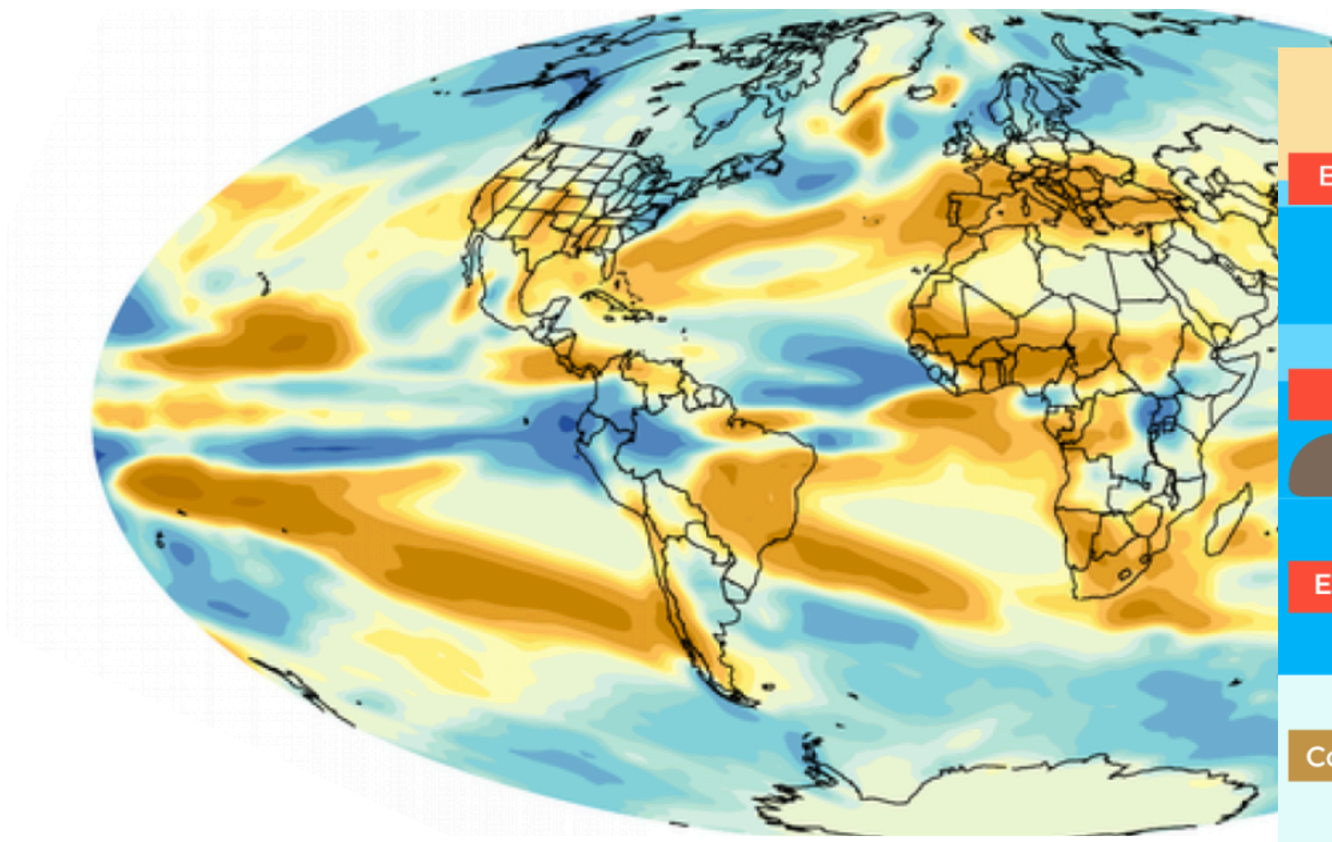
Causal inference for scientific discovery in fluid dynamics

Adrian Lozano Duran
Caltech

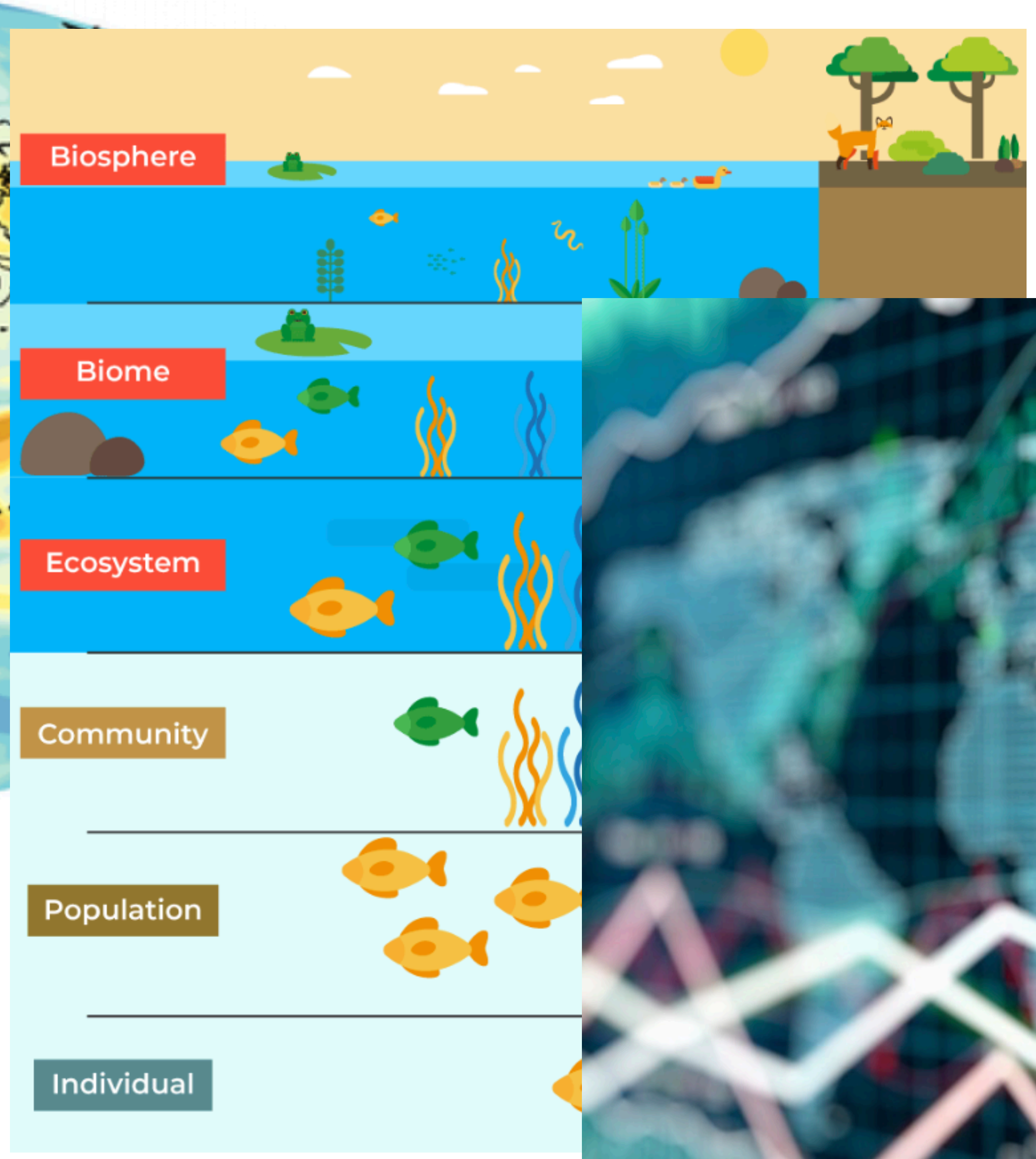
ERCOFTAC, ML for Fluids
March 4, 2026

ML for turbulence closures

Causality in Science

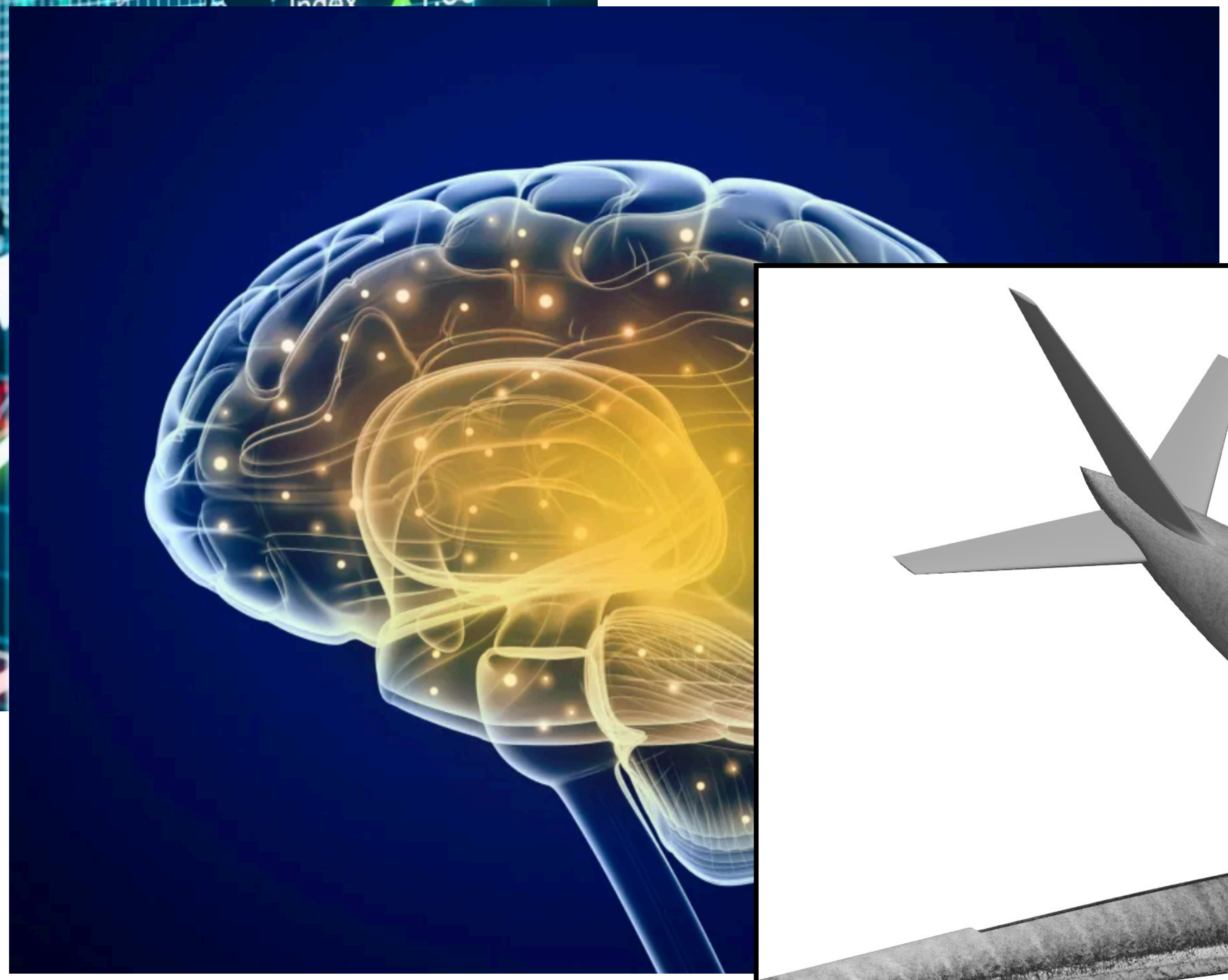


Climate

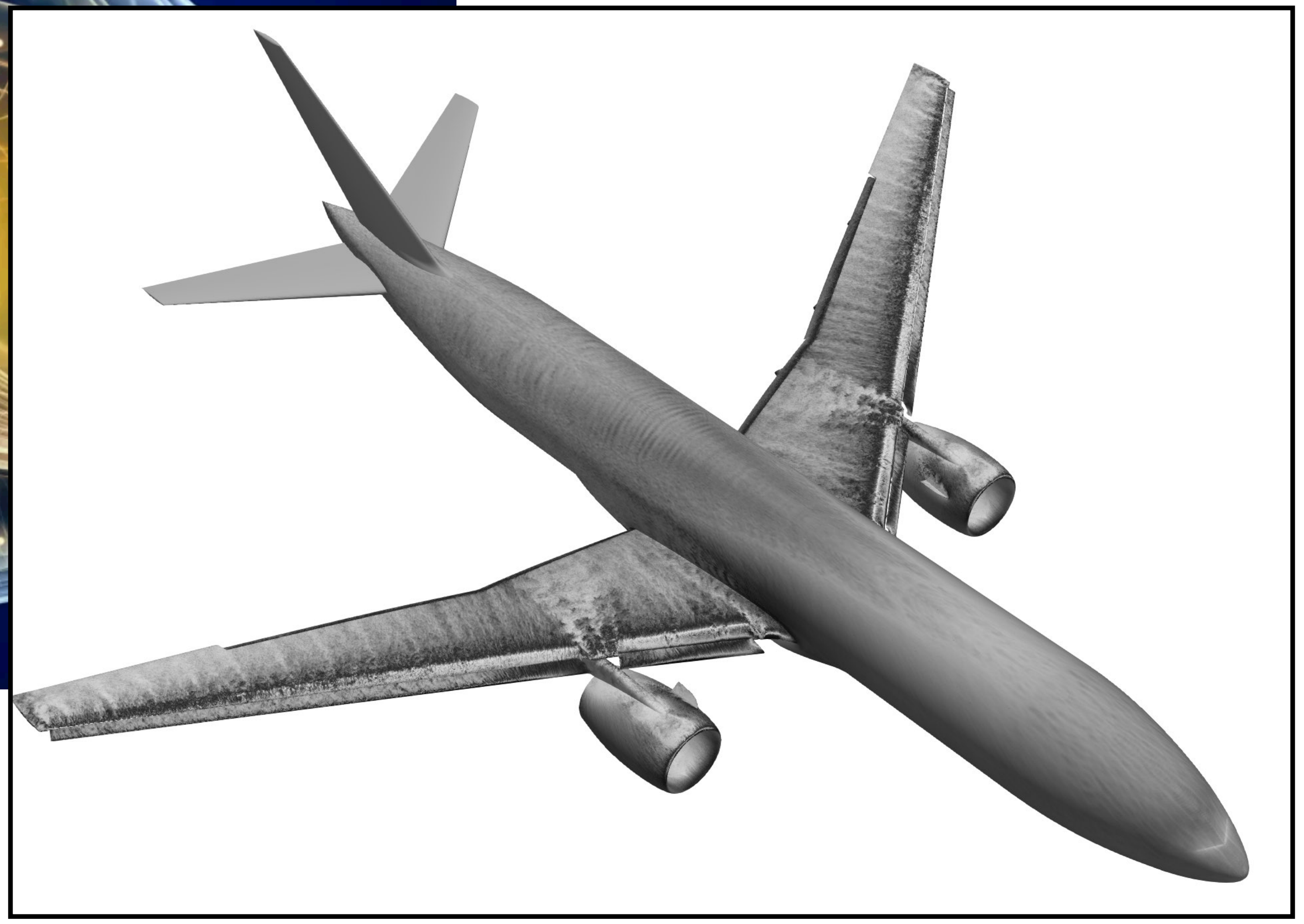


Ecology

Economics



Neuroscience



Fluid dynamics

. . .

Outline

- **What is causality?**
- **Frameworks for causal inference**
  - Interventional vs. observational
- **Three level of causality**
  - Average causality
  - State-dependent causality
  - Space-time causality
- **Limitations**

Outline

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Related publications at

adrianld.mit.edu

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“Causality is the mechanism by which one event contributes to the genesis of another”

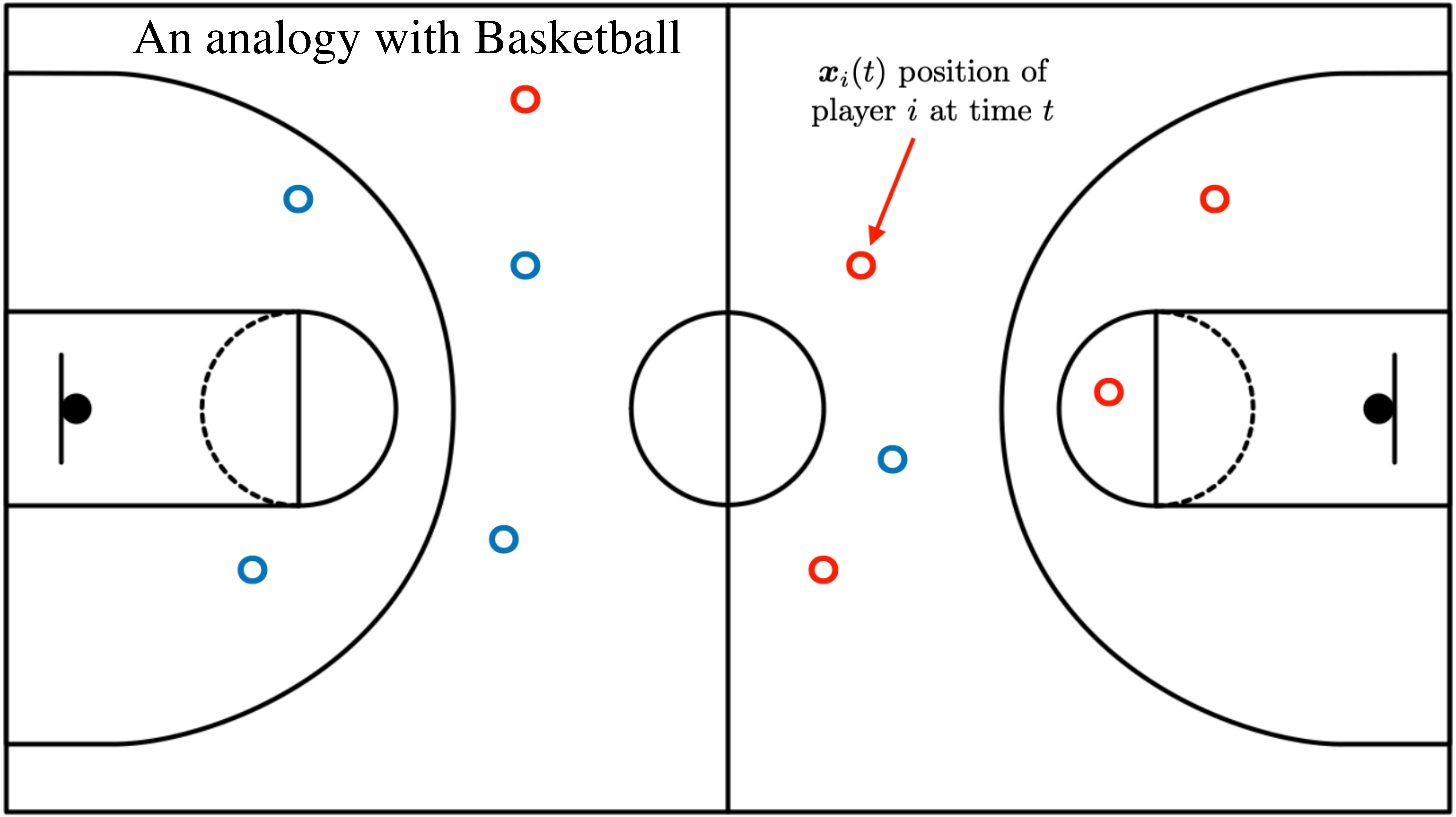
What is causality?

Credit: Laura Prescott

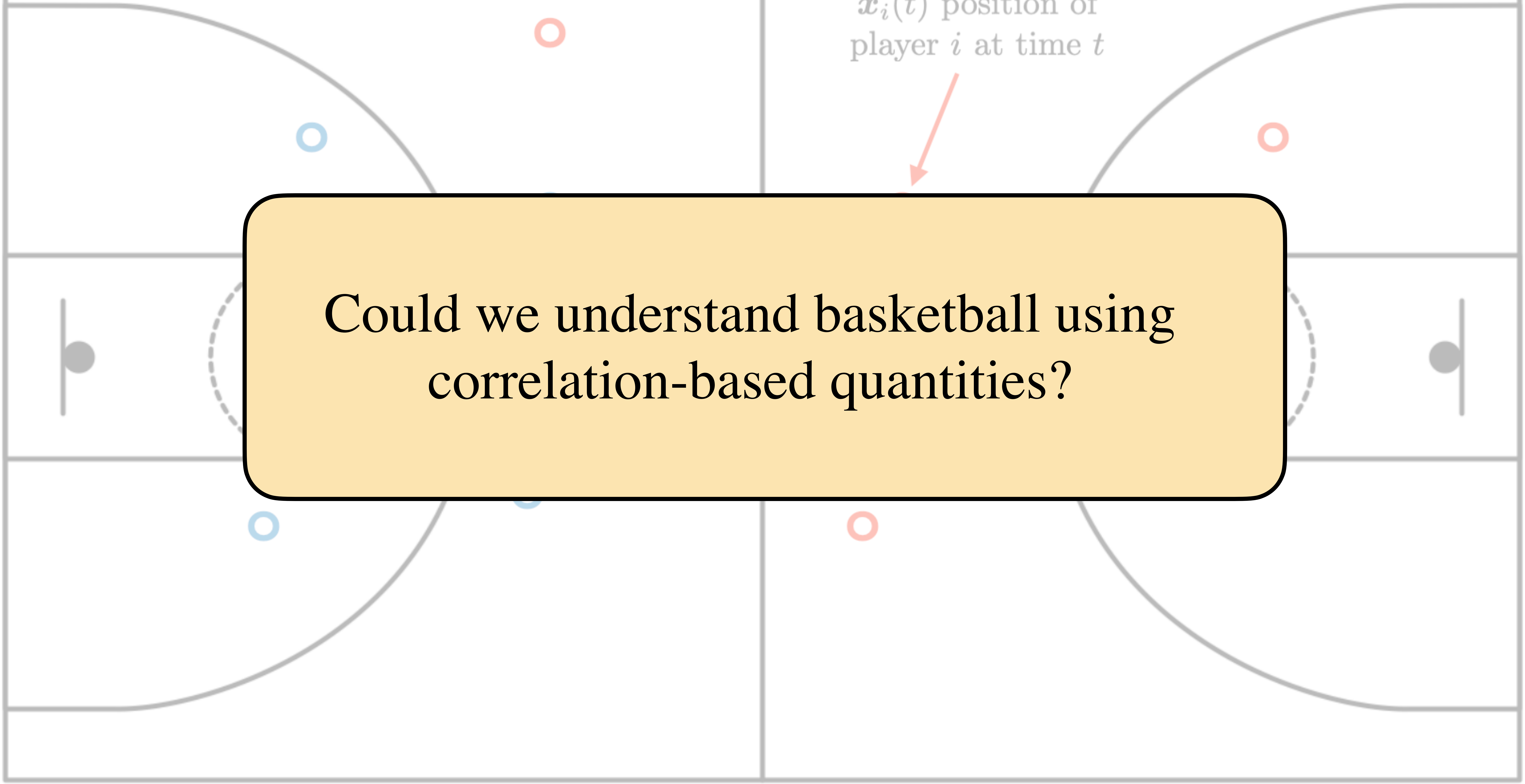
“Causality” in turbulence research

- Space/Temporal correlations
- One/two-point statistics
- Energy budget
- Linear stability analisys
- Modal decomposition
- ...

