.12	0.20	**0.32**
Stroke T1w	ATLAS	0.24	0.24	0.11	0.22	**0.31**

P. Liu et al.: *U*nraveling *N*ormal *A*natomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

[*Summary*] Modality-Agnostic Foundation Model | ***Ready-to-Use Software @ FreeSurfer***





✓ Out-of-the-Box Usage

✓ Offline Fine-Tuning

P. Liu et al.: `Brain-ID`: Learning Contrast-Agnostic Anatomical Representations for Brain Imaging. ***ECCV*** (2024)

P. Liu et al.: Pathology-Enhanced Pulse-Sequence-Invariant Representations for Brain MRI. ***MICCAI*** (2024)

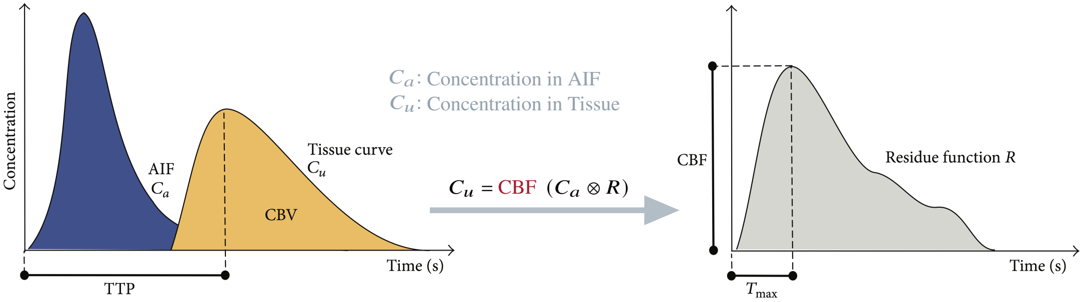
P. Liu et al.: Unraveling Normal Anatomy via Fluid-Driven Anomaly Randomization. ***CVPR*** (2025)

P. Liu et al.: A Modality-Agnostic Multi-Task Foundation Model for Human Brain Imaging. *Under Review at* ***IEEE TMI*** (2025)

Robust and Interpretable Learning for Modern Healthcare (Appendix)

Stroke | Ischemic Stroke | Perfusion Imaging - Conventional *Voxel-Wise* Analysis

Conventional Perfusion Summary Maps *(CBF, CBV, MTT, TTP, T_{max} ...)*

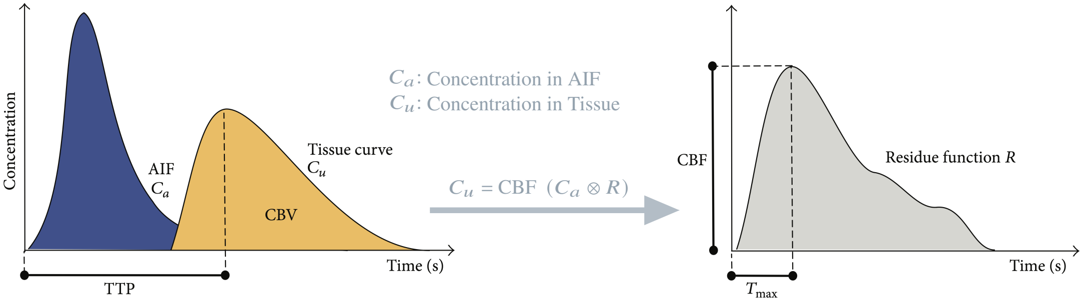


CBF: Cerebral Blood Flow | T_{max}: Time To Max | MTT: Mean Transit Time = CBV / CBF
TTP: Time To Peak | CBV: Cerebral Blood Volume | AIF: Arterial Input Function

F. Scalzo & D. Liebeskind: Perfusion Angiography in Acute Ischemic Stroke. *Computational and Mathematical Methods in Medicine* (2016)

Stroke | Ischemic Stroke | Perfusion Imaging - Conventional *Voxel-Wise* Analysis

✗ ***Variation** in (1) AIF Selection, (2) CA Injection Rate, (3) Deconvolution Algorithm (⊗), ...*