An analogy with Basketball

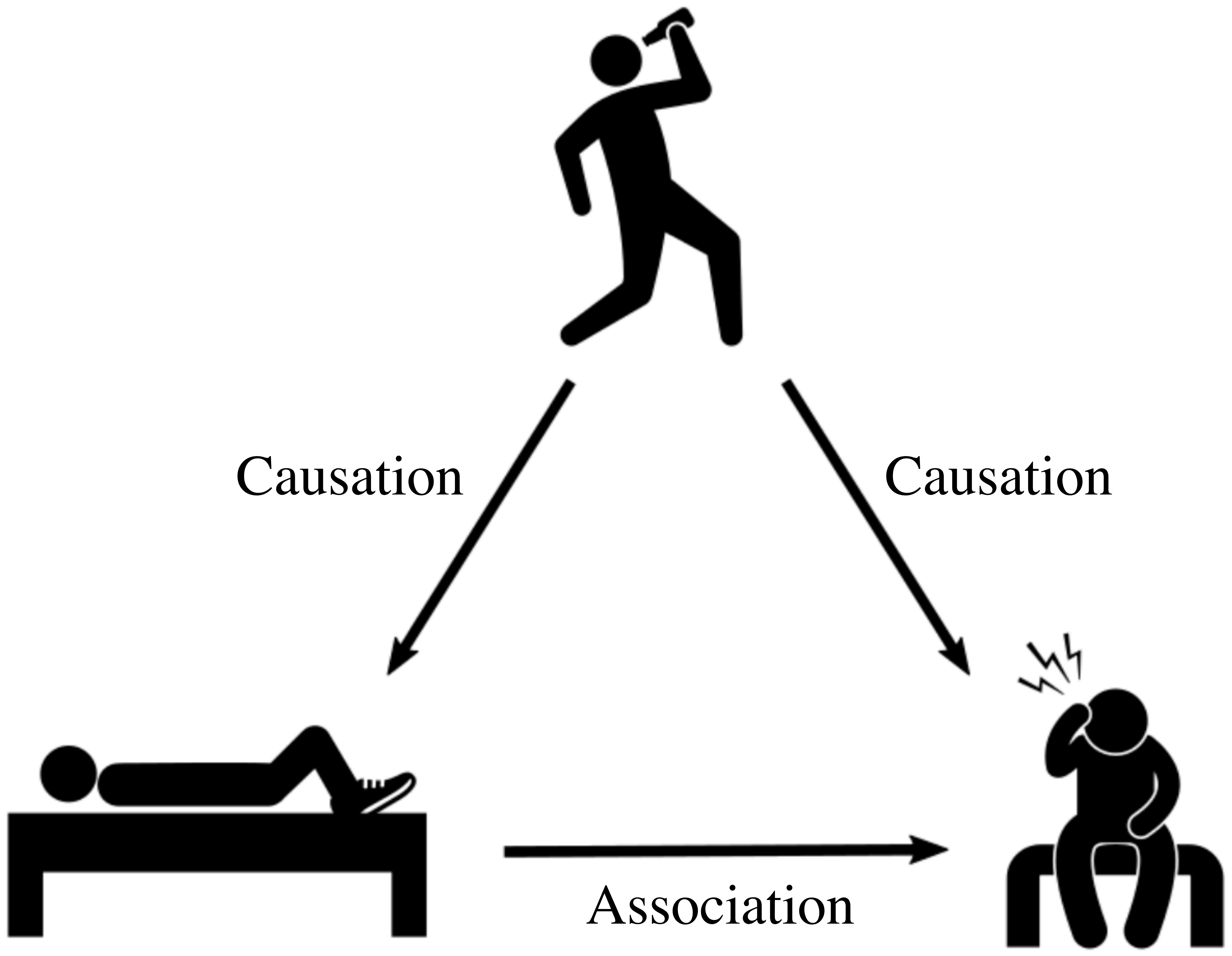


An analogy with Basketball

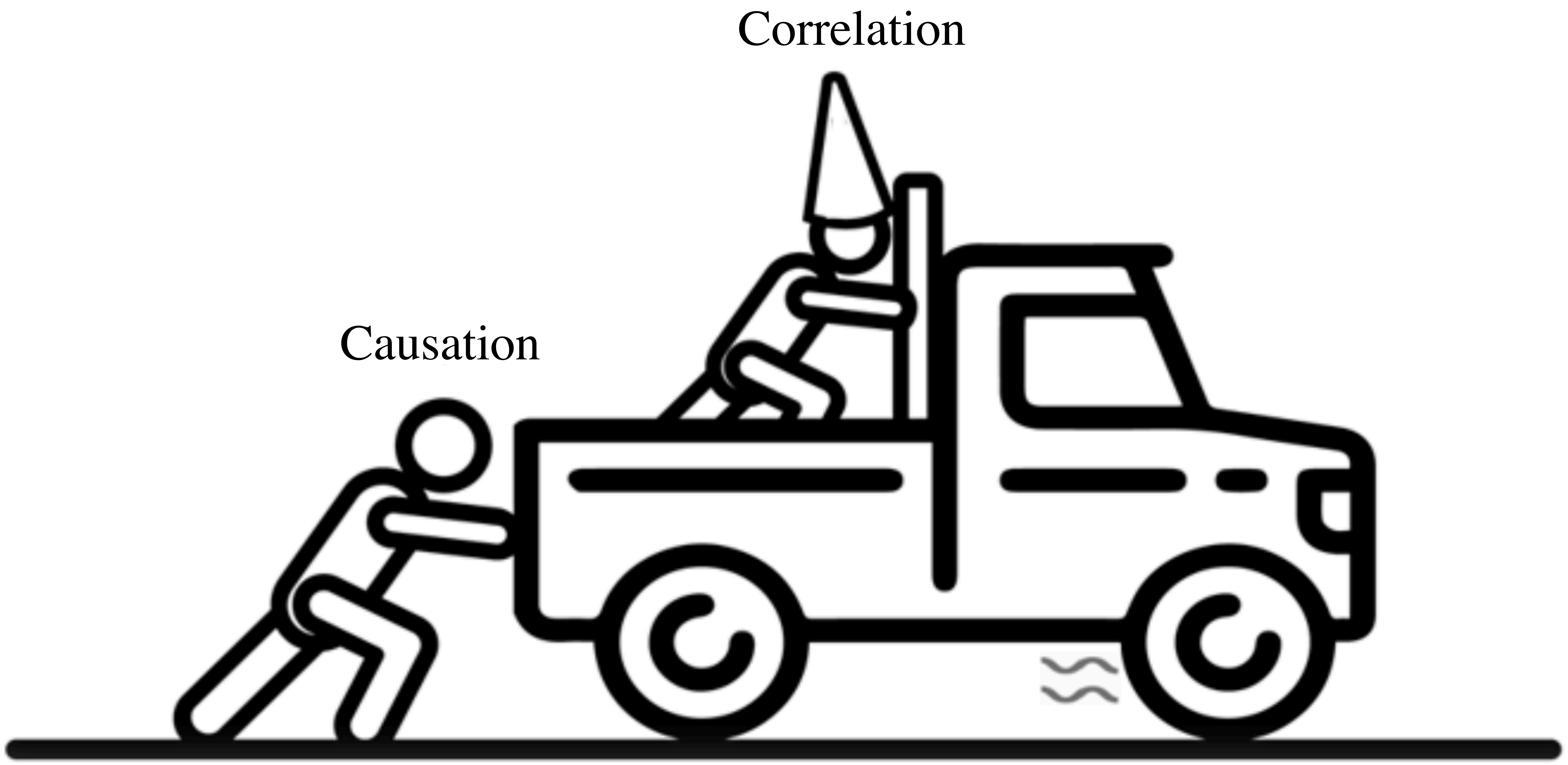


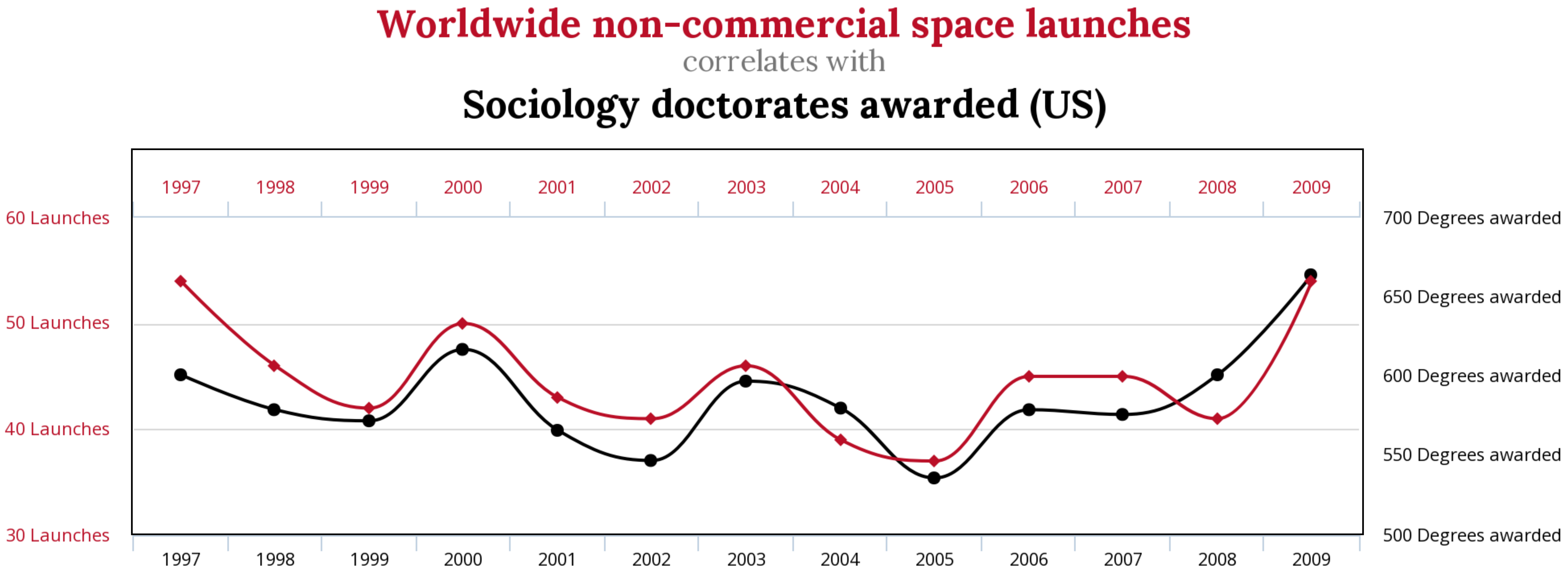
Could we understand basketball using correlation-based quantities?

Causality ≠ Association



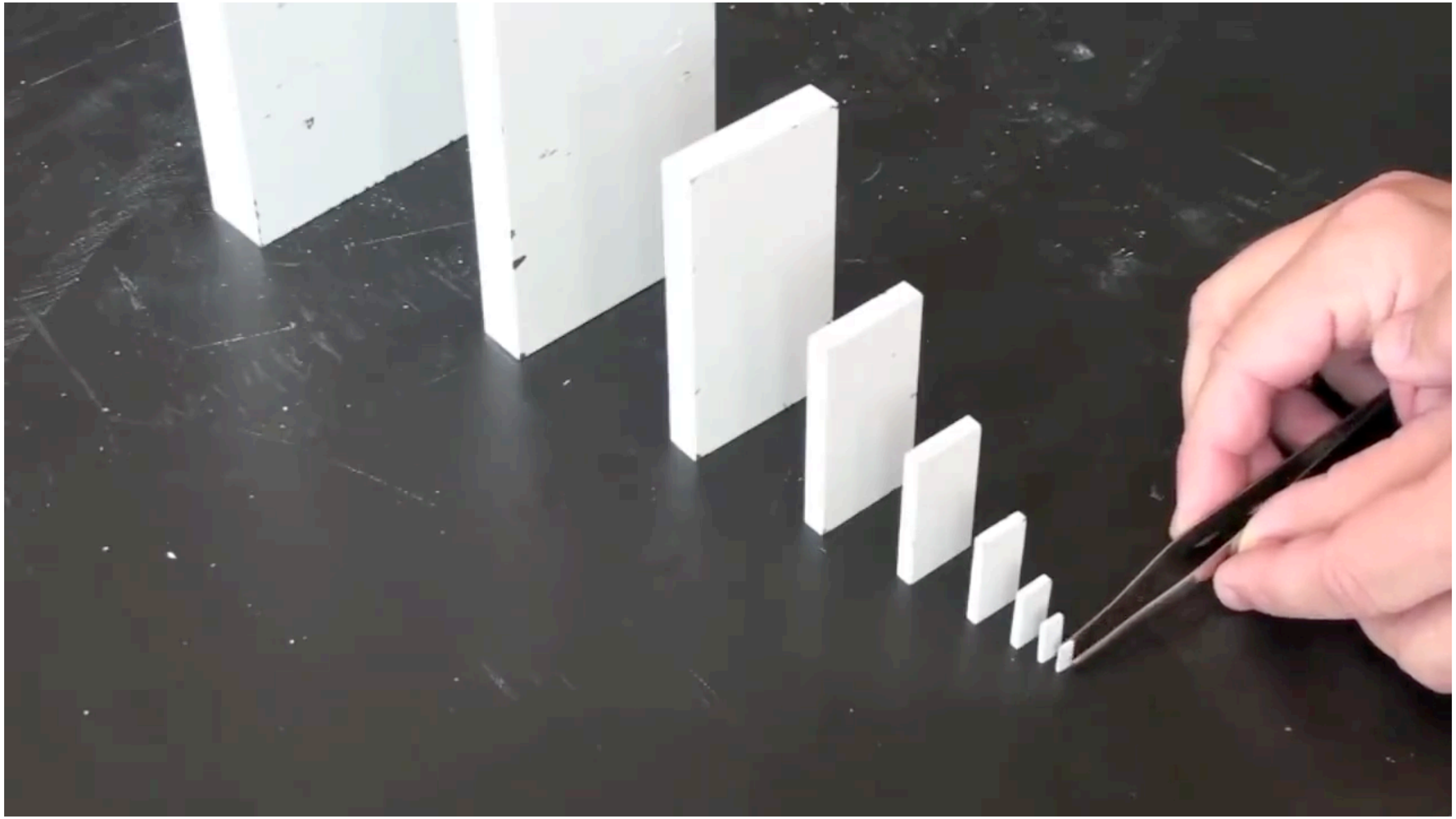
Causality ≠ Correlation



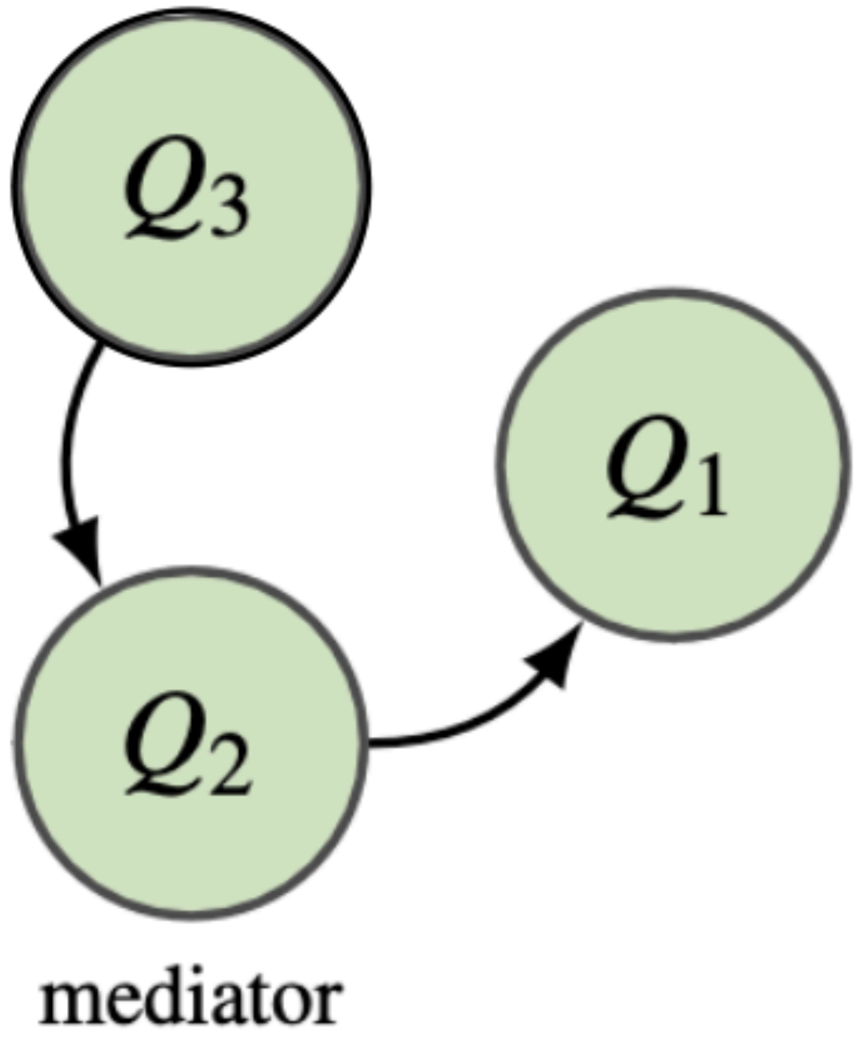


Worldwide non-commercial space launches
correlates with
Sociology doctorates awarded (US)
60 Launches
50 Launches
40 Launches
30 Launches
700 Degrees awarded
650 Degrees awarded
600 Degrees awarded
550 Degrees awarded
500 Degrees awarded
1997
1998
1999
2000
2001
2002
2003
2004
2005
2006
2007
2008
2009

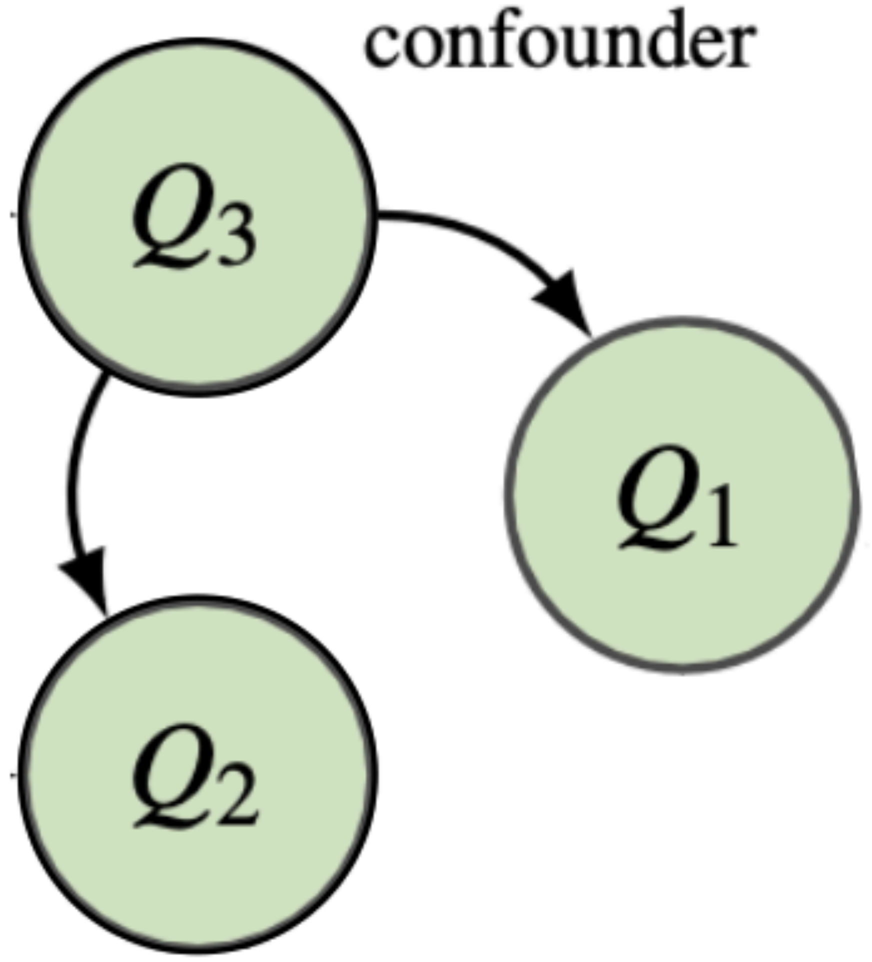
Causality ≠ Strength



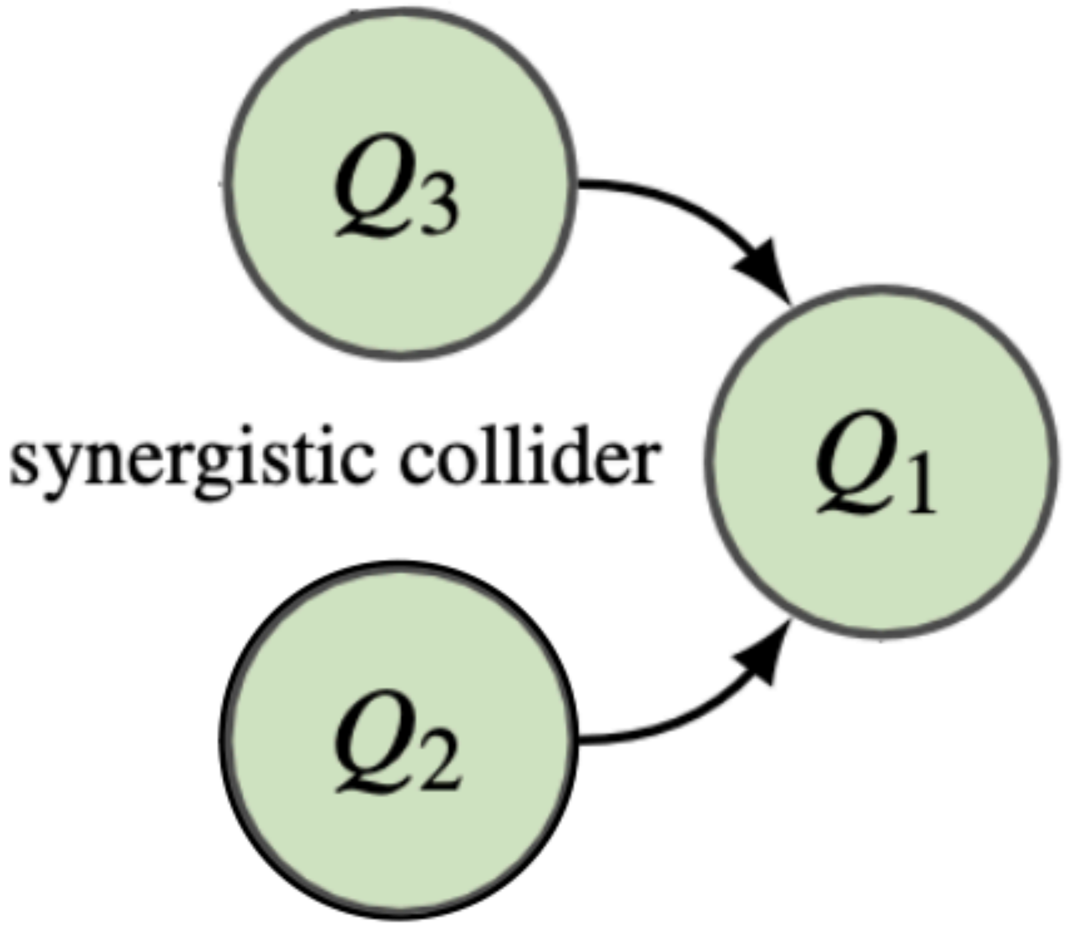
Fundamental interactions in causality



education level → job skills → income



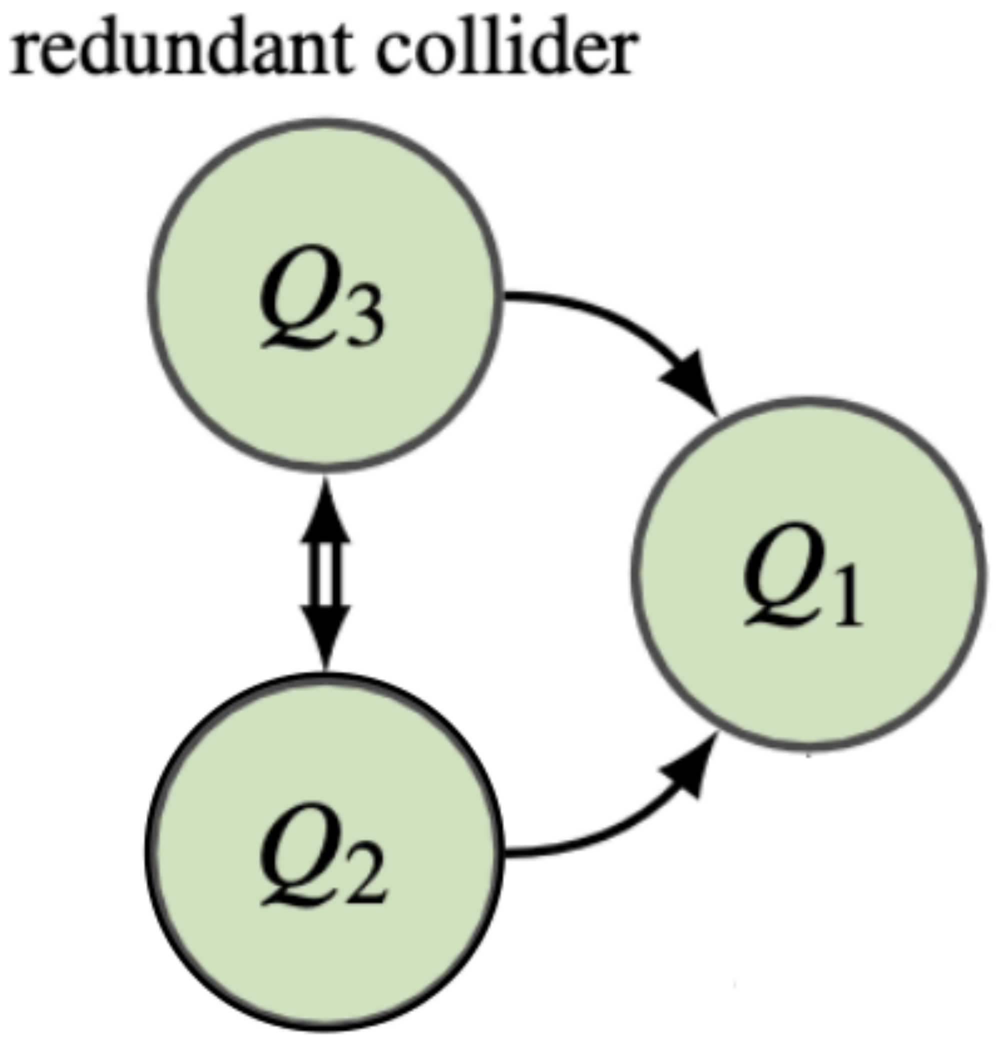
Rainy season → umbrella sales
→ raincoat sales



only drug A→ not recovery

only drug B→ not recovery

drug A + drug B→ recovery



smart student
hard-working student → good grades

Why causal analysis in fluid dynamics?

Physical insight

Causality-preserving reduced-order models

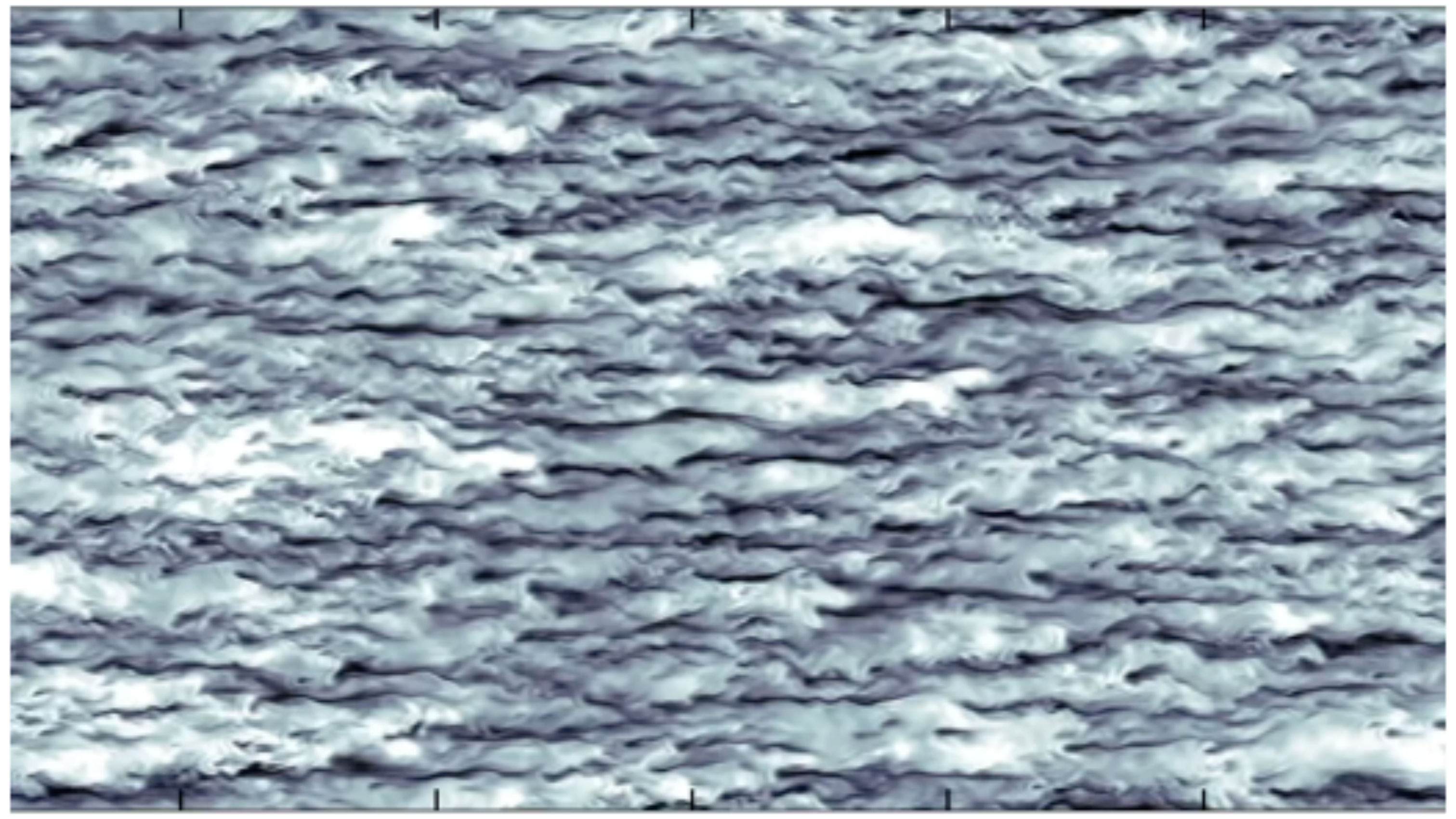
Causality-driven control

Why causal analysis in fluid dynamics?

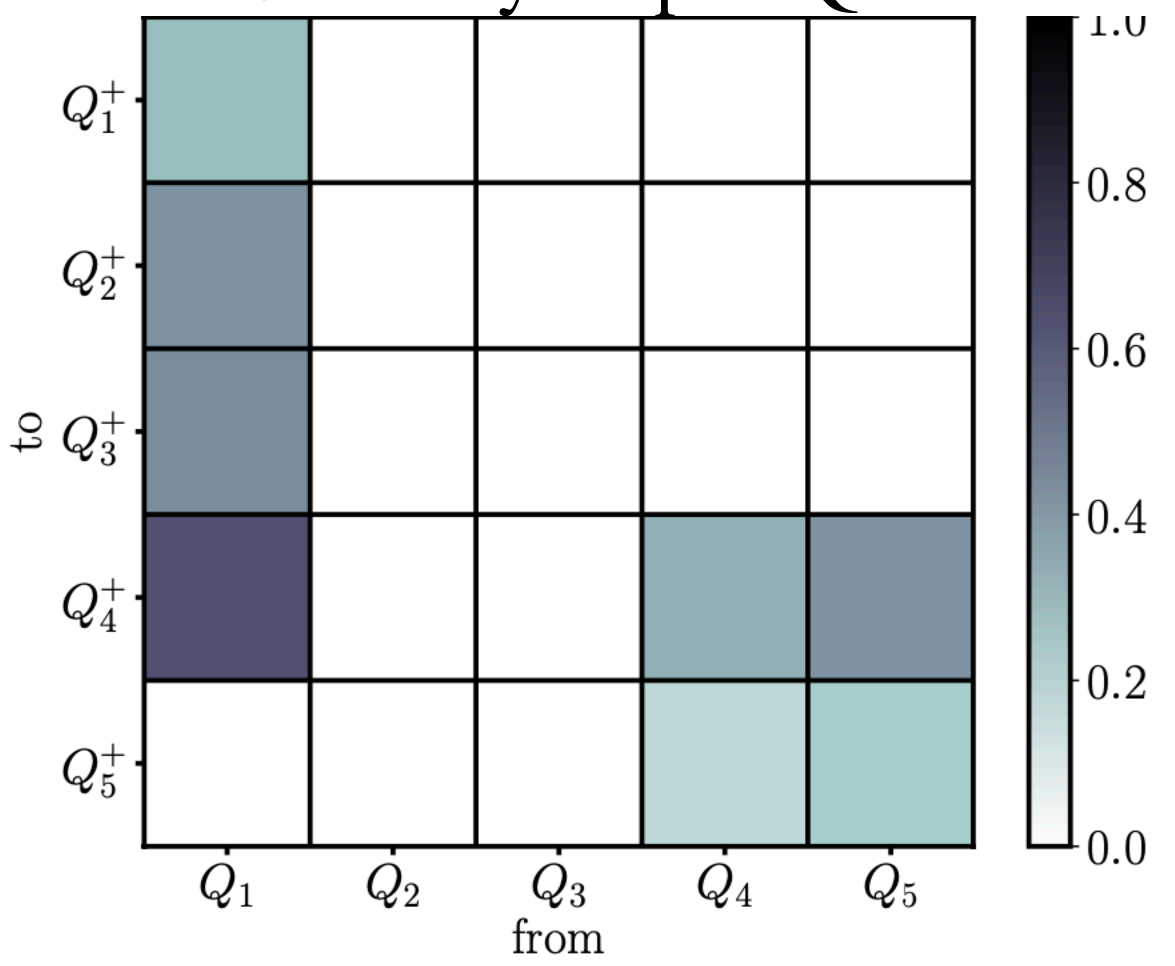
Physical insight

Causality-preserving reduced-order models

Causality-driven control

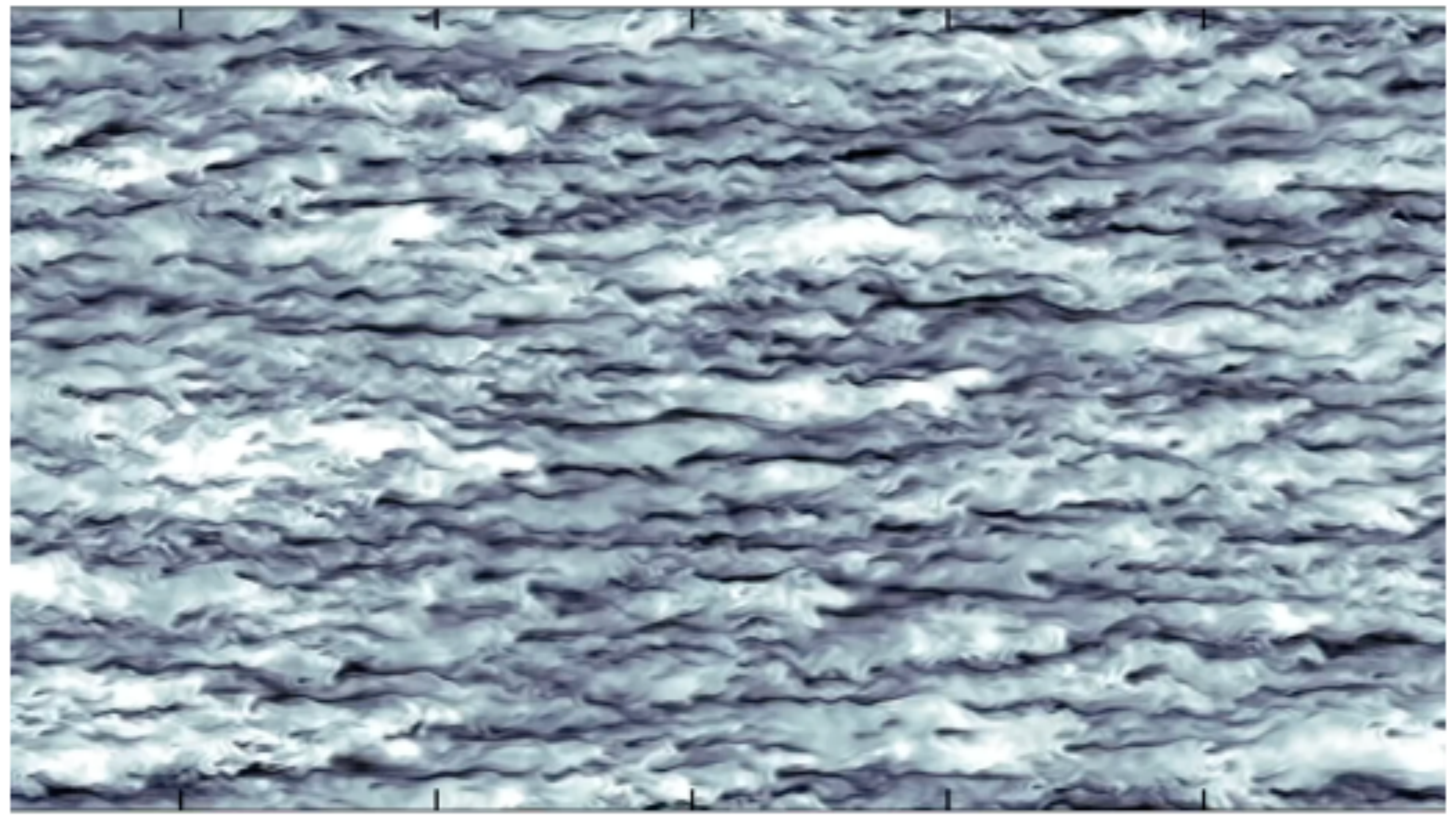


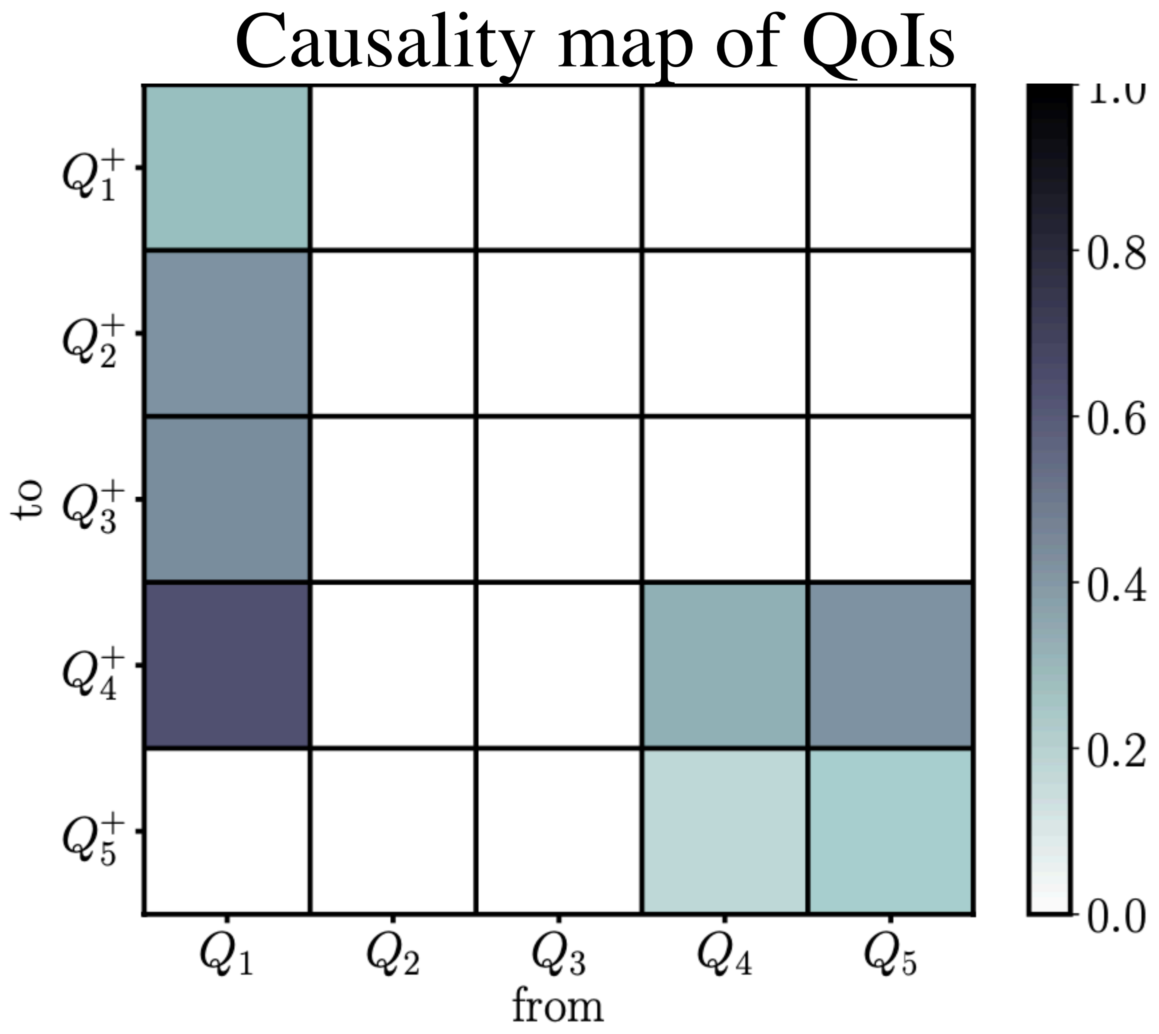
Causality map of QoIs



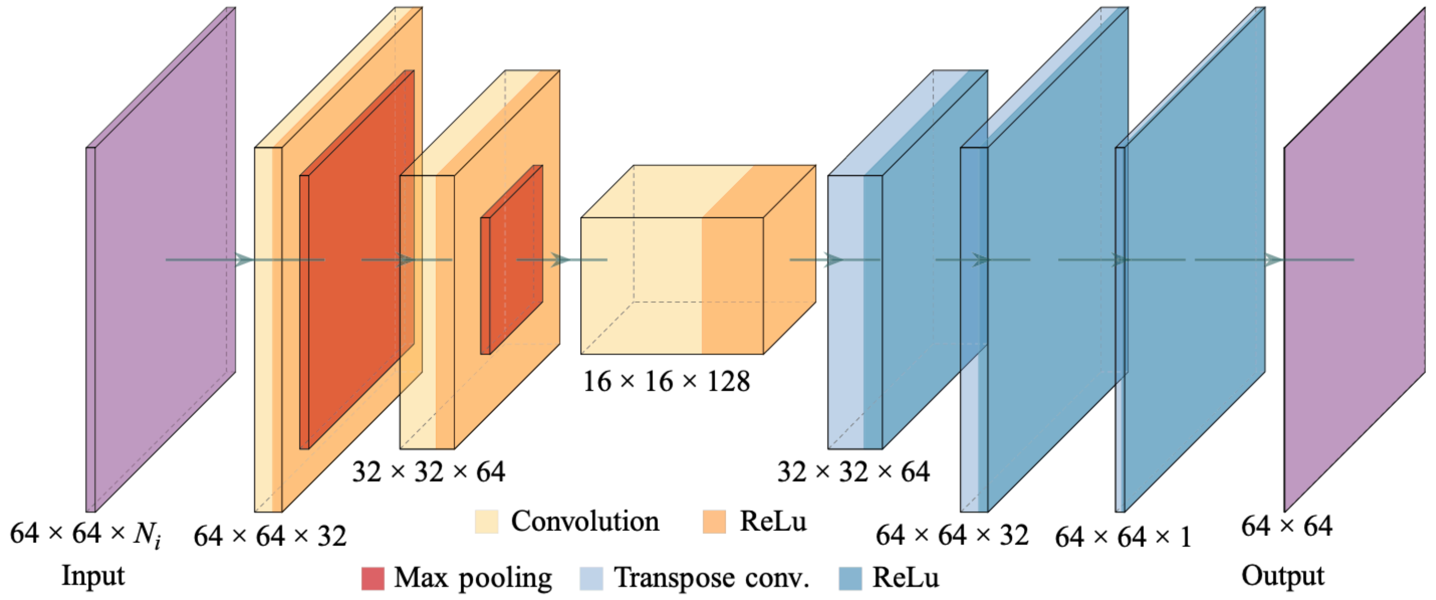
Why causal analysis in fluid dynamics?

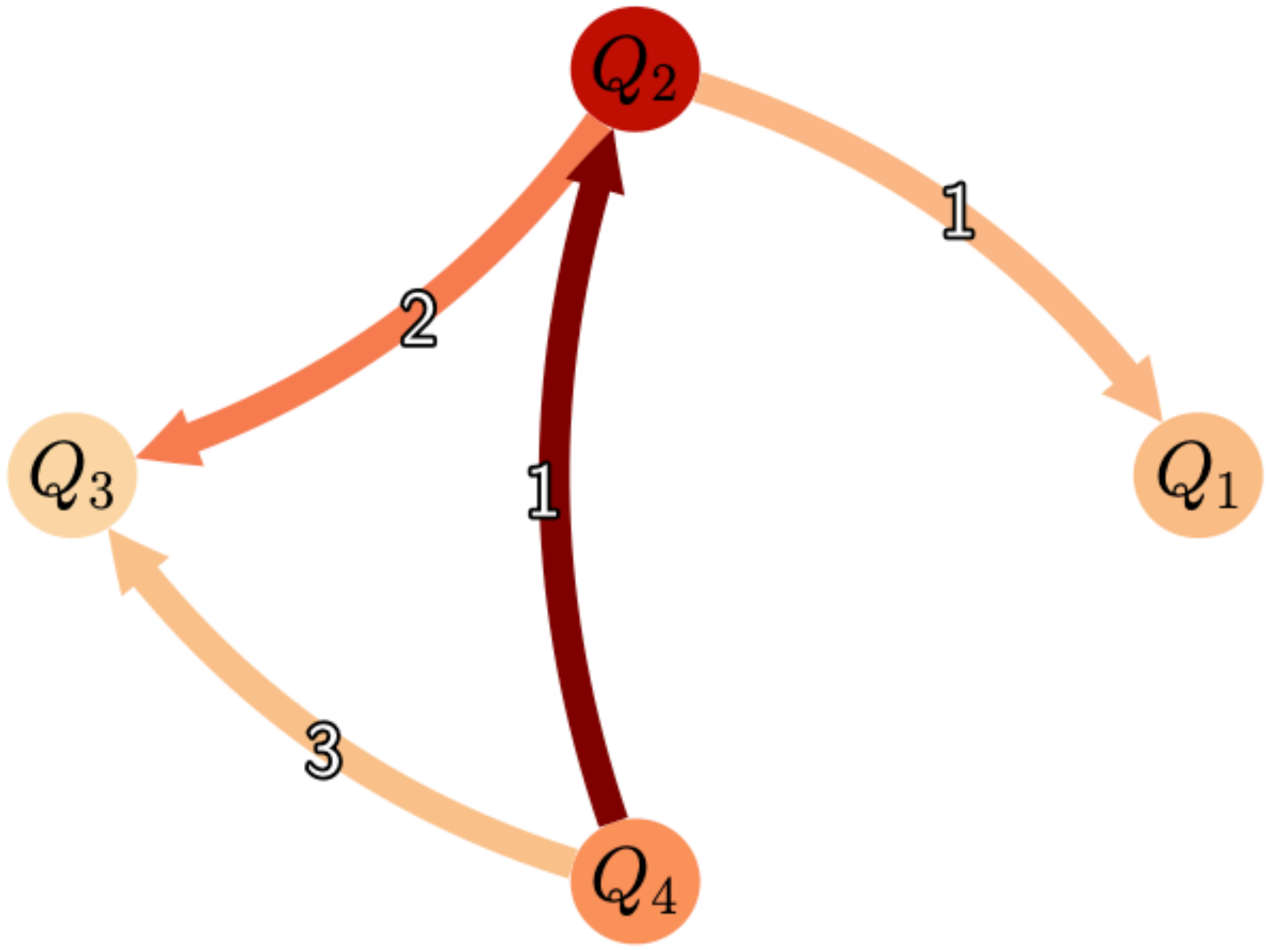
Physical insight





Causality-preserving reduced-order models

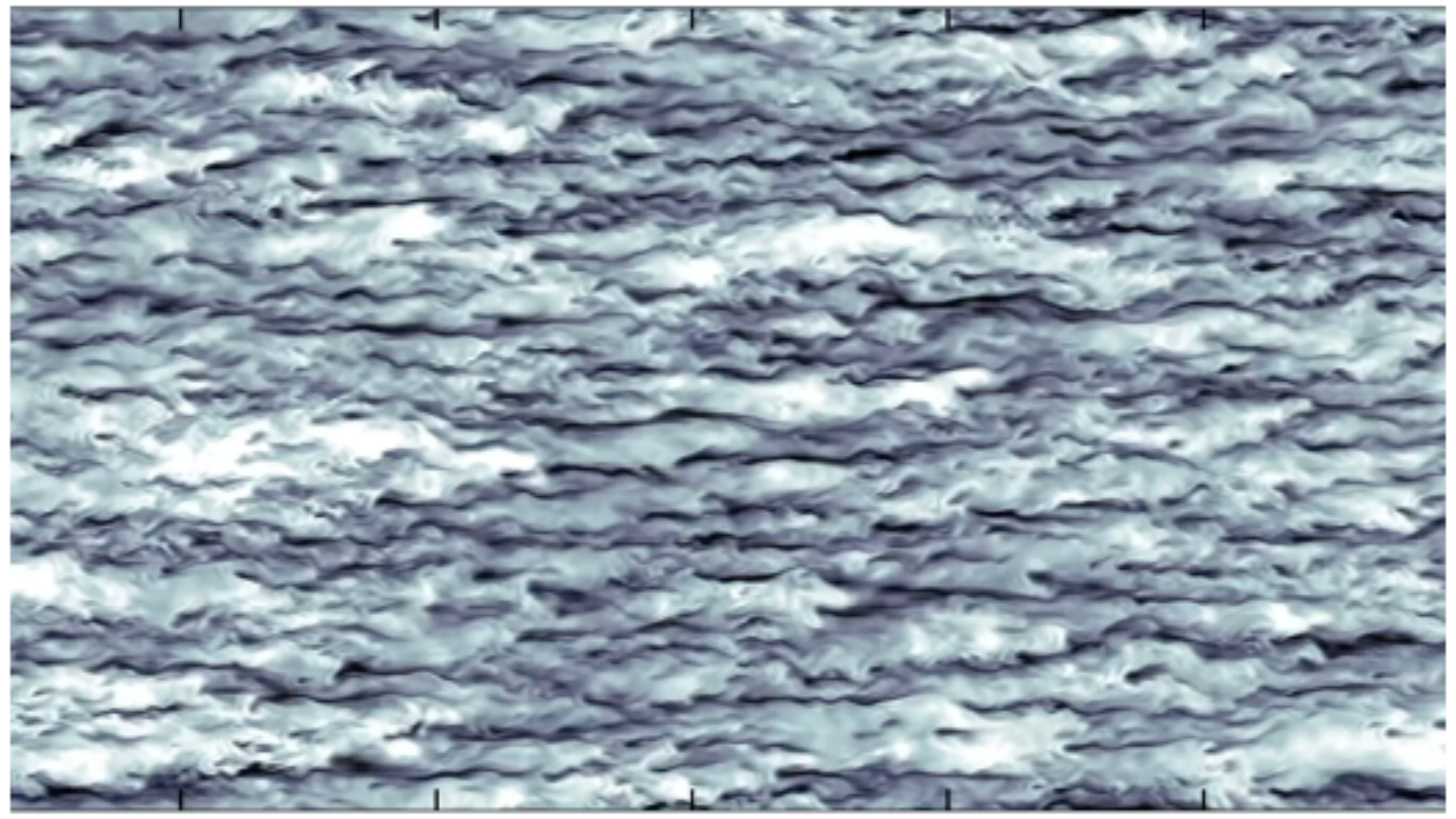




Causality-driven control

Why causal analysis in fluid dynamics?

Physical insight



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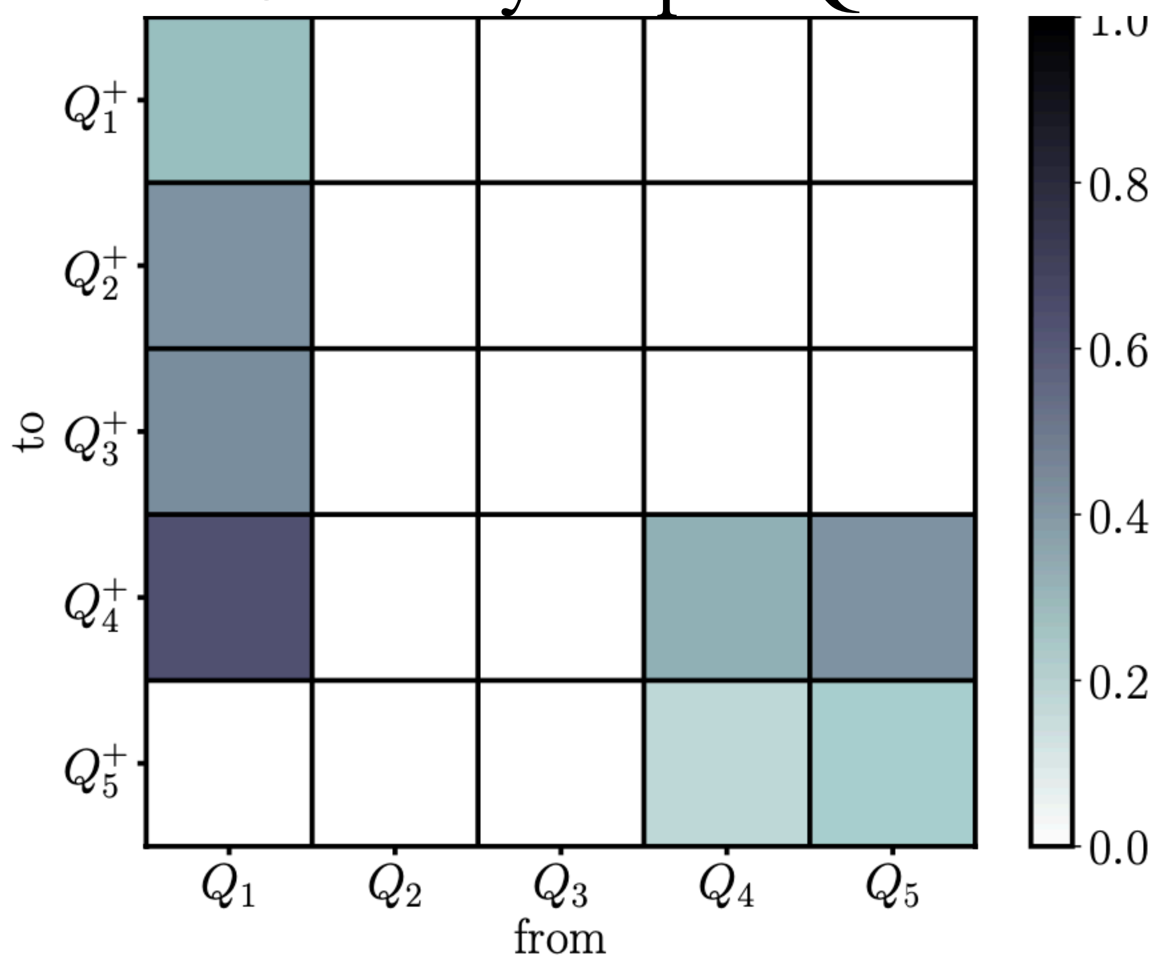