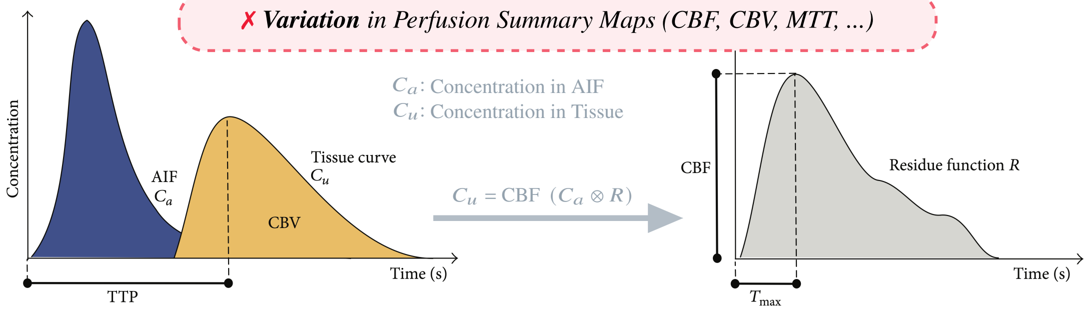
CBF: Cerebral Blood Flow | T_{max}: Time To Max | MTT: Mean Transit Time = CBV / CBF
TTP: Time To Peak | CBV: Cerebral Blood Volume | AIF: Arterial Input Function

F. Calamante: Arterial Input Function in Perfusion MRI: A Comprehensive Review. *Progress in Nuclear Magnetic Resonance Spectroscopy* (2013)

Stroke | Ischemic Stroke | Perfusion Imaging - Conventional *Voxel-Wise* Analysis

✗ ***Variation*** *in (1) AIF Selection, (2) CA Injection Rate, (3) Deconvolution Algorithm (⊗), ...*

✗ ***Variation*** *in Perfusion Summary Maps (CBF, CBV, MTT, ...)*



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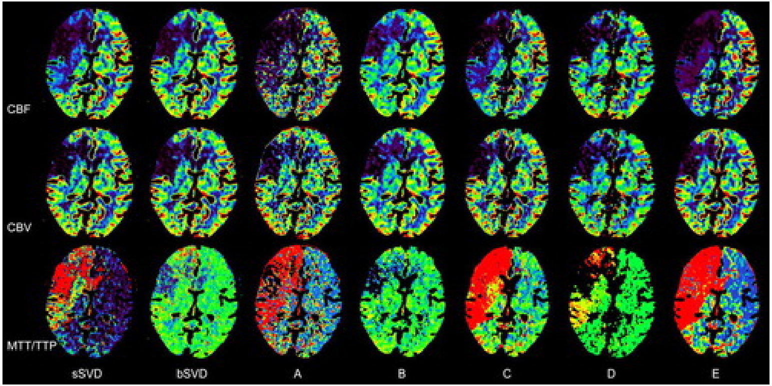
F. Calamante: Arterial Input Function in Perfusion MRI: A Comprehensive Review. *Progress in Nuclear Magnetic Resonance Spectroscopy* (2013)

Stroke | Ischemic Stroke | Perfusion Imaging - Conventional *Voxel-Wise* Analysis



Perfusion summary maps generated from ***identical source*** data using ***different software***

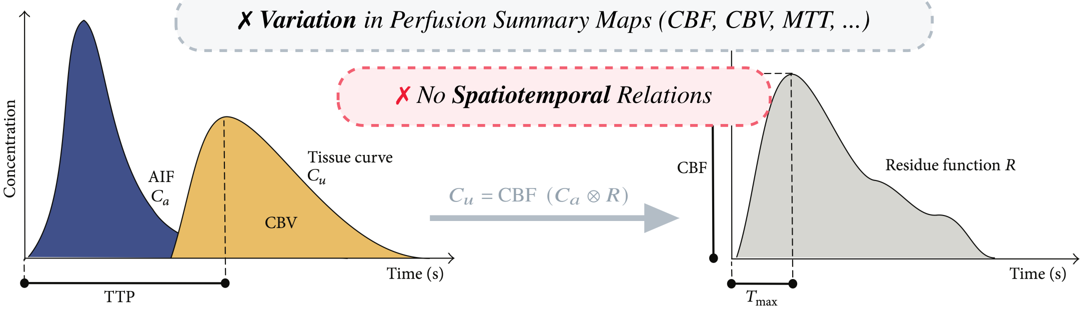
K. Kudo et al.: Differences in CT Perfusion Maps Generated by Different Commercial Software. *Radiology* (2009)