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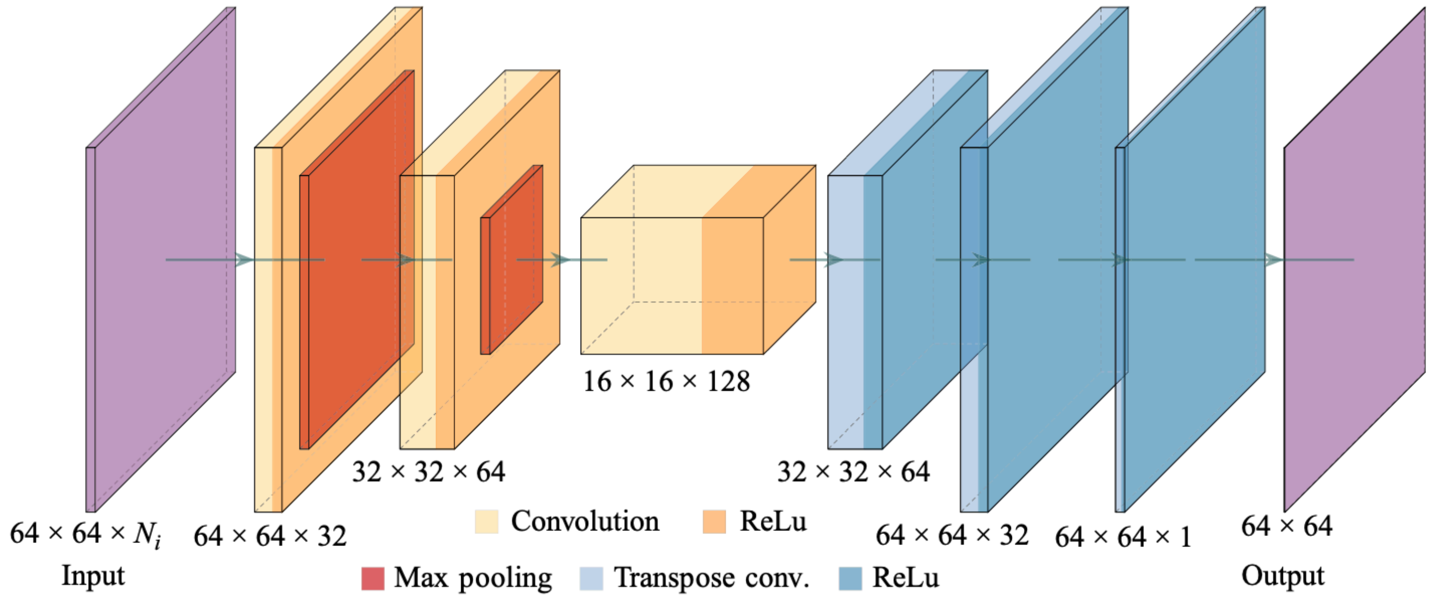
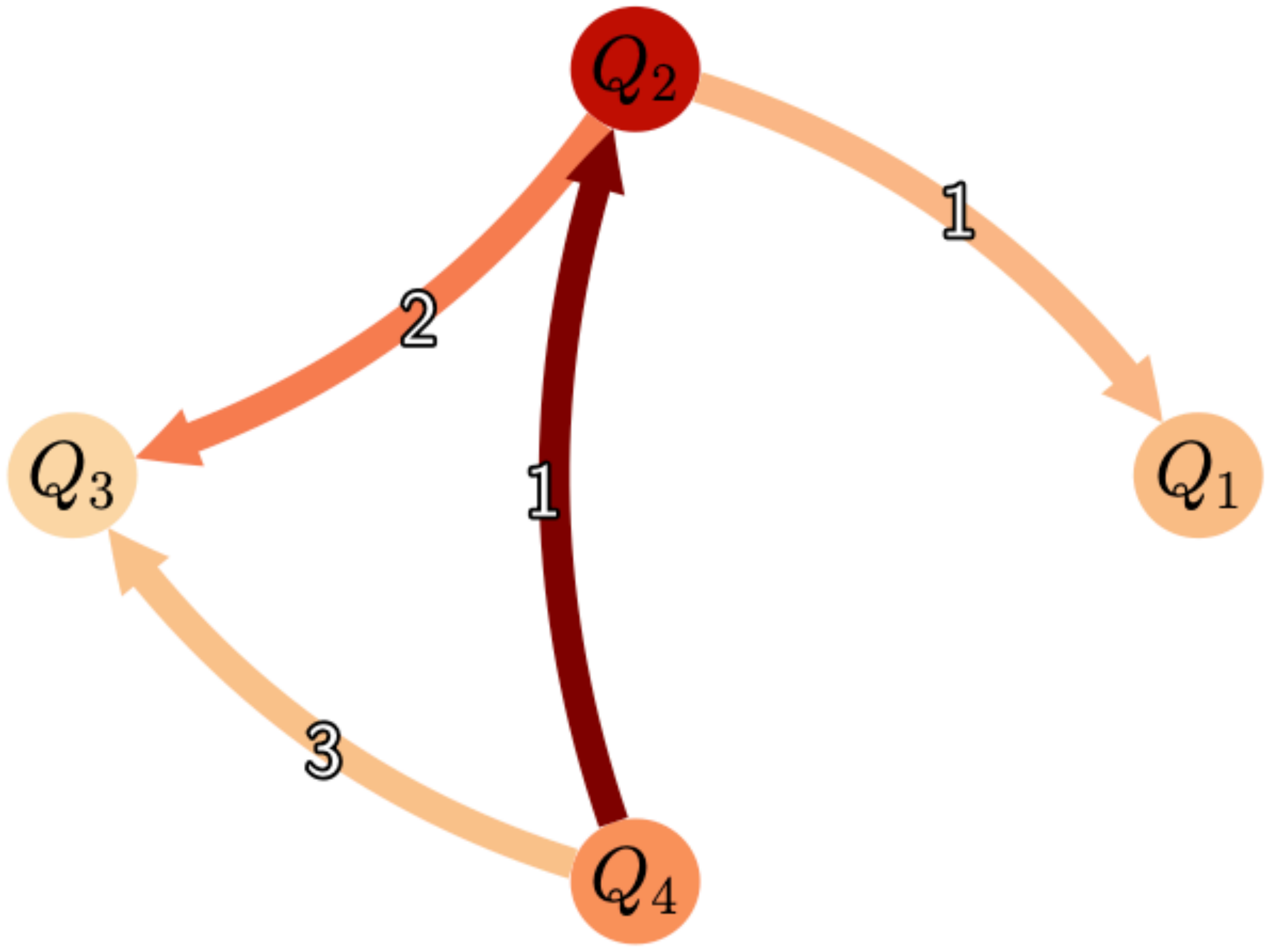
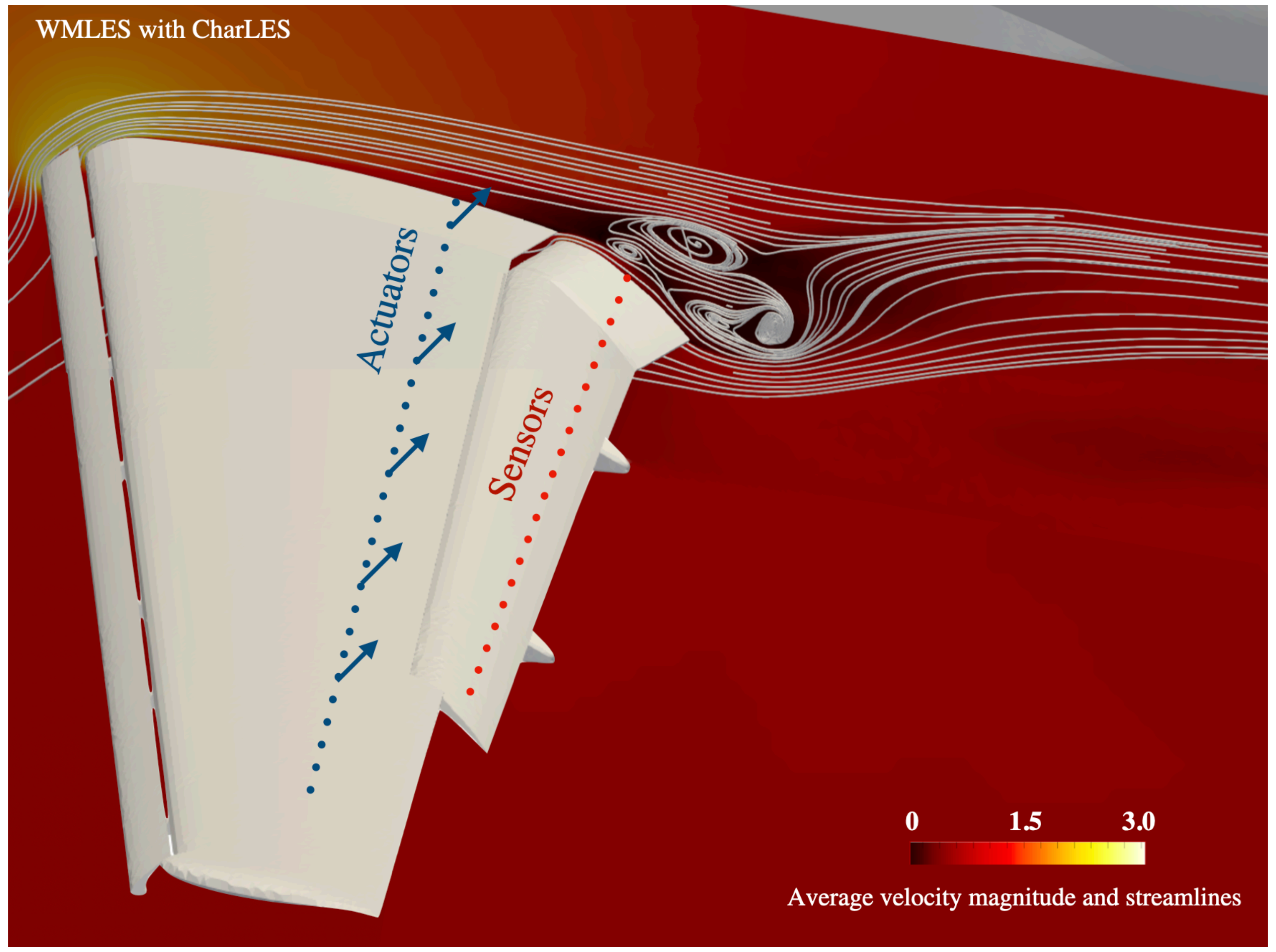




Causality-driven control



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Causality with **Interventions**

Modify the system and observe the consequences

Causality with **Interventions**

Modify the system and observe the consequences

Challenges:

- Impossible: interventions to assess the causality in the stock market in 2008 not possible
- Ethical problems: manipulating living organisms or altering natural environmental conditions
- Taking the system out of its natural attractor
- What interventions to perform?
- Even if interventions are possible, quantity of interest might not be straight forward to intervene

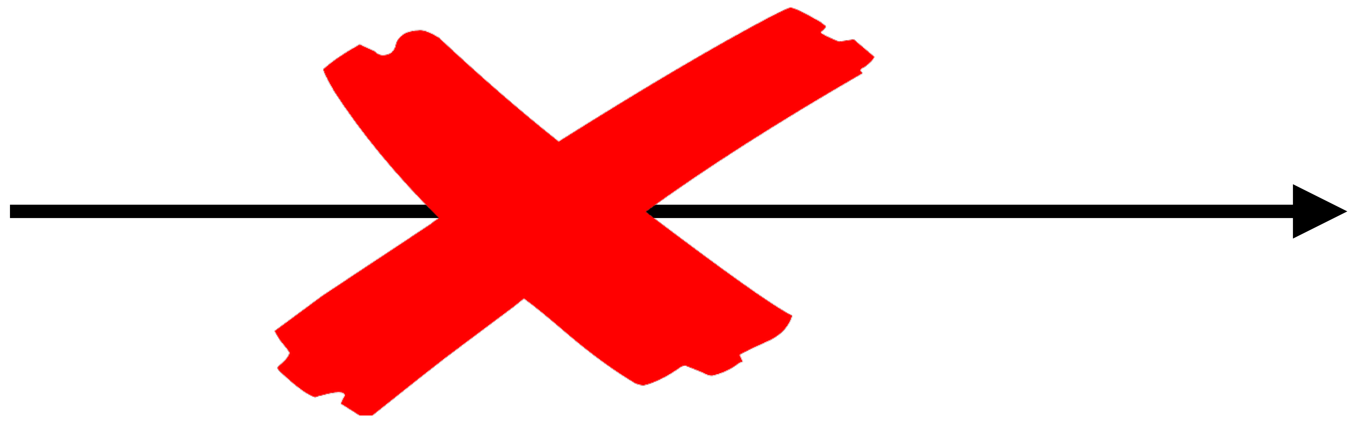
Causality with **Interventions**

Alexander the Great

Alexander the Great, victorious over Darius at the Battle of Gaugamela by Jacques Courtois

Causality with **Interventions**

Alexander the Great



Causality?

Alexander the Great, victorious over Darius at the Battle of Gaugamela by Jacques Courtois

Causality with **Interventions**

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Challenges:

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↓

Observational methods for causal inference

Causality with **Observations**

Infer causal relationship by observing the system in its 'natural' state without disturbances

- **Model forecasting methods:**
  - Granger causality (Granger, 1969)
  - Conditional GC (Barrett, 2010)
  - …
- **Statistical independence relations in data:**
  - Structural causal model (Pearl, 1995)
  - PC (Peter and Clark,)
  - tsPC (Spirtes, 2004)
  - PCMCI (Runge, 2019)
  - …
- **Randomized experiments:**
  - Potential outcomes (Rubin, 2007)
  - …
- **Information-theoretic methods:**
  - Transfer entropy (Schreiber, 2000)
  - Liang's information flow (Liang, 2008)
  - Information flux (Lozano-Duran, 2022)
  - SURD (Martinez-Sanchez, 2024)
  - …
- **Attractor reconstruction:**
  - Convergent cross-mapping (Sugihara, 2012)
  - Partial convergent cross-mapping (Long, 2020)
  - …

See reviews: Pearl (2009), Camps-Valls (2022), Runge (2023)

Two Nobel Prizes in Economic Sciences

Granger Causality, 2003

Sir Clive Granger

U. Nottingham and UCSD

Natural Experiments, 2021

MIT, UC Berkeley and Stanford

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Three levels of causality

Average Causality

State-dependent Causality

Space-time Causality


Mixing
MINUTE
PHYSICS


Mixing
[redacted]
MINUTE
PHYSICS


Both cases comply with conservation of mass, energy and momentum
But the information flow in the system is very different
MINUTE
PHYSICS

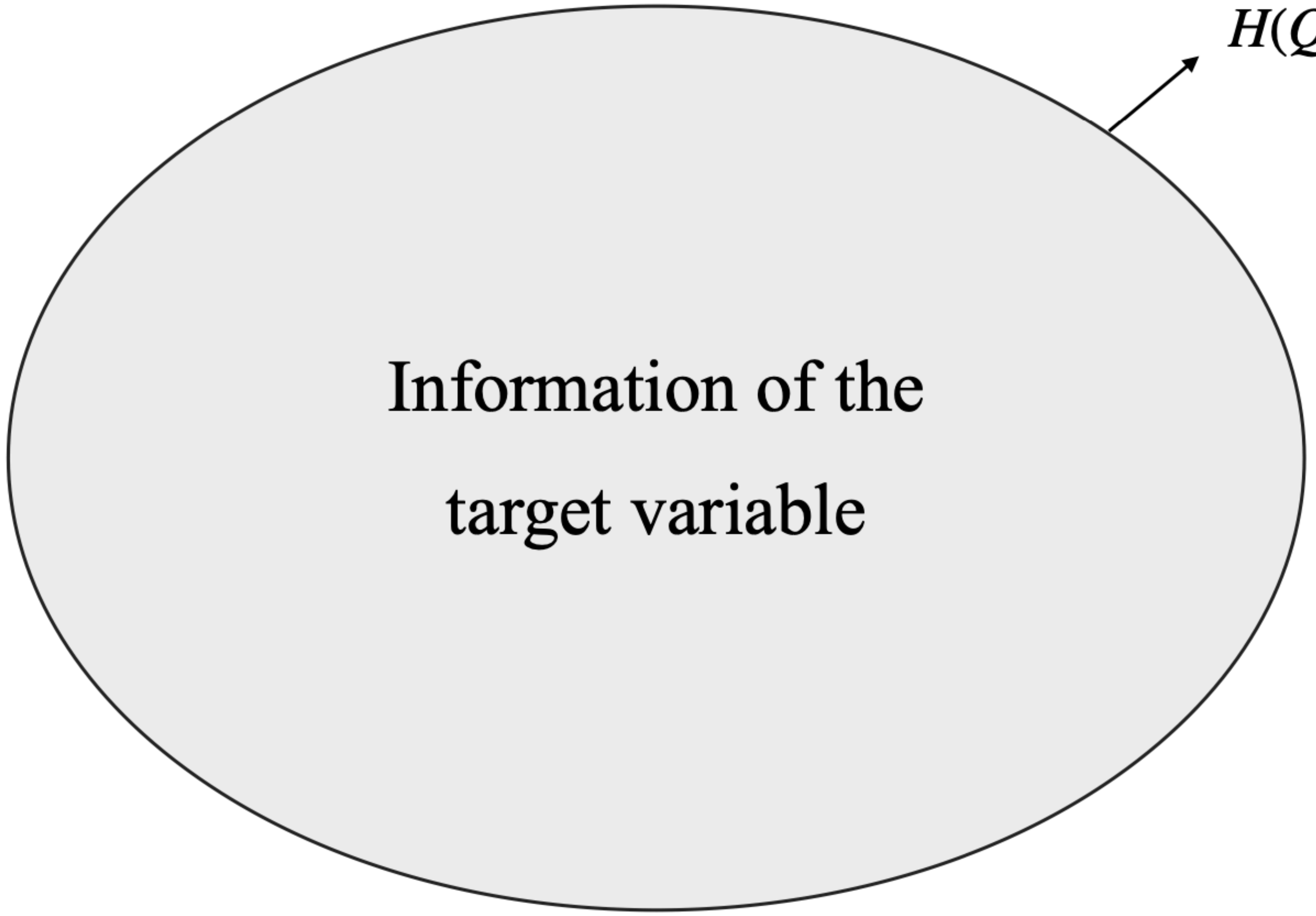
Average causality: Method

“Causality is the mechanism by which one event contributes to the genesis of another” (Pearl 2008)

Average causality: Method

Quantify the causality from observed variables $\boldsymbol{Q} = [Q_1, Q_2]$ to target variable $Q_j^+ = Q_j(t + \Delta T)$

$H(Q_j^+) \equiv$ information of the target variable Q_j^+



Martinez-Sanchez, Arranz, Lozano-Duran, Nat. Comm., 2024

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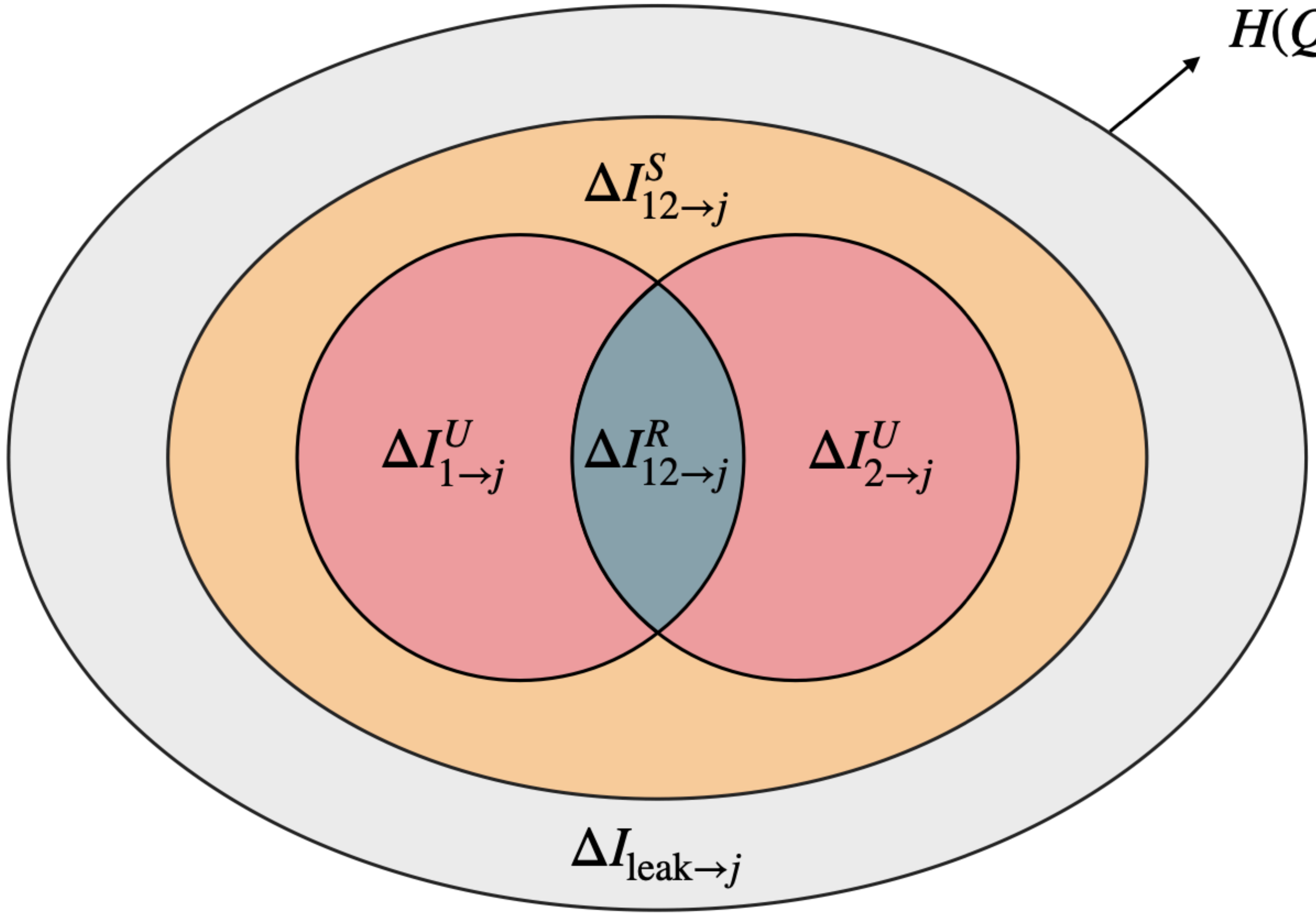

$$H(Q_j^+) = \Delta I^S_{\boldsymbol{i}\to j} + \Delta I^U_{i\to j} + \Delta I^R_{\boldsymbol{i}\to j} + \Delta I_{\mathrm{leak}\to j}$$

Forward-in-time propagation of information equation

Martinez-Sanchez, Arranz, Lozano-Duran, Nat. Comm., 2024

Average causality: Method

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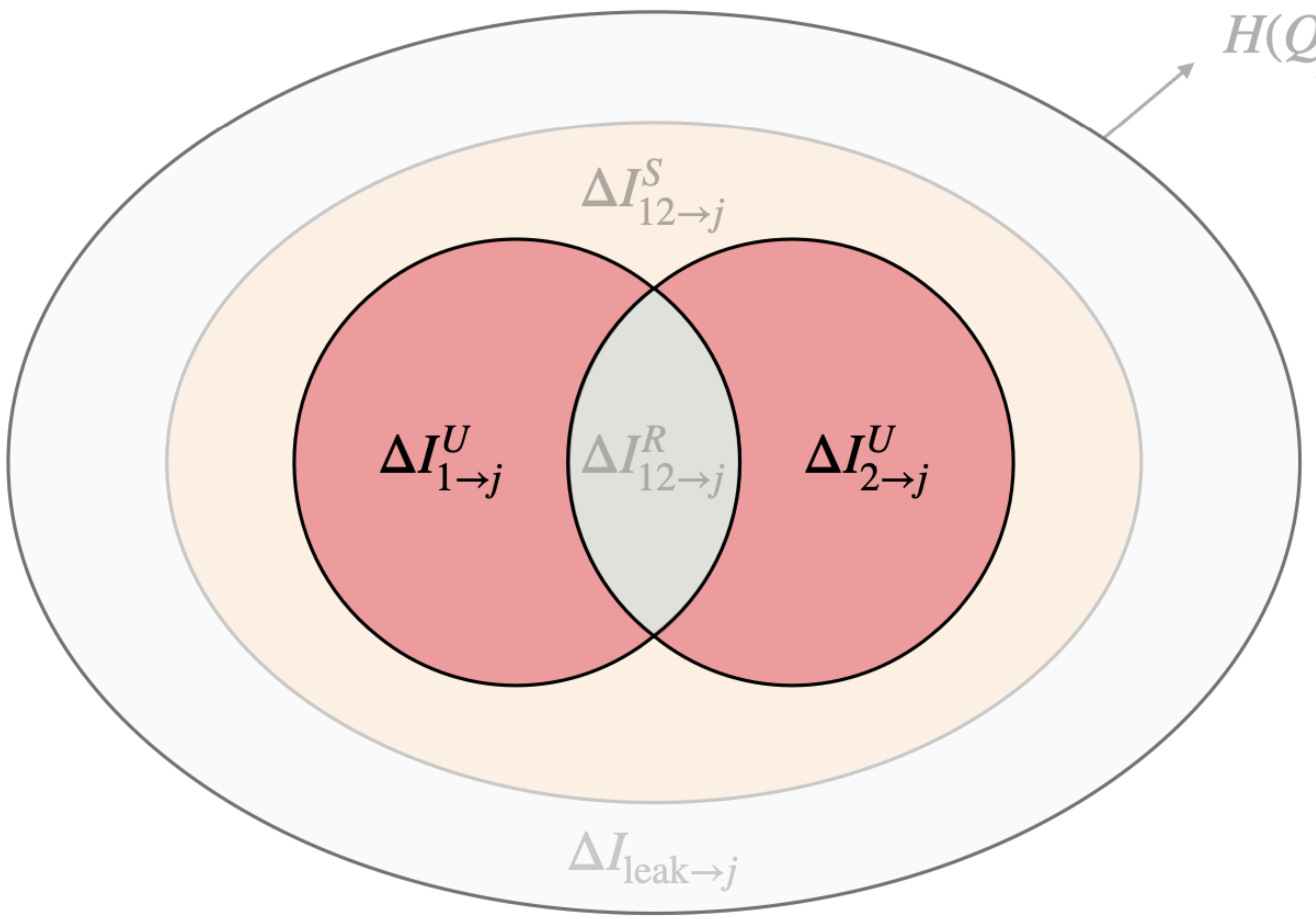

$$H(Q_j^+) = \Delta I^S_{\boldsymbol{i}\to j} + \boxed{\Delta I^U_{i\to j}} + \Delta I^R_{\boldsymbol{i}\to j} + \Delta I_{\text{leak}\to j}$$

Unique causality

Q_i contains unique information about Q_j^+

Rainy season → umbrella sales

Martinez-Sanchez, Arranz, Lozano-Duran, Nat. Comm., 2024

Average causality: Method

Quantify the causality from observed variables $\boldsymbol{Q} = [Q_1, Q_2]$ to target variable $Q_j^+ = Q_j(t + \Delta T)$

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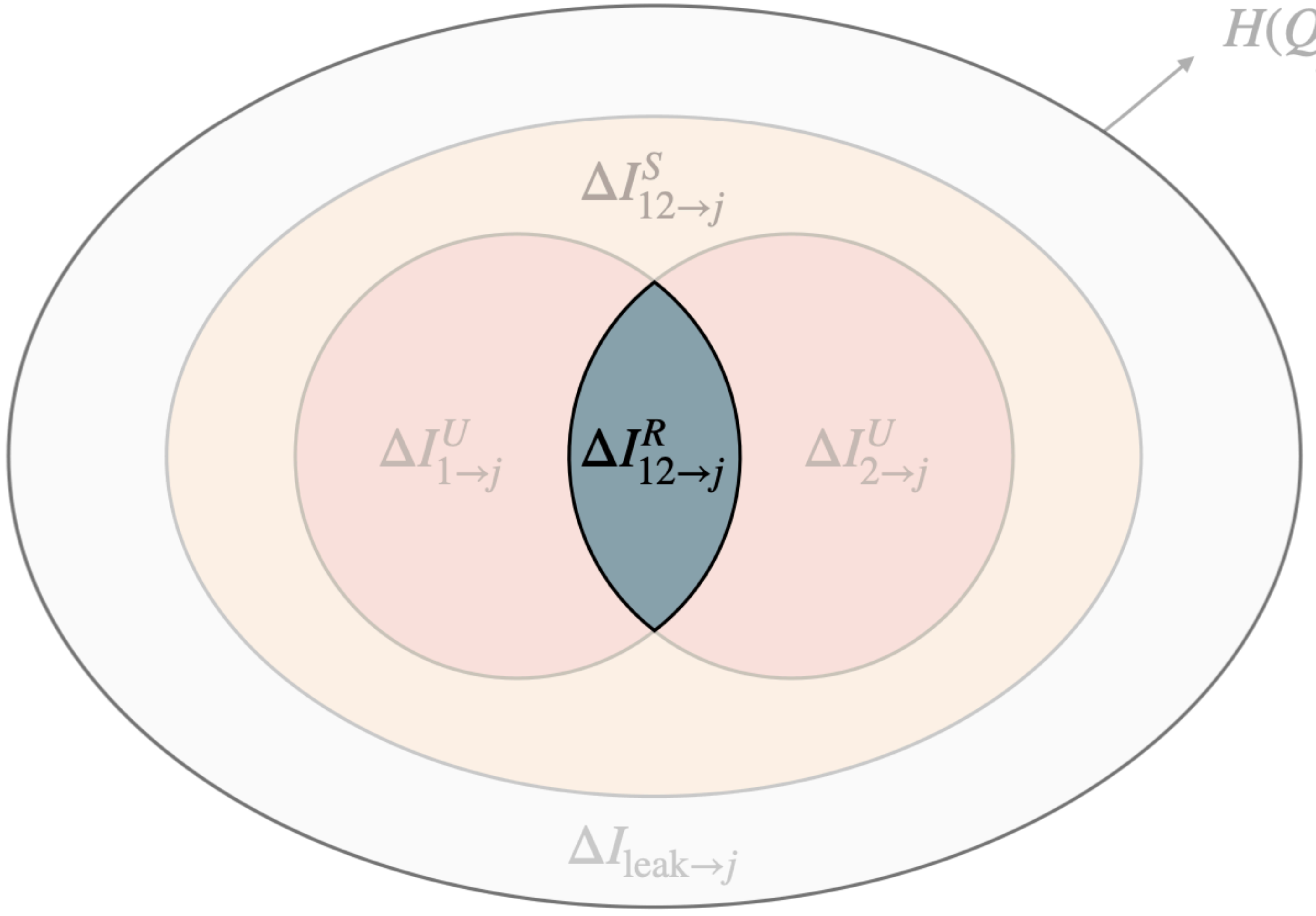


$$H(Q_j^+) = \Delta I^S_{\boldsymbol{i}\to j} + \Delta I^U_{i\to j} + \Delta I^R_{\boldsymbol{i}\to j} + \Delta I_{\mathrm{leak}\to j}$$

Redundant causality

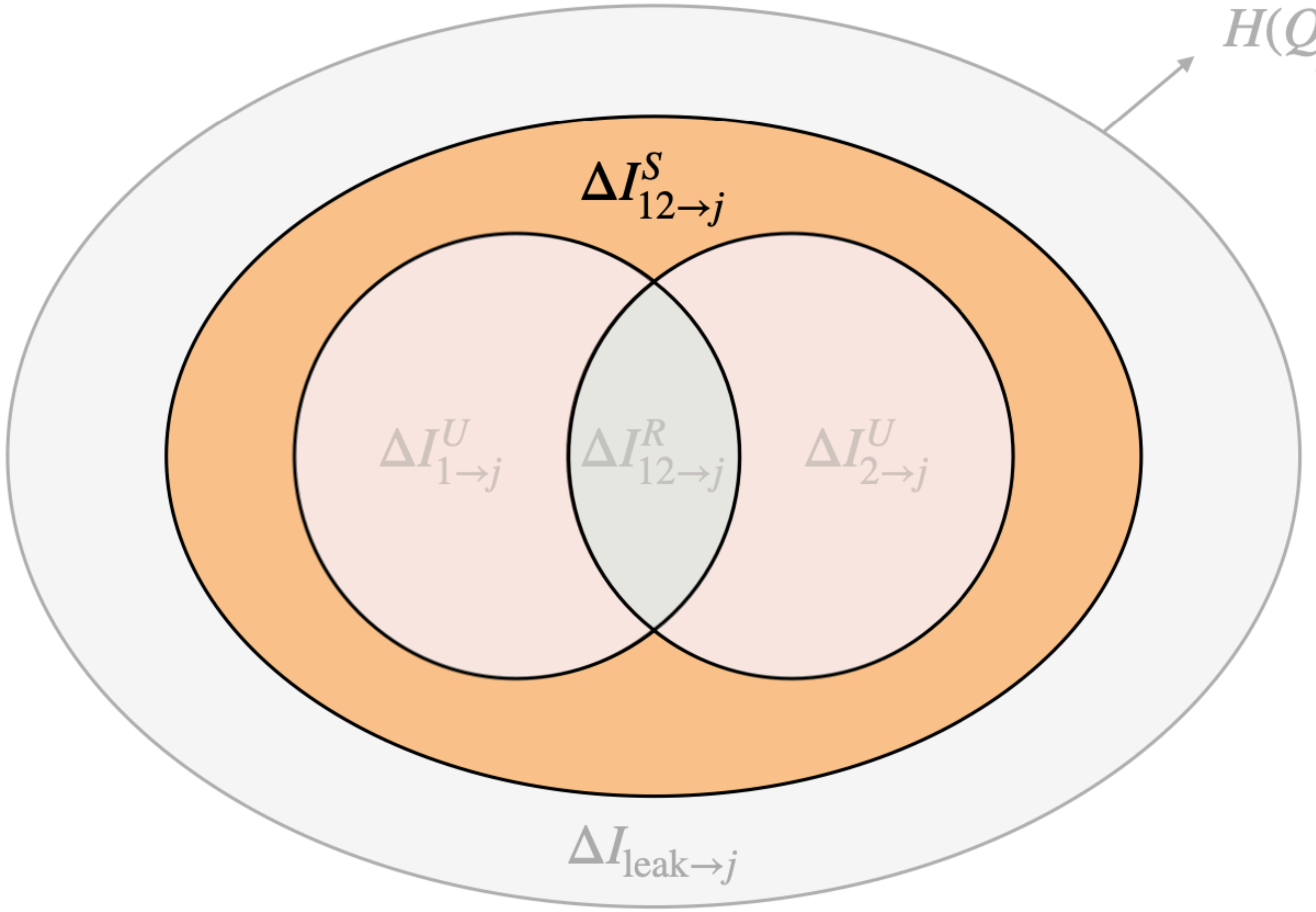
Q_1 and Q_2 contain the same information about Q_j^+

smart student
hard-working student $\rightarrow$ good grades

Martinez-Sanchez, Arranz, Lozano-Duran, Nat. Comm., 2024

Average causality: Method

Quantify the causality from observed variables $\boldsymbol{Q} = [Q_1, Q_2]$ to target variable $Q_j^+ = Q_j(t + \Delta T)$



$H(Q_j^+) \equiv$ information of the target variable Q_j^+

$$H(Q_j^+) = \boxed{\Delta I^S_{i\to j}} + \Delta I^U_{i\to j} + \Delta I^R_{i\to j} + \Delta I_{\mathrm{leak}\to j}$$

Synergistic causality

Q_1 and Q_2 together yield more information about Q_j^+

only drug A→ not recovery

only drug B→ not recovery

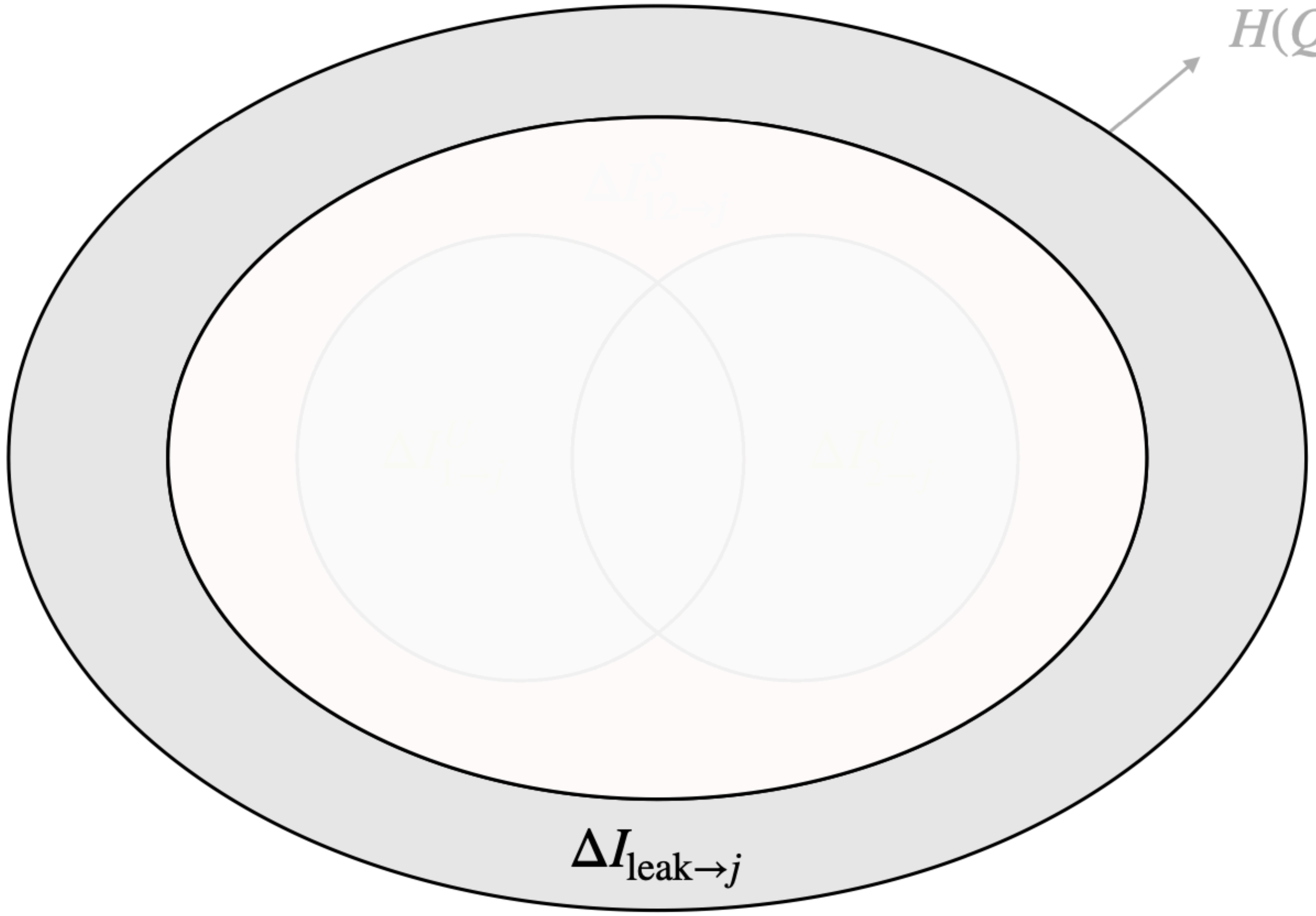
drug A + drug B→ recovery

Martinez-Sanchez, Arranz, Lozano-Duran, Nat. Comm., 2024

Average causality: Method

Quantify the causality from observed variables $\boldsymbol{Q} = [Q_1, Q_2]$ to target variable $Q_j^+ = Q_j(t + \Delta T)$

$H(Q_j^+) \equiv$ information of the target variable Q_j^+



$$H(Q_j^+) = \Delta I^S_{\boldsymbol{i}\to j} + \Delta I^U_{i\to j} + \Delta I^R_{\boldsymbol{i}\to j} + \Delta I_{\mathrm{leak}\to j}$$

Causality leak

Effect from unobserved variables that influence Q_j^+

Martinez-Sanchez, Arranz, Lozano-Duran, Nat. Comm., 2024

Average causality: Method

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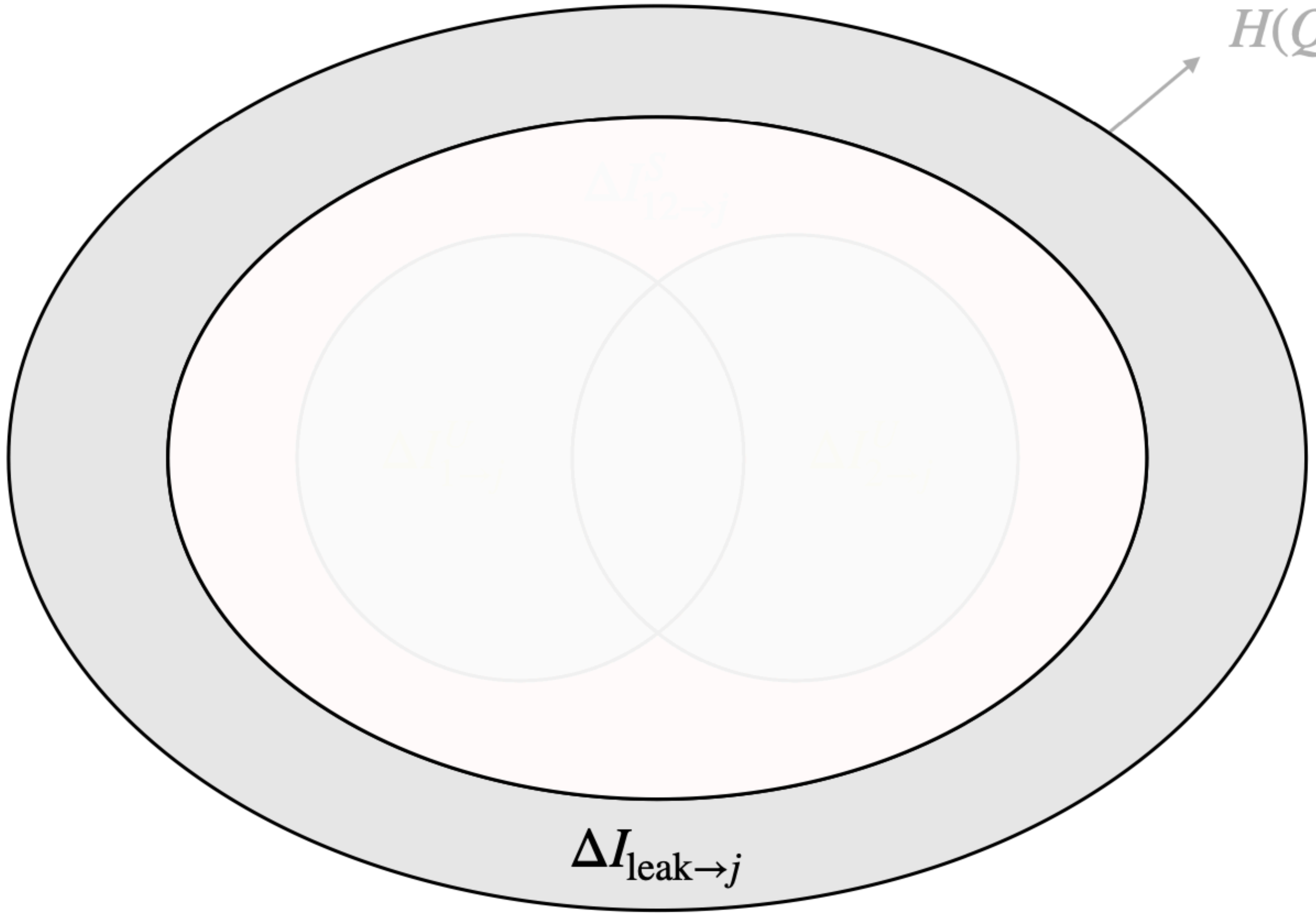


$$H(Q_j^+) = \Delta I^S_{\boldsymbol{i}\to j} + \Delta I^U_{i\to j} + \Delta I^R_{\boldsymbol{i}\to j} + \Delta I_{\mathrm{leak}\to j}$$

Causality & predictability

For any model: $Q_j^{+\mathrm{model}} = f(\boldsymbol{Q})$

$$||Q_j^+ - Q_j^{+\mathrm{model}}|| \geq c\exp[-\Delta I^S_{i\to j} - \Delta I^U_{i\to j} - \Delta I^R_{i\to j}]$$

Martinez-Sanchez, Arranz, Lozano-Duran, Nat. Comm., 2024

Computation of Information in high-dimensional spaces

We quantify causality as increments of mutual information between different combinations of $\boldsymbol{Q}$ and Q_O

$$I(Q_O;\boldsymbol{Q}) = \mathbb{E}_{p(q_O,\boldsymbol{q})} \log \frac{p(q_O,\boldsymbol{q})}{p(q_O)p(\boldsymbol{q})} = D_{\mathrm{KL}}\left(p(q_O,\boldsymbol{q}) \| p(q_O)p(\boldsymbol{q})\right)$$

MINE: Mutual Information Neural Estimator (Donsker-Varadhan (DV) representation)

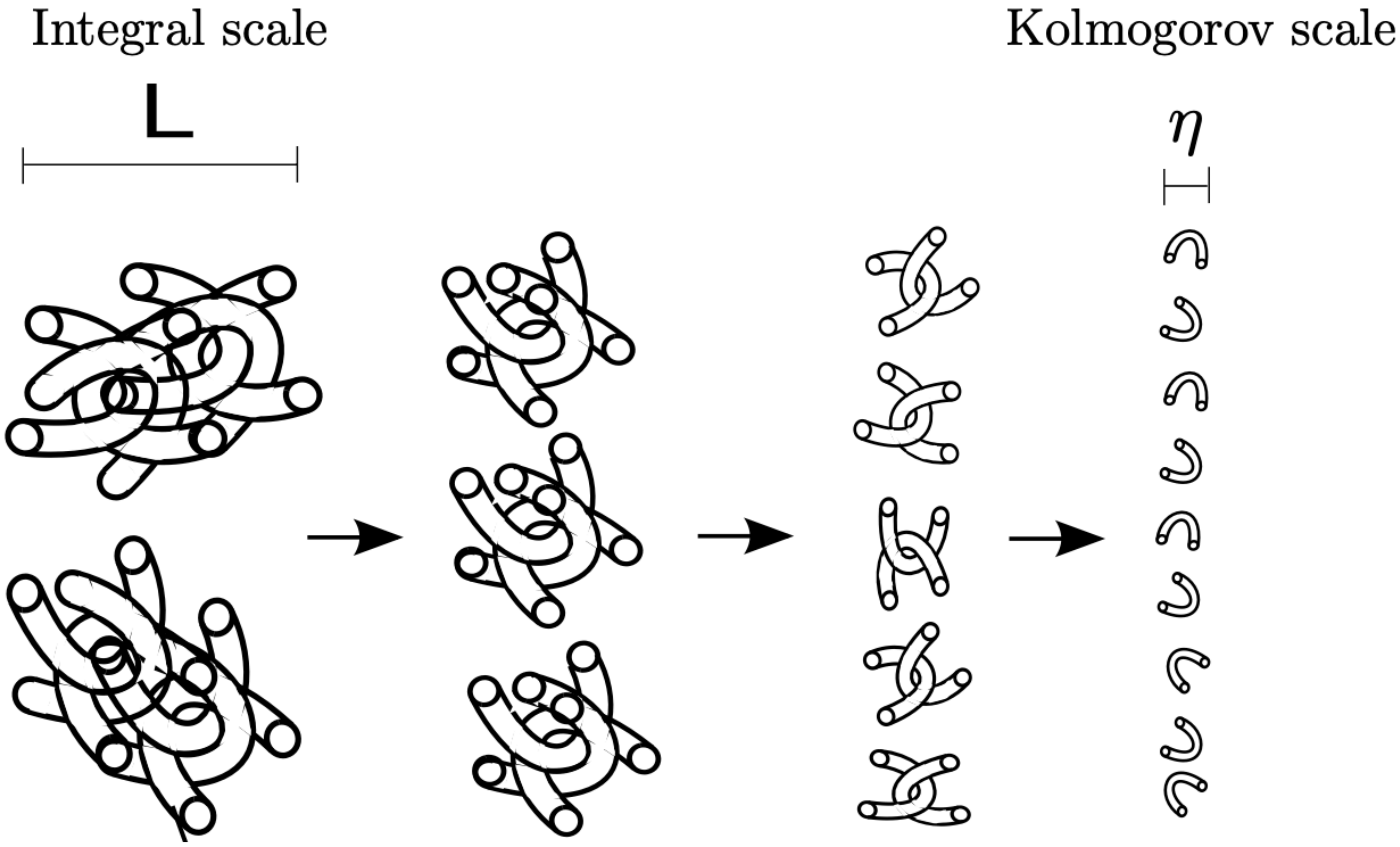
$$\hat{I}_\theta(Q_O;\boldsymbol{Q}) \leftarrow \frac{1}{m}\sum_{k=1}^{m} F_\theta\left(q_{O,k},\boldsymbol{q}_k\right) - \log\left(\frac{1}{m}\sum_{k=1}^{m} e^{F_\theta\left(\tilde{q}_{O,k},\boldsymbol{q}_k\right)}\right)$$

$m \equiv$ number of samples

$\tilde{q}_O \equiv$ randomly shuffled q_O

Donsker &Varadhan (*Comm. Pure Appl. Math.*, 1983), Belghazi *et al.* (*ICML*, 2018)

Average causality: Application



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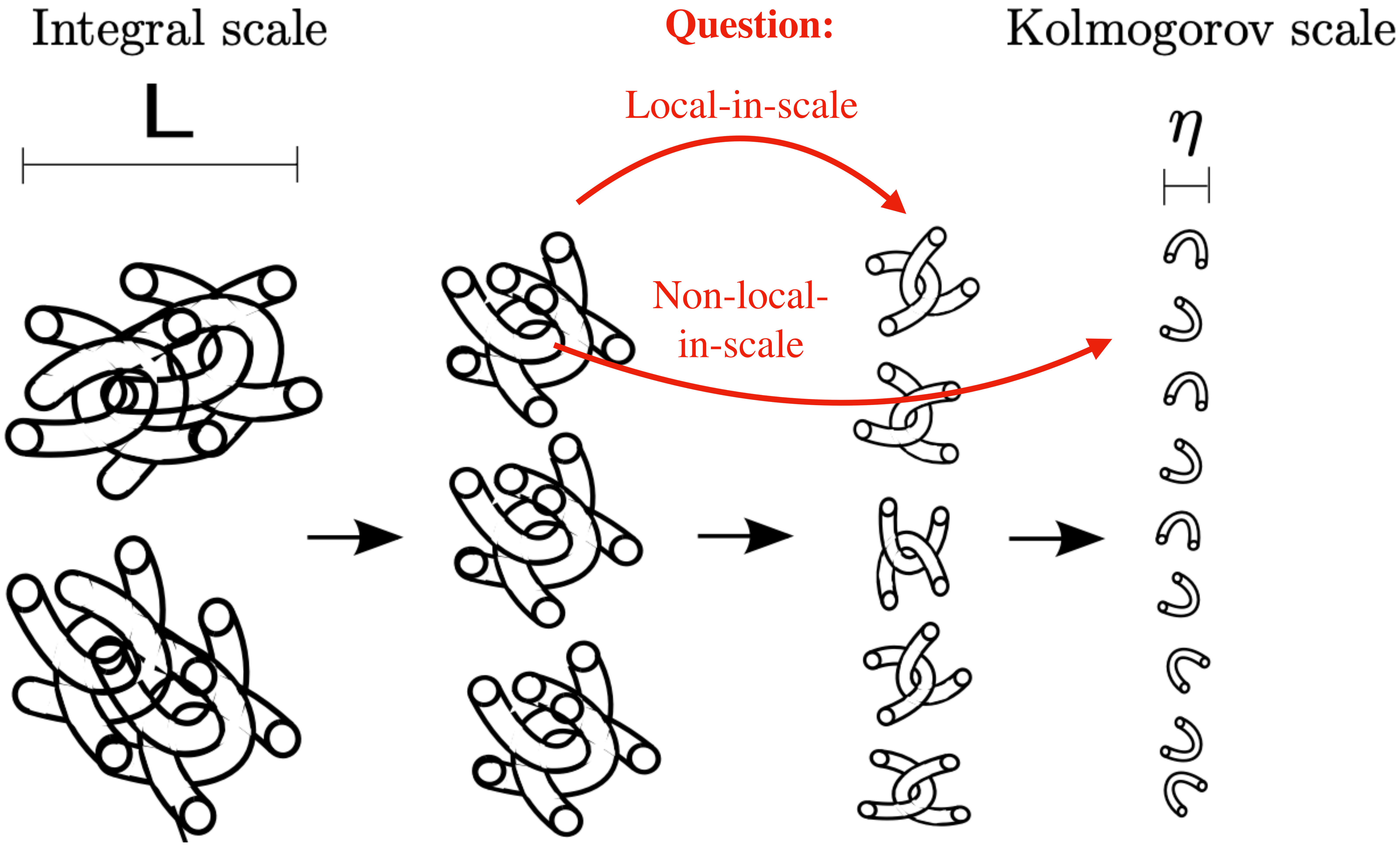