Stroke | Ischemic Stroke | Perfusion Imaging - Conventional *Voxel-Wise* Analysis

✗ ***Variation*** *in (1) AIF Selection, (2) CA Injection Rate, (3) Deconvolution Algorithm (⊗), ...*

✗ ***Variation*** *in Perfusion Summary Maps (CBF, CBV, MTT, ...)*

✗ *No **Spatiotemporal** Relations*



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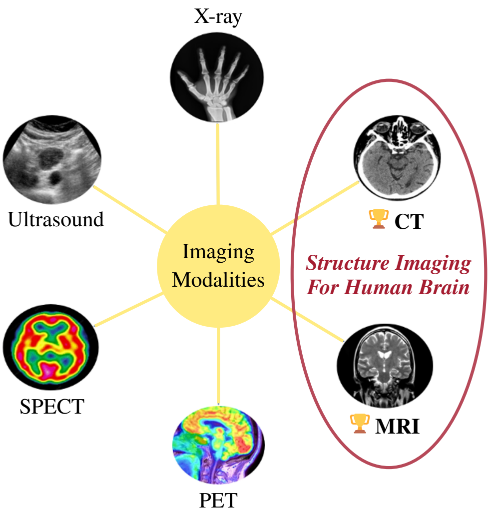
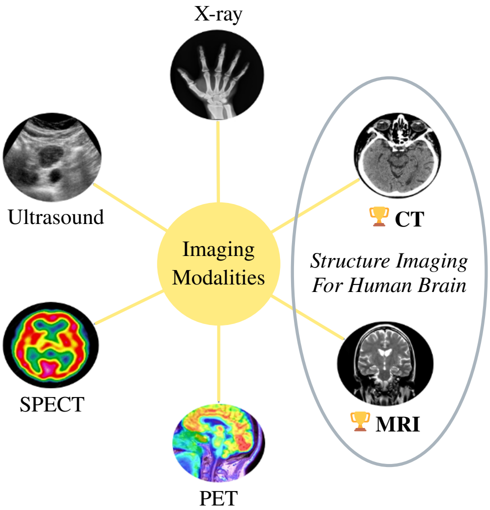
F. Calamante: Arterial Input Function in Perfusion MRI: A Comprehensive Review. *Progress in Nuclear Magnetic Resonance Spectroscopy* (2013)

Medical Imaging Techniques | *CT* & *MRI*



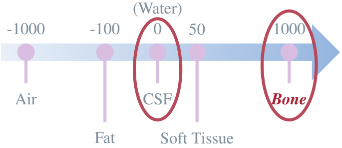
Medical Imaging Techniques | *CT* & *MRI*



CT

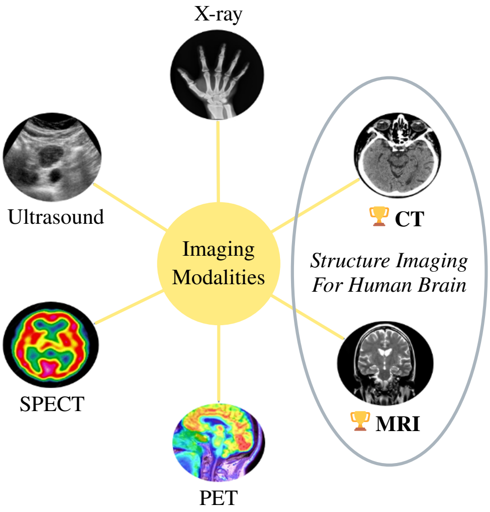
Bones
Fluid
Tumors
Vascular Disease

Hounsfield Units (HU)



MRI

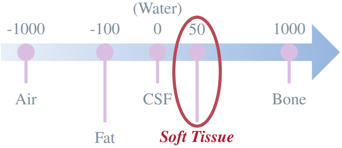
Medical Imaging Techniques | *CT* & *MRI*