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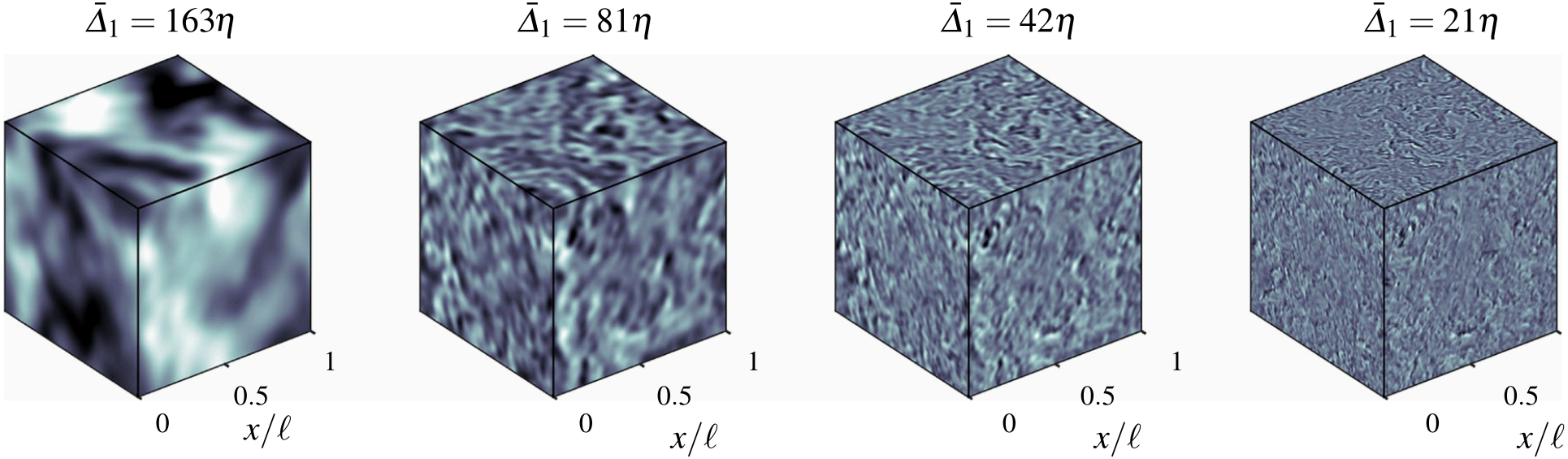
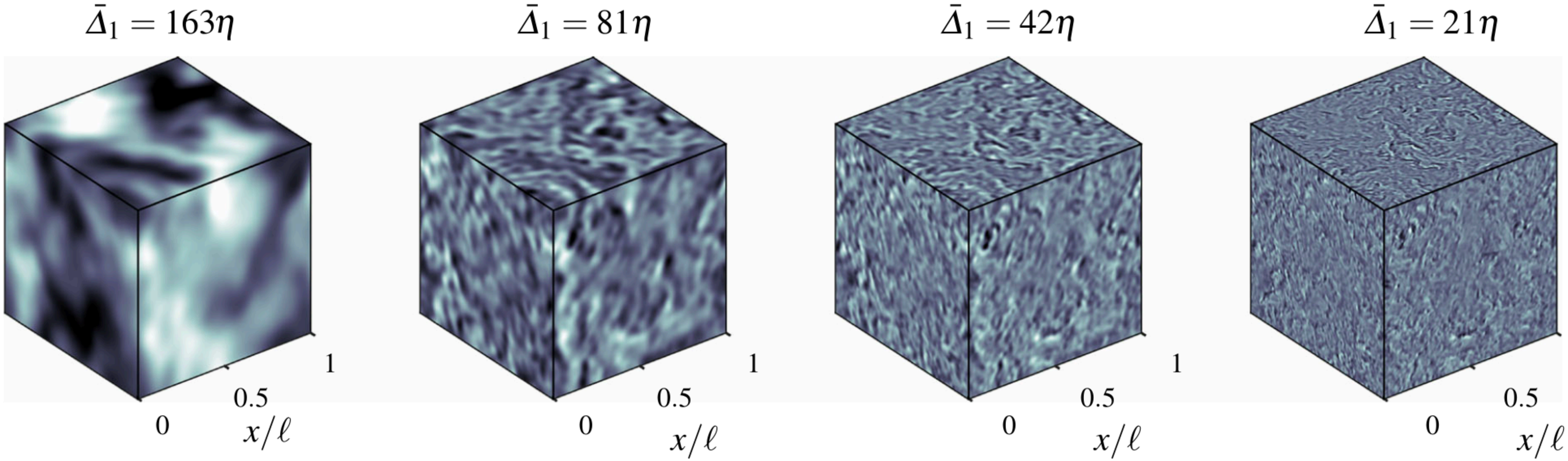


DNS of isotropic turbulence at $Re_\lambda \approx 400$

Filtered velocity field: $\bar{u}_i(\boldsymbol{x}, t) = \int_V \frac{\sqrt{\pi}}{\bar{\Delta}} \exp\left[-\pi^2(\boldsymbol{x} - \boldsymbol{x}')^2/\bar{\Delta}^2\right] u_i(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}'$

Average causality: Application



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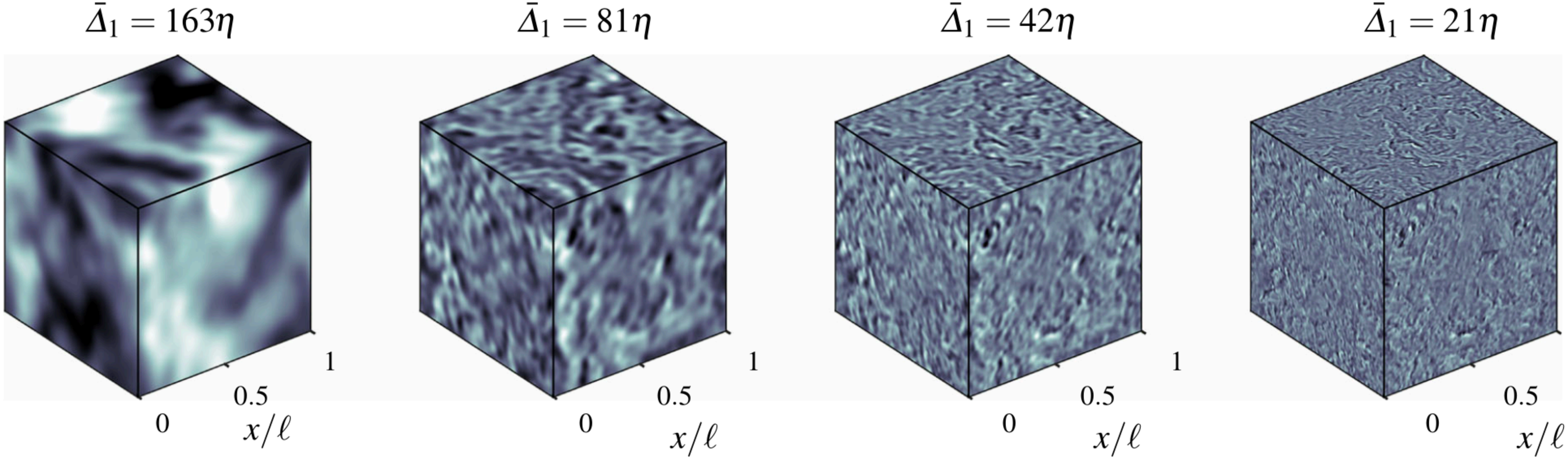
Inter-scale energy transfer: $\Sigma = (\overline{u_i u_j} - \bar{u}_i \bar{u}_j)\bar{S}_{ij}$

Average causality: Application



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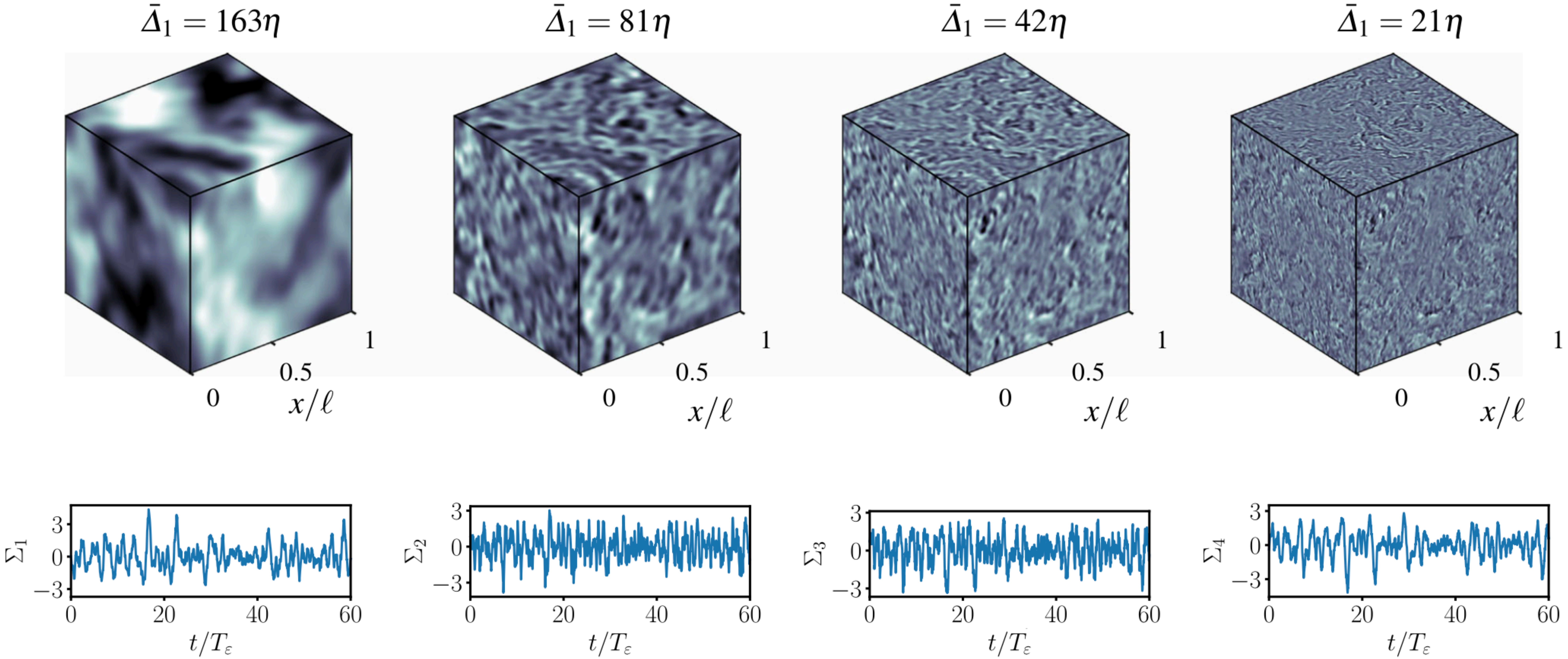
Inter-scale energy transfer: $\Sigma = (\overline{u_i u_j} - \bar{u}_i \bar{u}_j)\bar{S}_{ij}$

Energy transfer extracted for 4 filter widths and averaged in space: $\langle \Sigma_1 \rangle, \langle \Sigma_2 \rangle, \langle \Sigma_3 \rangle, \langle \Sigma_4 \rangle$

Average causality: Application



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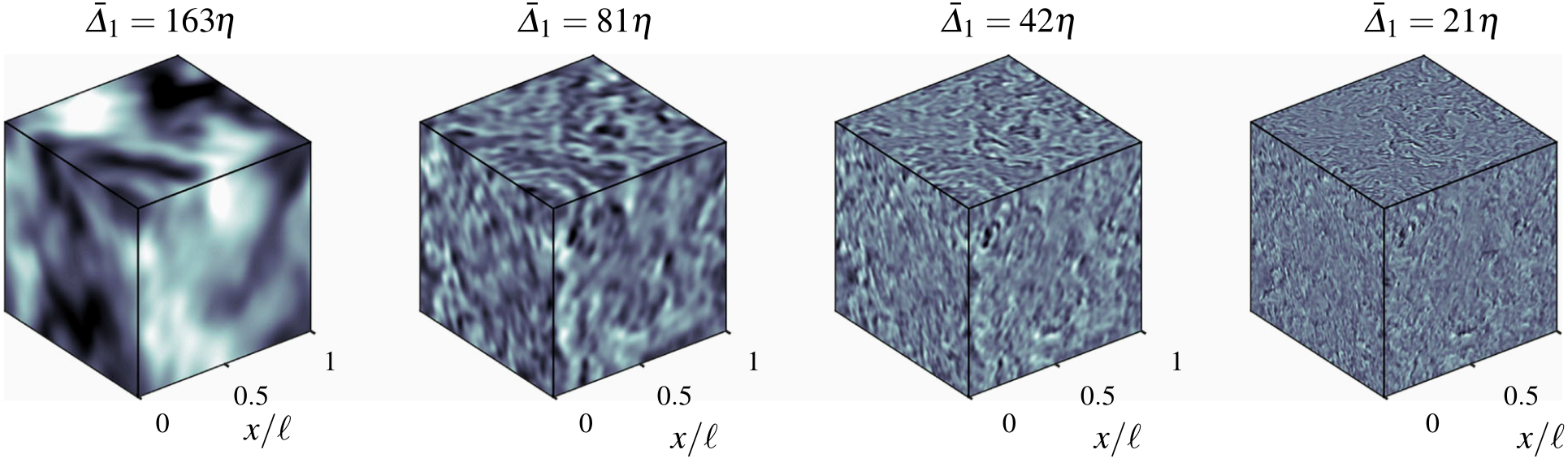
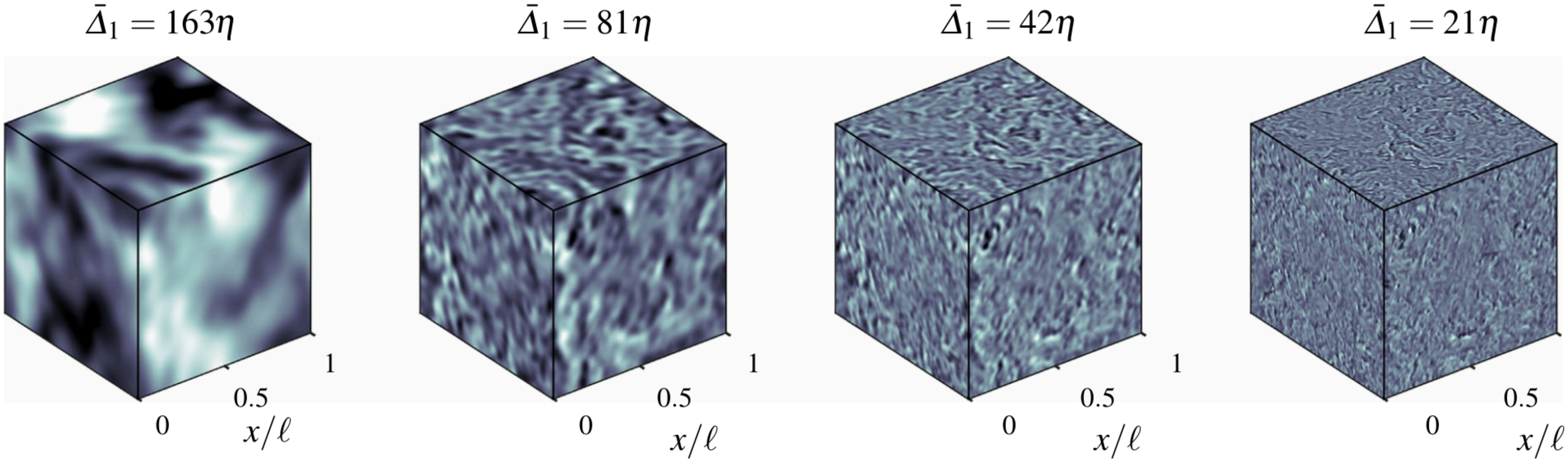


$$H(Q_j^+) = \underbrace{\Delta I^S_{i\to j}}_{\text{Synergistic causality}} + \underbrace{\Delta I^U_{i\to j}}_{\text{Unique causality}} + \underbrace{\Delta I^R_{i\to j}}_{\text{Redundant causality}} + \Delta I_{\text{leak}\to j}$$

Average causality: Application



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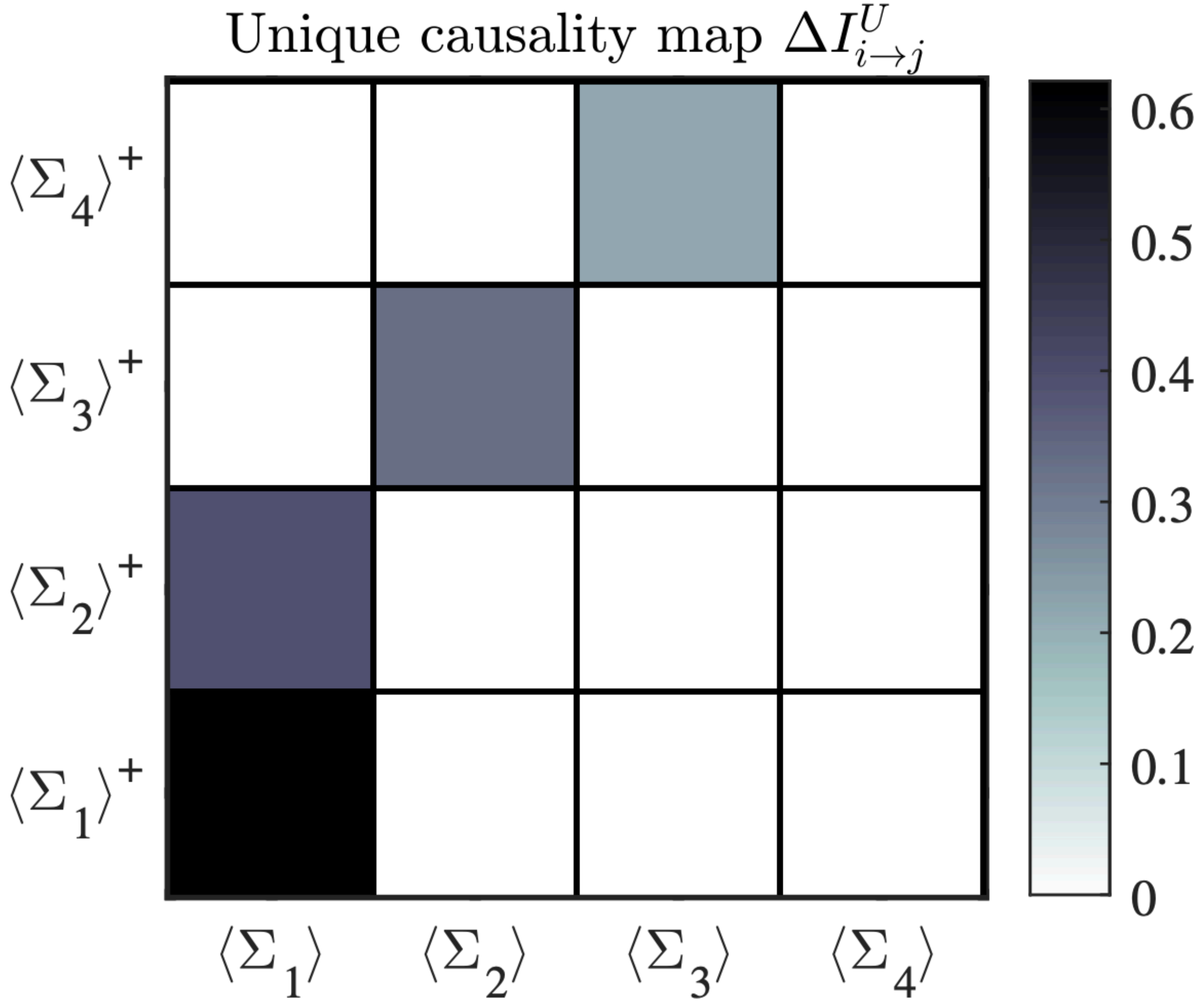
Synergistic causality

Unique causality

Redundant causality

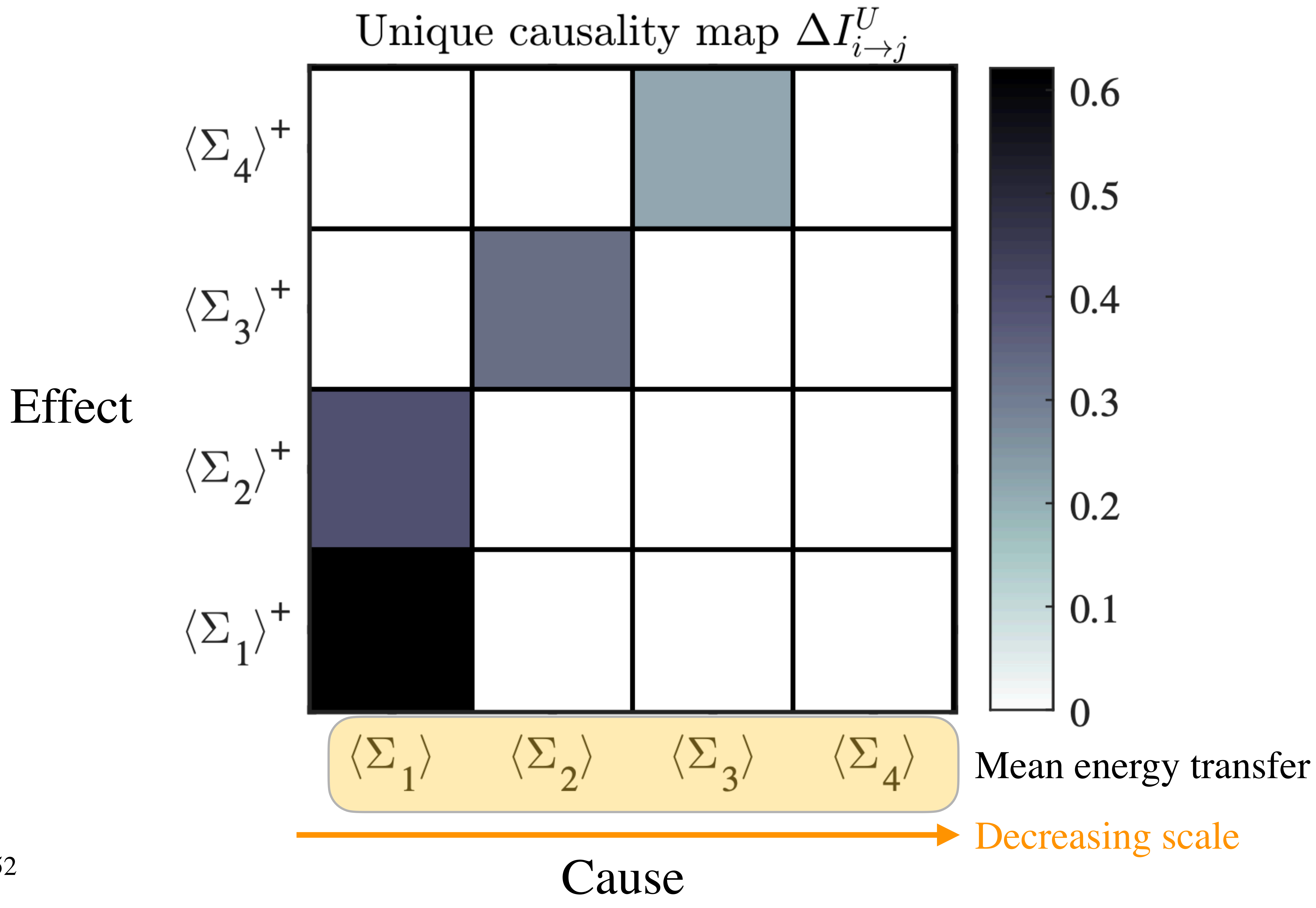
Average causality: Application

Effect

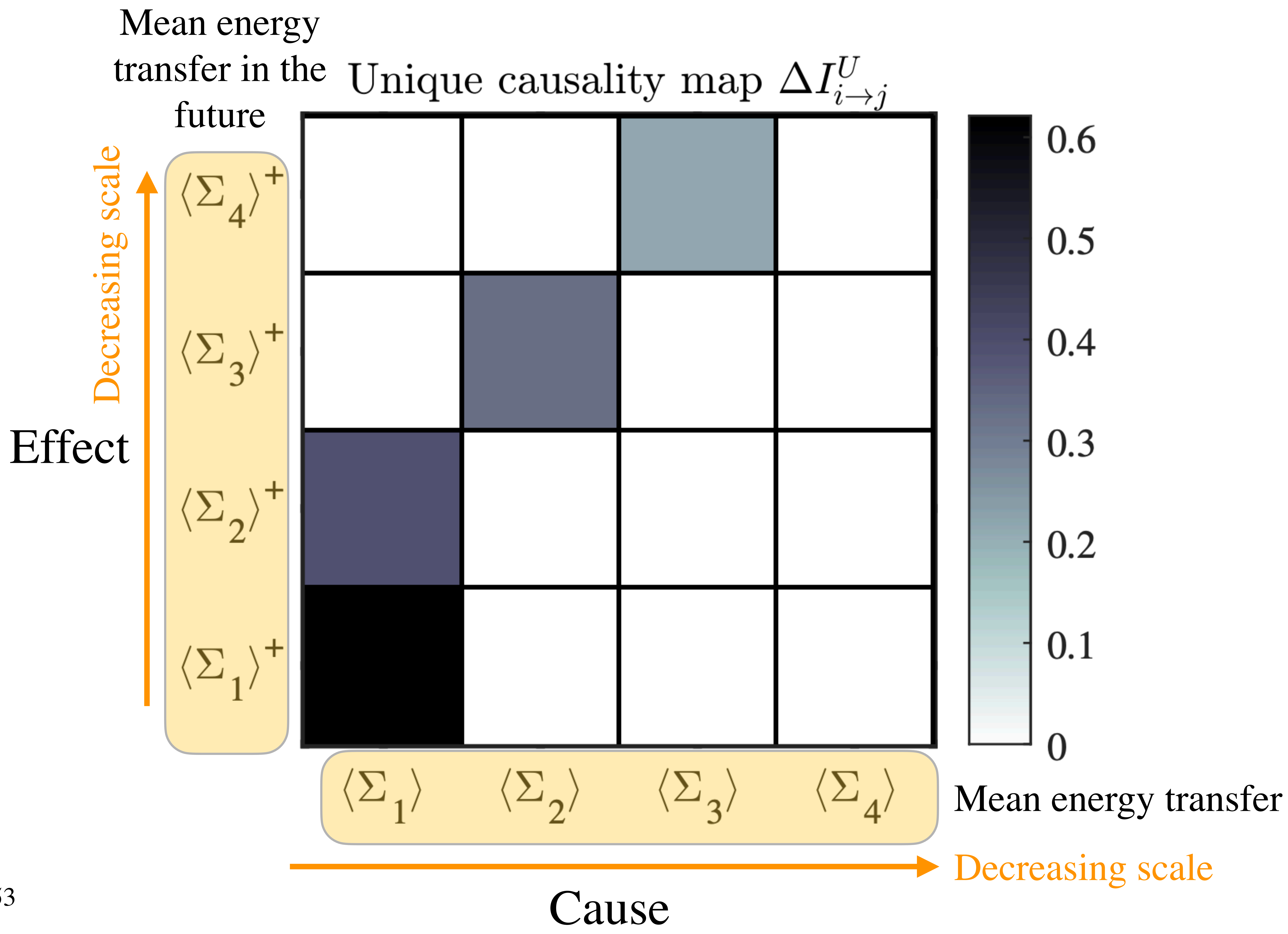


Cause

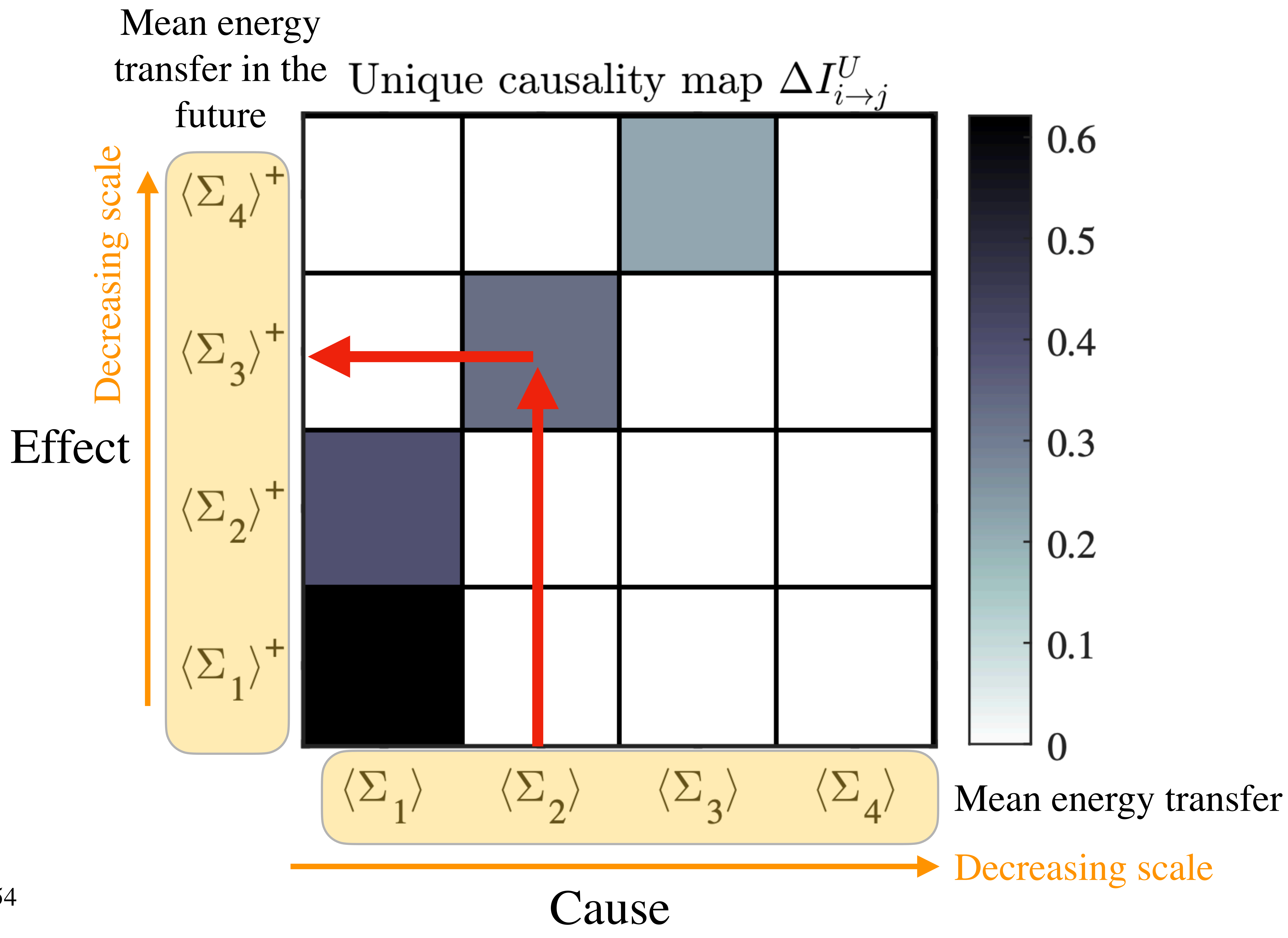
Average causality: Application



Average causality: Application

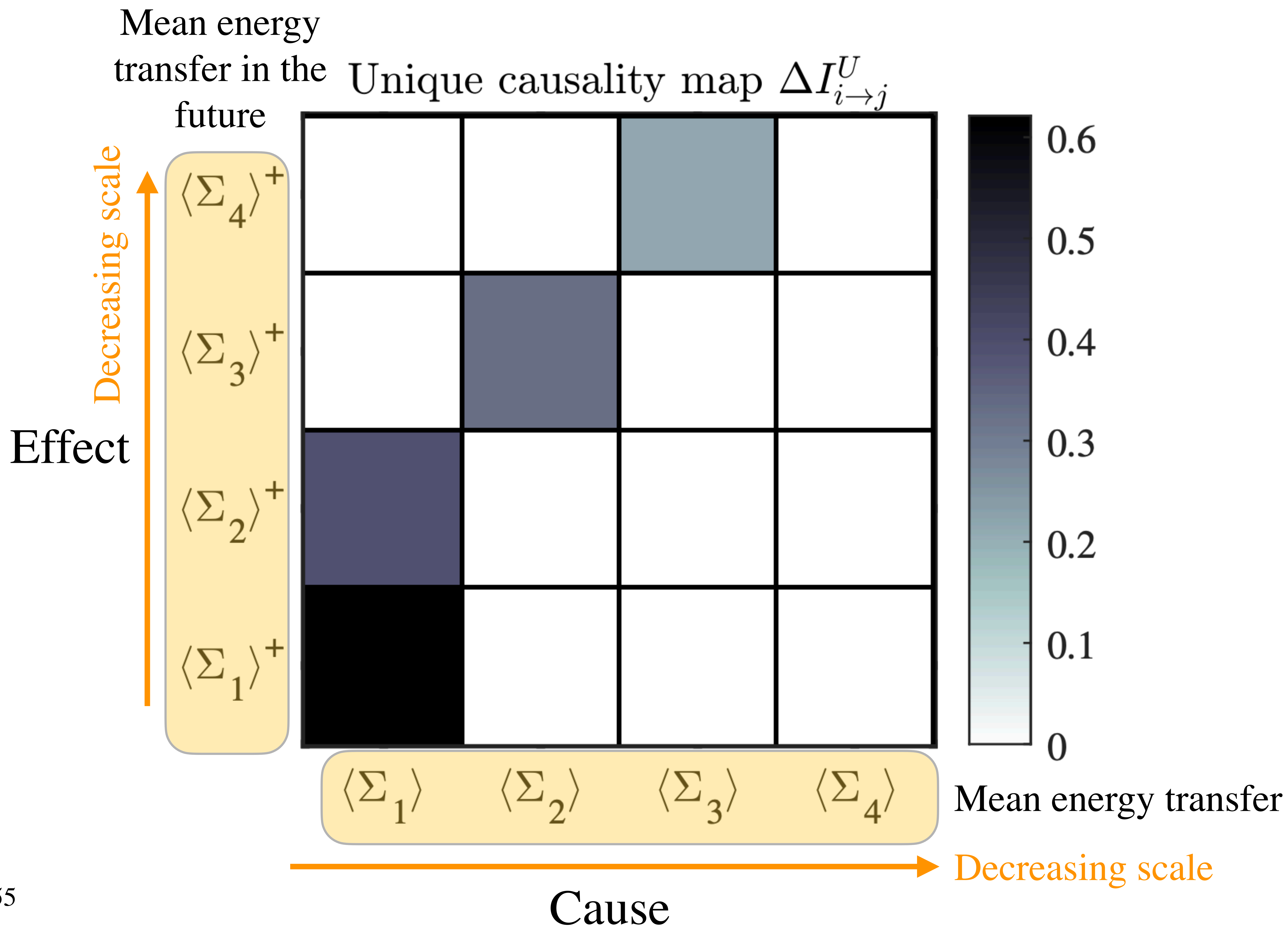


Average causality: Application



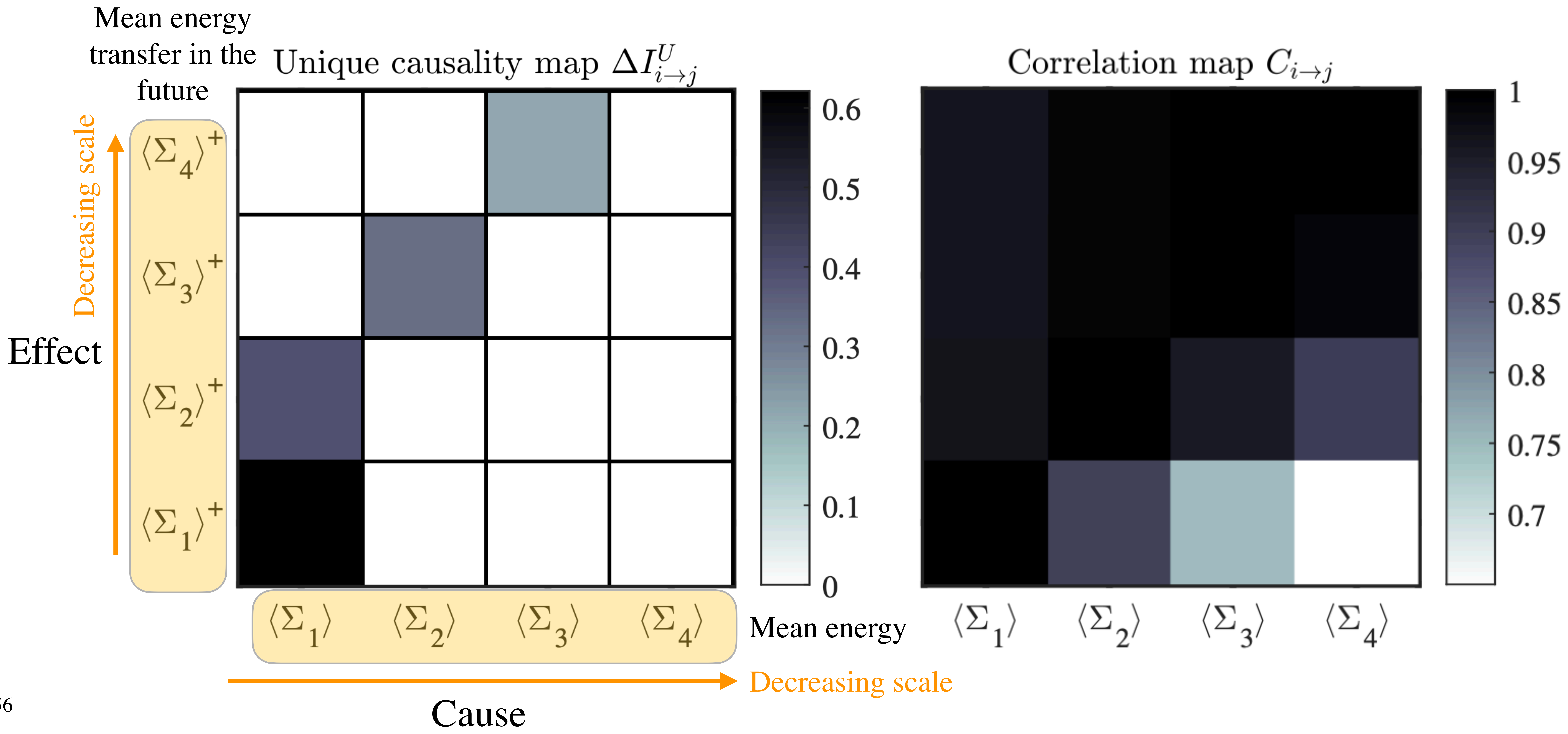
$$\langle \Sigma_2 \rangle \to \langle \Sigma_3^+ \rangle$$

Average causality: Application



Sequential-in-scale propagation of causality

Average causality: Application



Three levels of causality

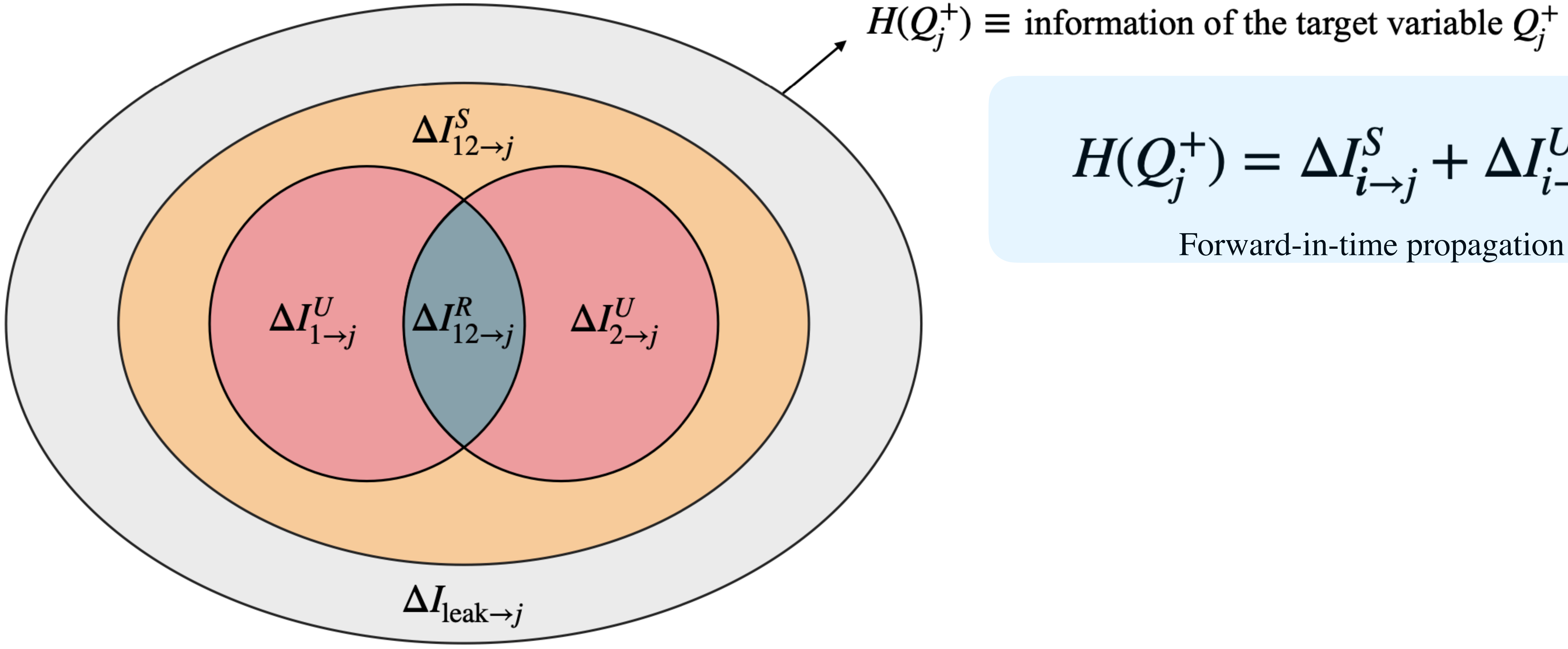
Average Causality

State-dependent Causality

Space-time Causality

State-dependent causality: Method

Quantify the causality from observed variables $\boldsymbol{Q} = [Q_1, Q_2]$ to target variable $Q_j^+ = Q_j(t + \Delta T)$

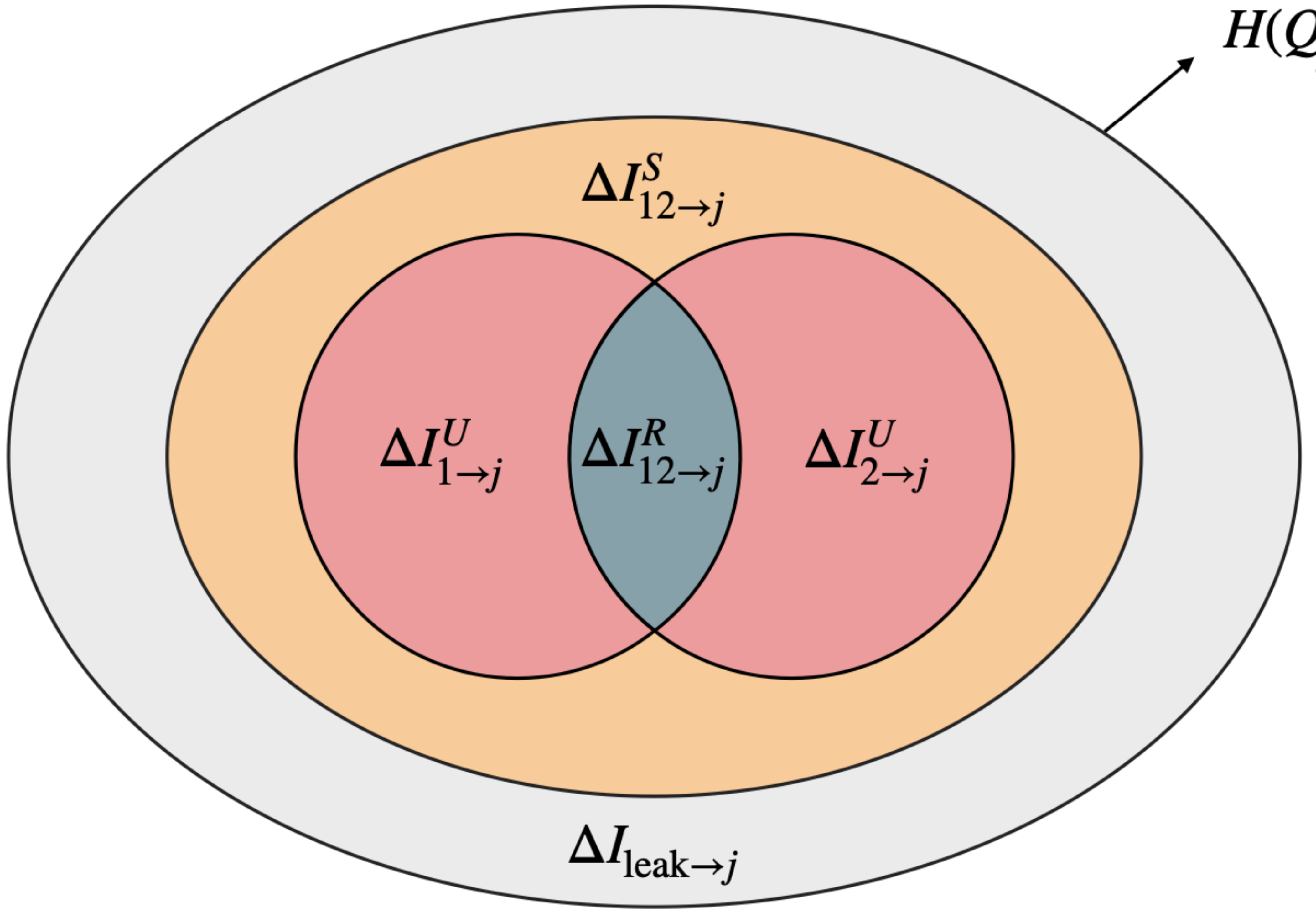


$$H(Q_j^+) = \Delta I^S_{\boldsymbol{i}\to j} + \Delta I^U_{i\to j} + \Delta I^R_{\boldsymbol{i}\to j} + \Delta I_{\text{leak}\to j}$$

Forward-in-time propagation of information equation

State-dependent causality: Method

Quantify the causality from observed variables $\boldsymbol{Q} = [Q_1, Q_2]$ to target variable $Q_j^+ = Q_j(t + \Delta T)$



$H(Q_j^+) \equiv$ information of the target variable Q_j^+

$$H(Q_j^+) = \Delta I^S_{\boldsymbol{i}\to j} + \Delta I^U_{i\to j} + \Delta I^R_{\boldsymbol{i}\to j} + \Delta I_{\mathrm{leak}\to j}$$

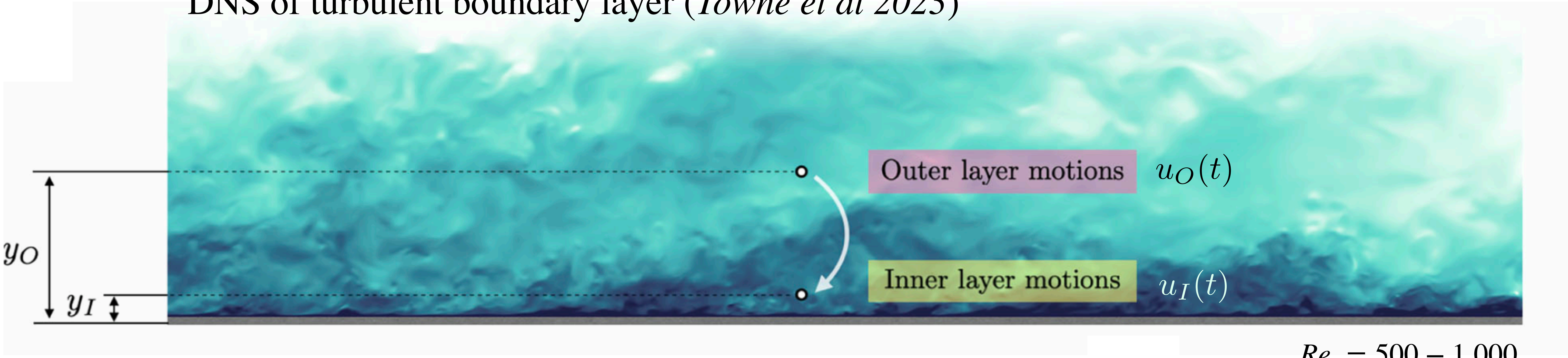
Forward-in-time propagation of information equation

$$\Delta I^\alpha_{\boldsymbol{i}\to j} = \sum_{q_j^+\in Q_j^+} \sum_{\boldsymbol{q}\in\boldsymbol{Q}} \Delta C^\alpha_{\boldsymbol{i}\to j} + \dots$$

Martinez-Sanchez, Lozano-Duran, Comm. Phys., 2025

State-dependent causality: Application

DNS of turbulent boundary layer (*Towne et al 2023*)



$Re_\tau = 500 - 1{,}000$

Question: Is there causality of outer layer velocity to the inner layer velocity?

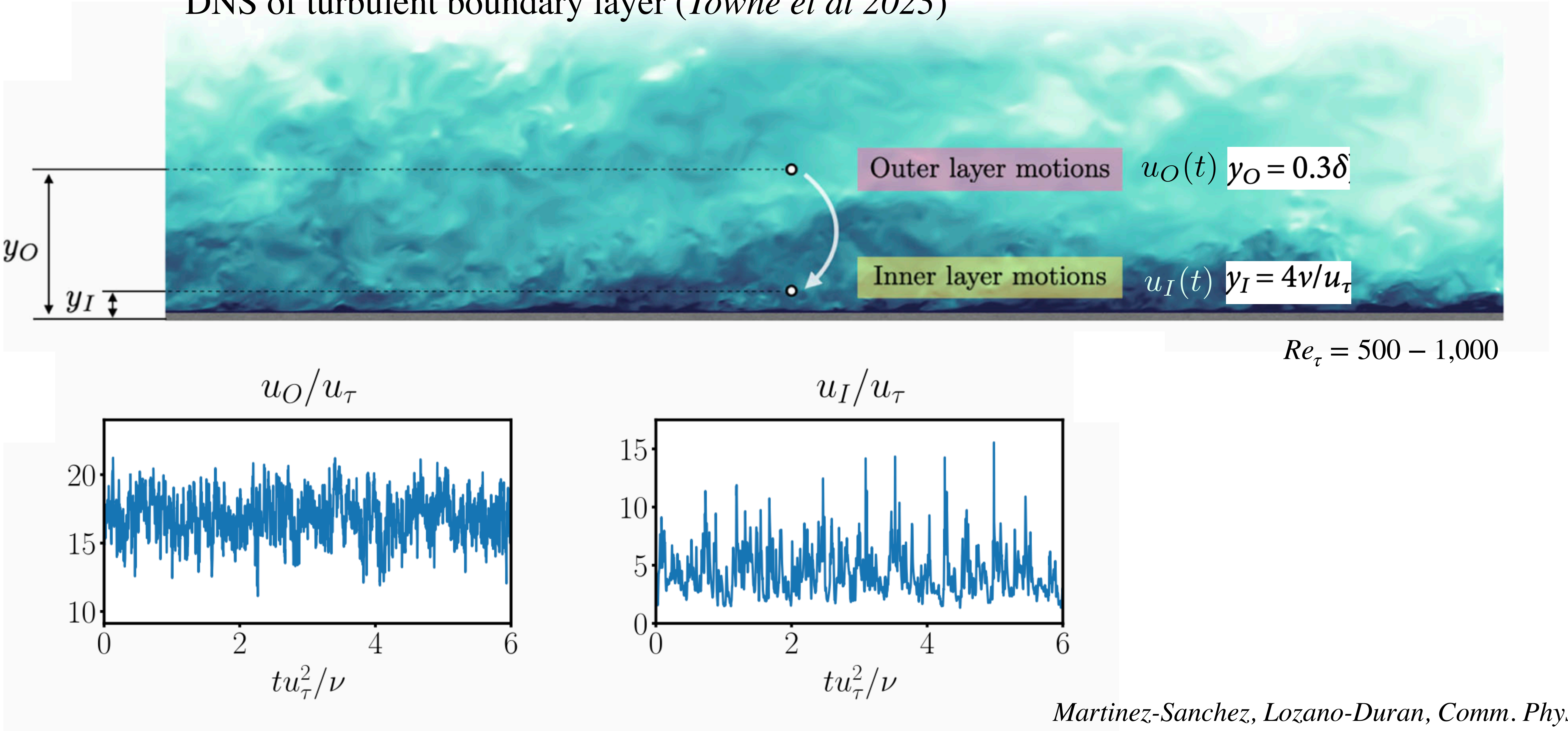
$y_O = 0.3\delta$

$y_I = 4\nu/u_\tau$

Martinez-Sanchez, Lozano-Duran, Comm. Phys., 2025

State-dependent causality: Application

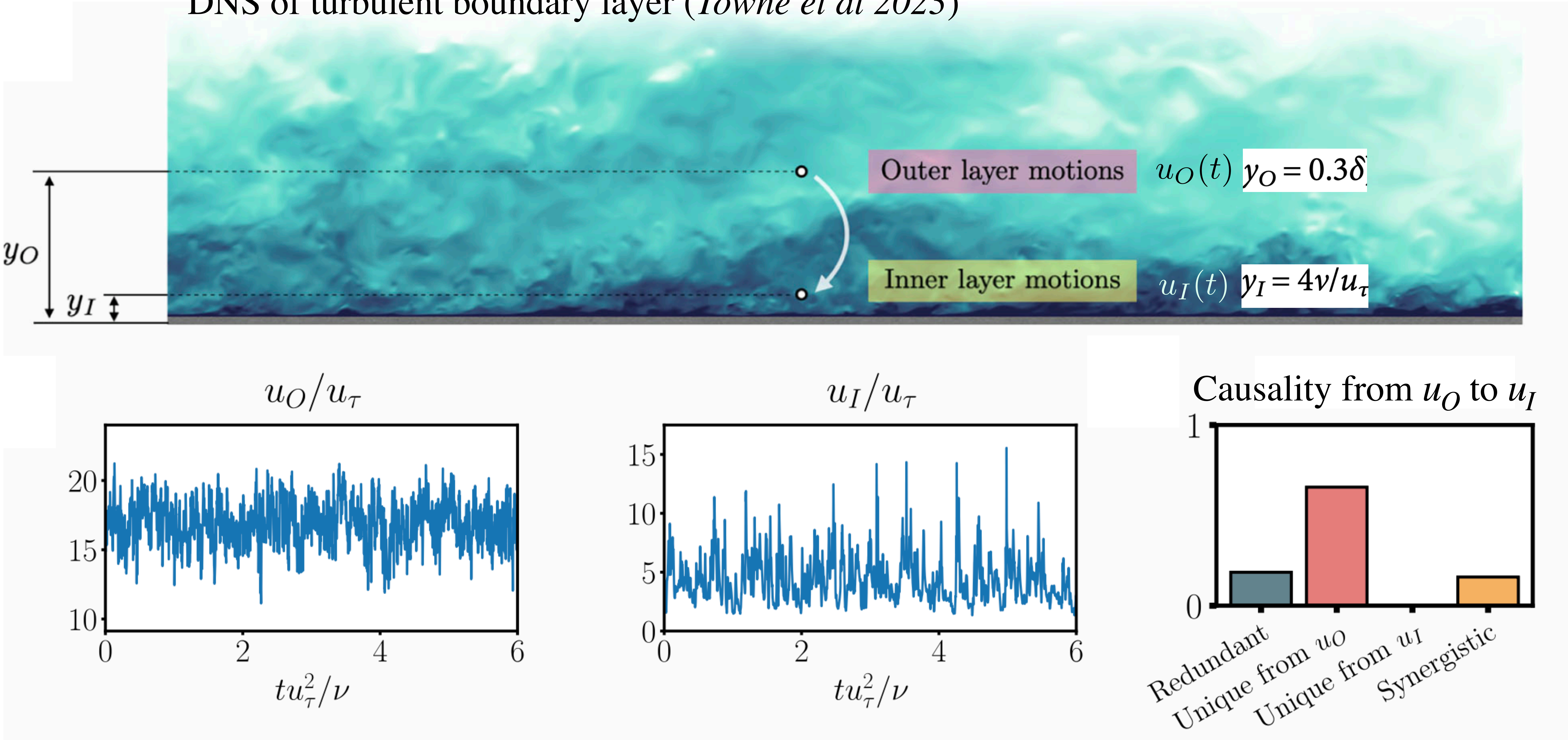
DNS of turbulent boundary layer (*Towne et al 2023*)