CT

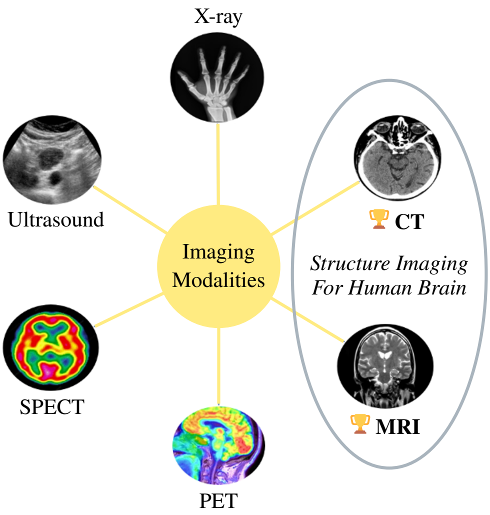
Bones
Fluid
Tumors
Vascular Disease

Hounsfield Units (HU)



MRI

Medical Imaging Techniques | *CT* & *MRI*



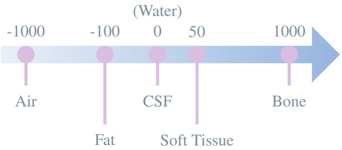
CT

Bones
Fluid
Tumors
Vascular Disease

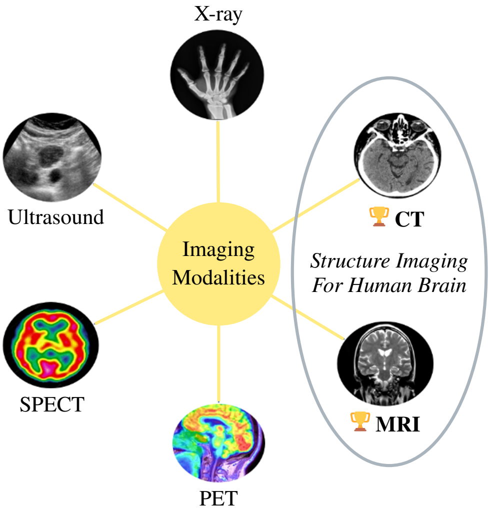
MRI

Soft Tissues
Tumors
Spinal Cords
Tendons/Joints

Hounsfield Units (HU)



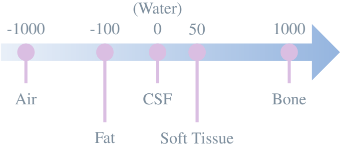
Medical Imaging Techniques | *CT* & *MRI*



CT

Bones
Fluid
Tumors
Vascular Disease

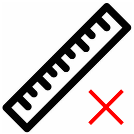
Hounsfield Units (HU)



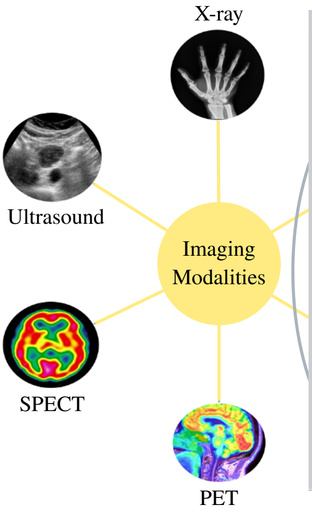
MRI

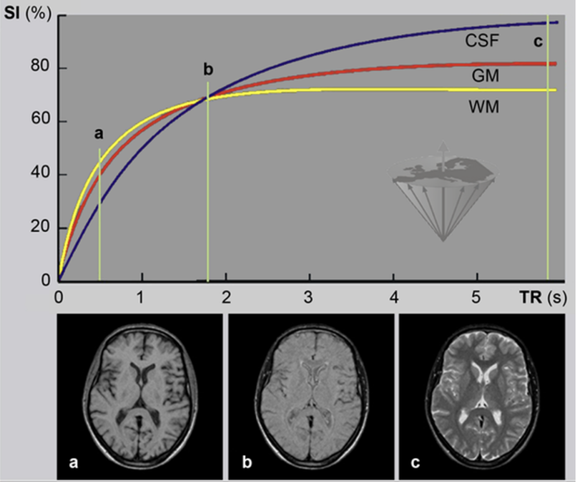
Soft Tissues
Tumors
Spinal Cords
Tendons/Joints

Non-Quantified Units



Medical Imaging Techniques | *CT* & *MRI*





*Signal-intensity (SI) behavior of a partial saturation pulse sequence - **All are T1w!***

MRI

Soft Tissues
Tumors
Spinal Cords
Tendons/Joints

Non-Quantified Units

The End

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Athinoula A. Martinos Center For Biomedical Imaging