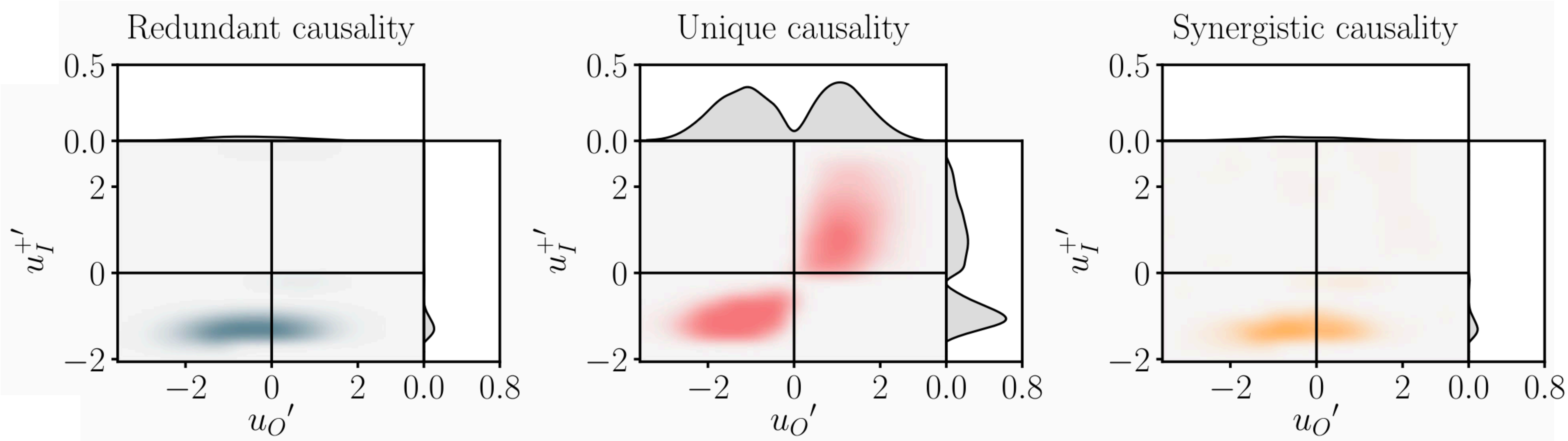
Martinez-Sanchez, Lozano-Duran, Comm. Phys., 2025

State-dependent causality: Application

DNS of turbulent boundary layer (*Towne et al 2023*)

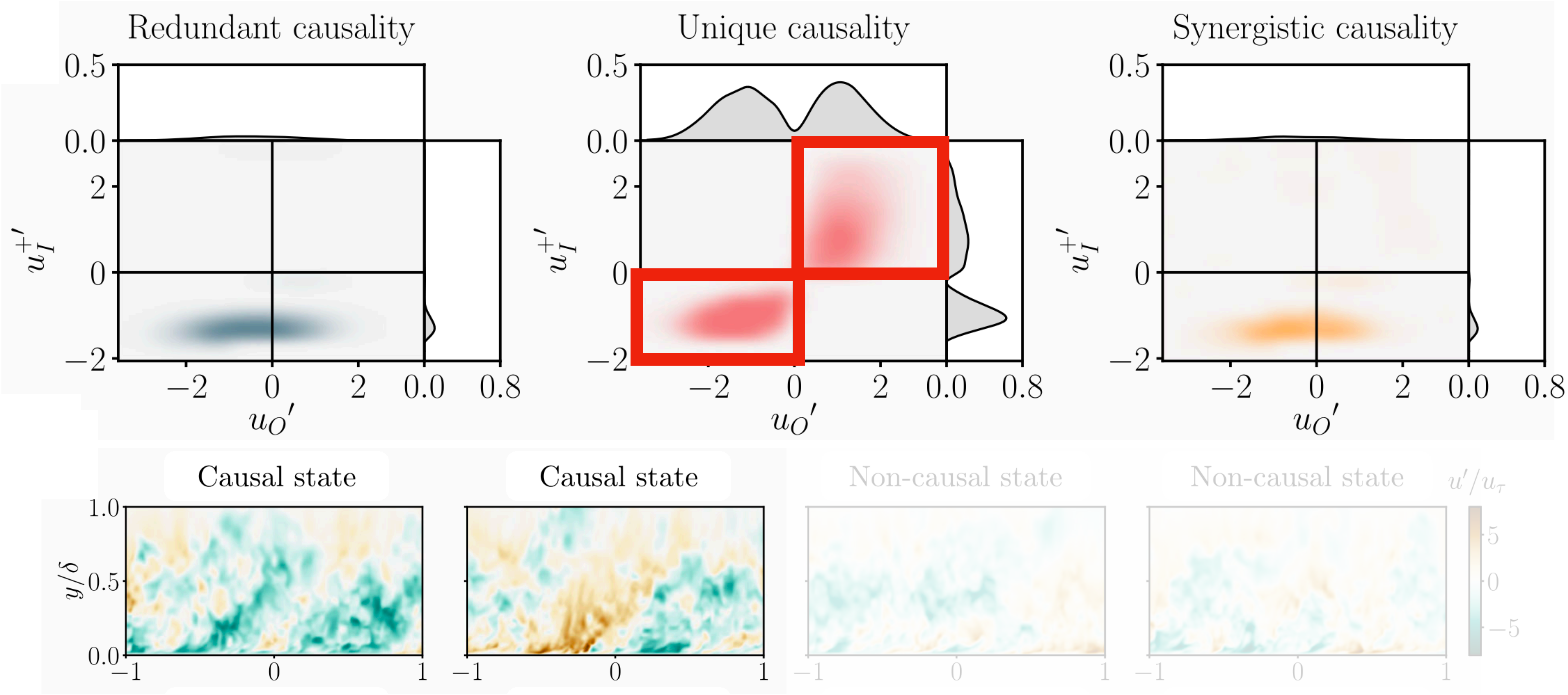


State-dependent causality: Application

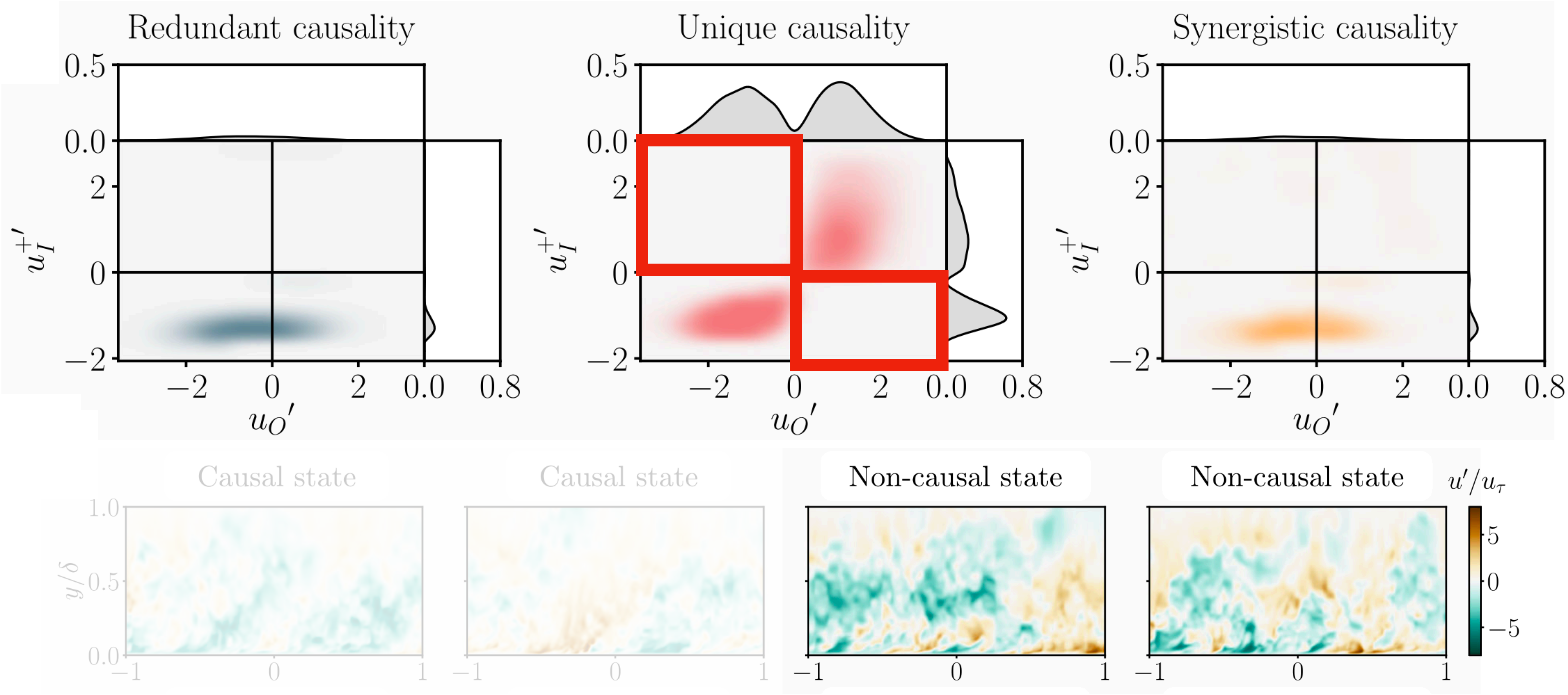


Martinez-Sanchez, Lozano-Duran, Comm. Phys., 2025

State-dependent causality: Application



State-dependent causality: Application



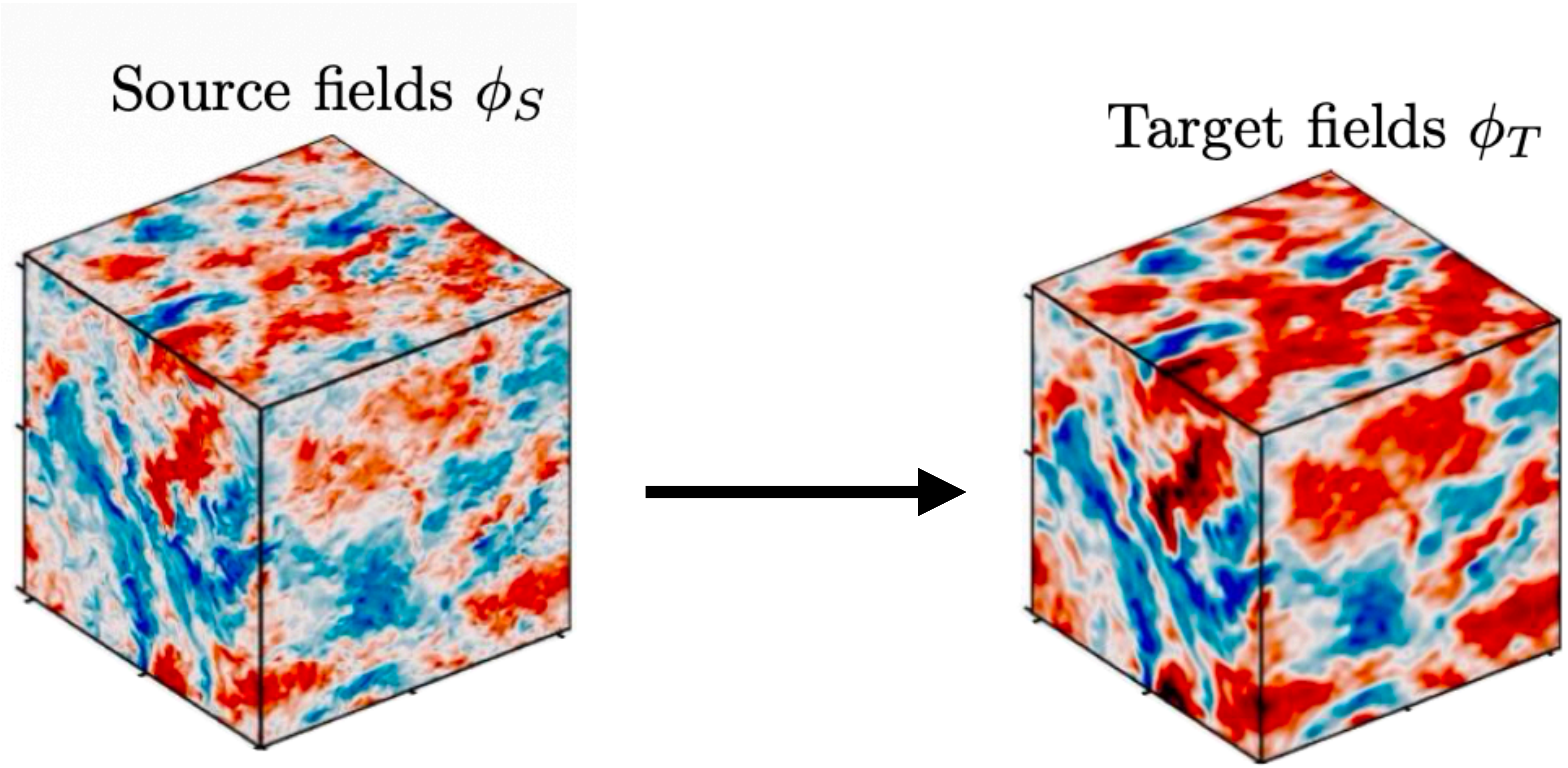
Three levels of causality

Average Causality

State-dependent Causality

Space-time Causality

Space-time causality: Method

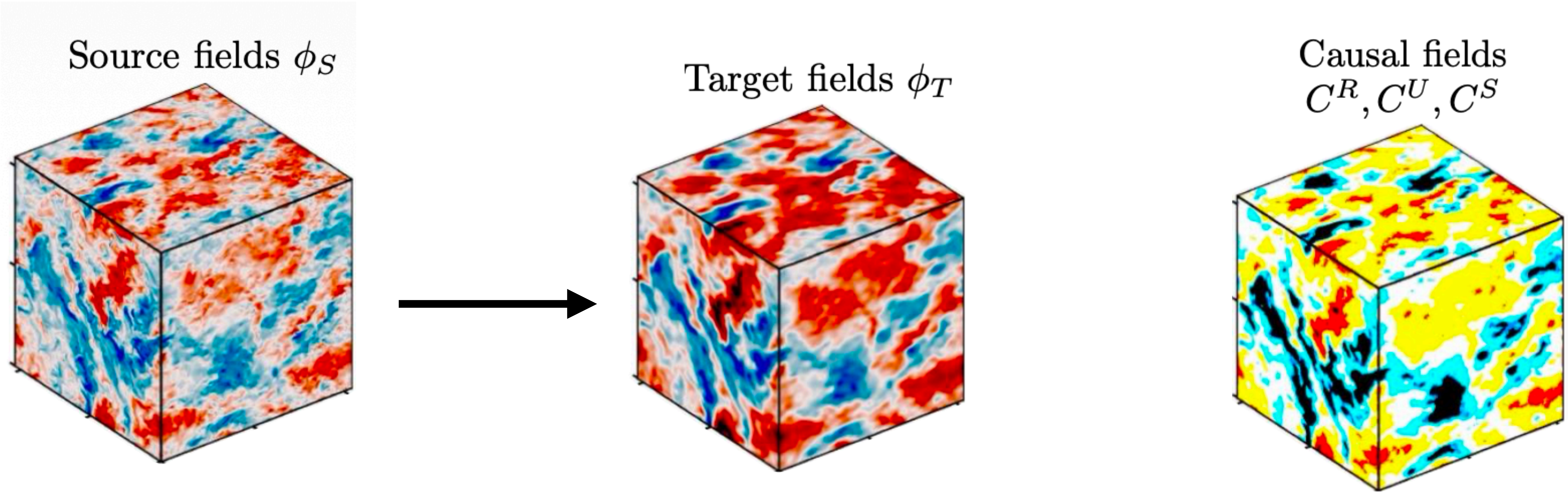


Cause? Effect?

Space-time causality:
When and **where** the source field is causal to the target and by how much?

Martinez-Sanchez, Uyumaz, Lozano-Duran, 2026

Space-time causality: Method



Cause?

Effect?

Space-time causality:
When and **where** the source field is causal to the target and by how much

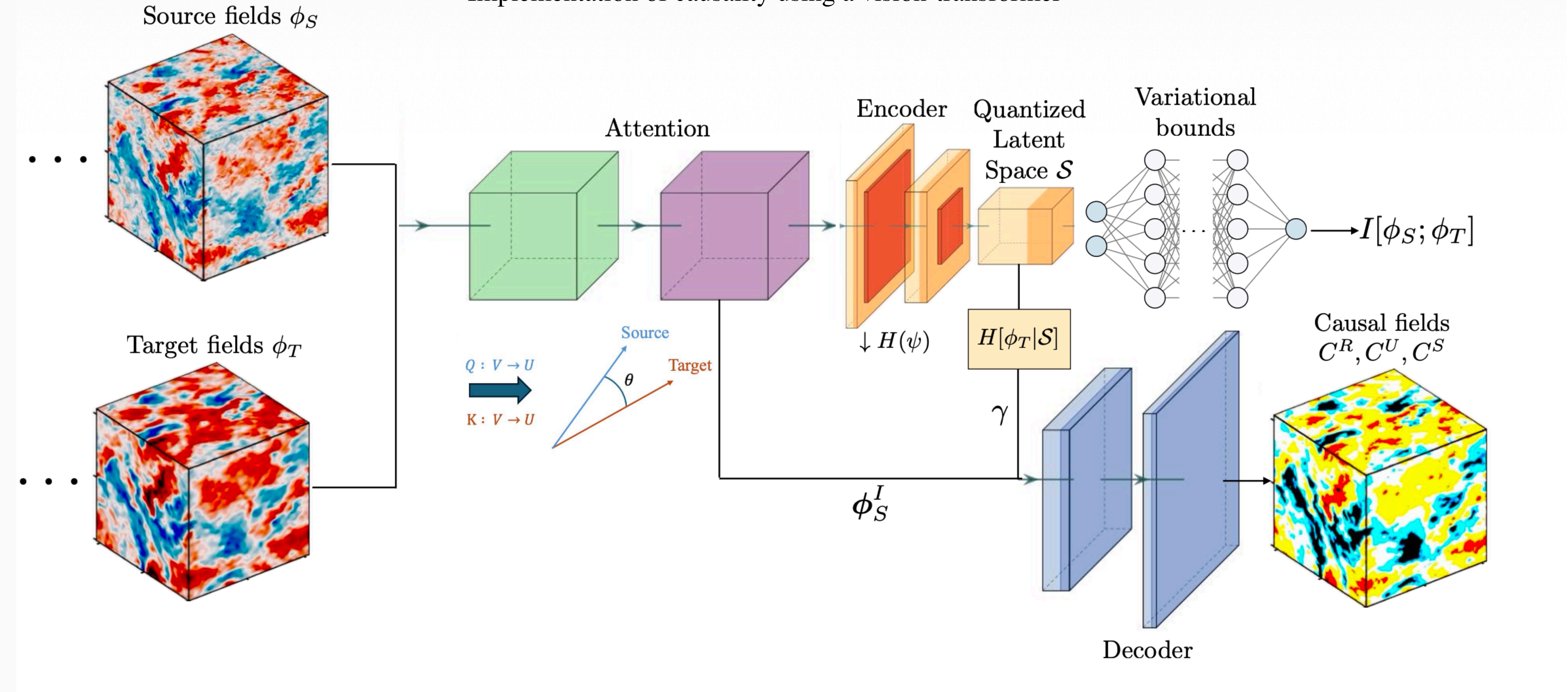
Quantification of causality

$$\phi_S^I(\boldsymbol{x}, t) = \arg\min_{\boldsymbol{\psi}} \left\{ H[\boldsymbol{\psi}] \;\middle|\; \boldsymbol{\psi} \in F(\boldsymbol{\phi}_S),\ I[\boldsymbol{\psi}; \boldsymbol{\phi}_T] = I[\boldsymbol{\phi}_S; \boldsymbol{\phi}_T] \right\} \quad \text{with} \quad \|\boldsymbol{\phi}_S - \boldsymbol{\phi}_S^I\| \text{ minimized}$$

Martinez-Sanchez, Uyumaz, Lozano-Duran, 2026

Space-time causality: Method

Implementation of causality using a vision-transformer

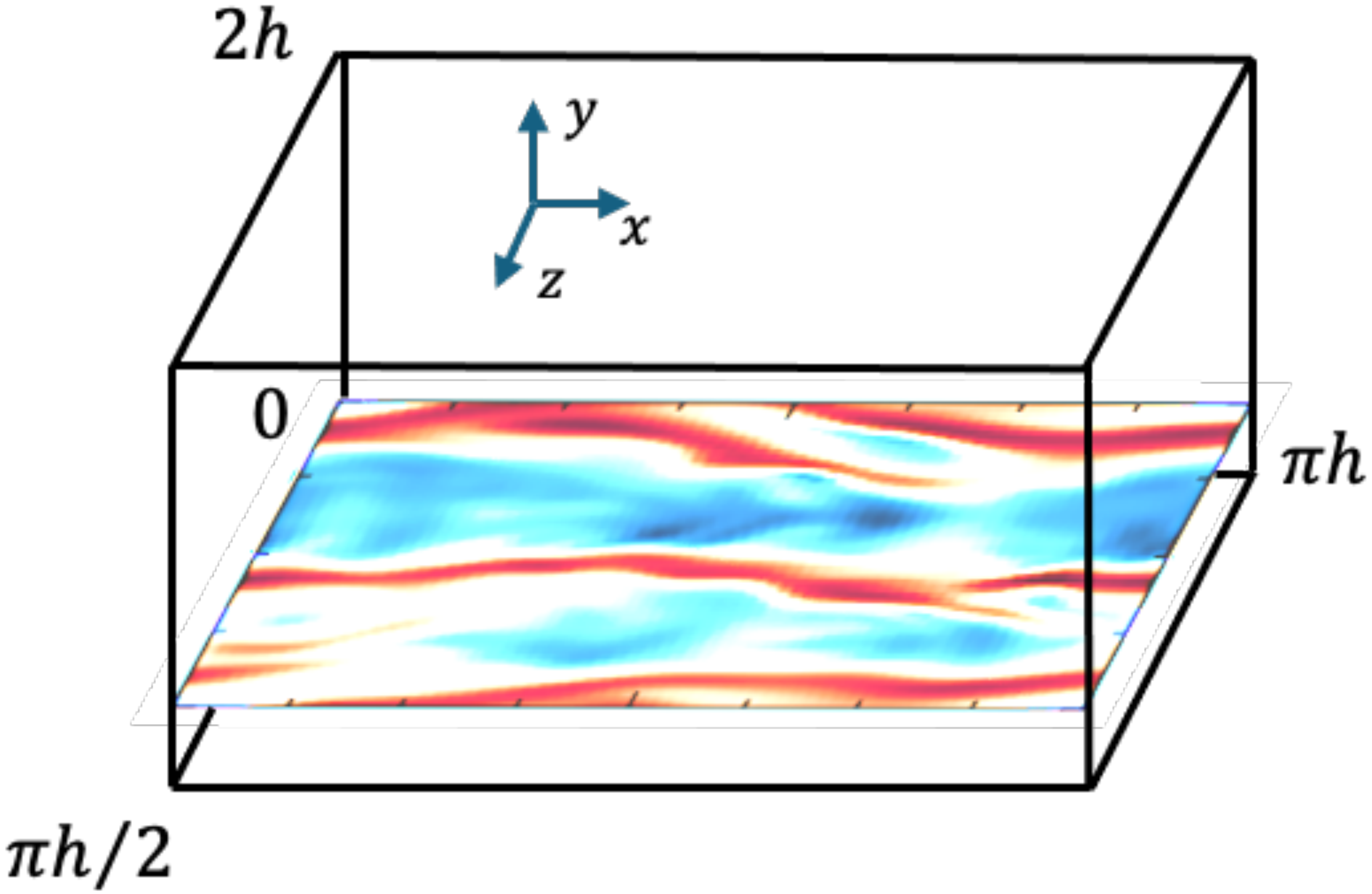


Space-time causality: Application

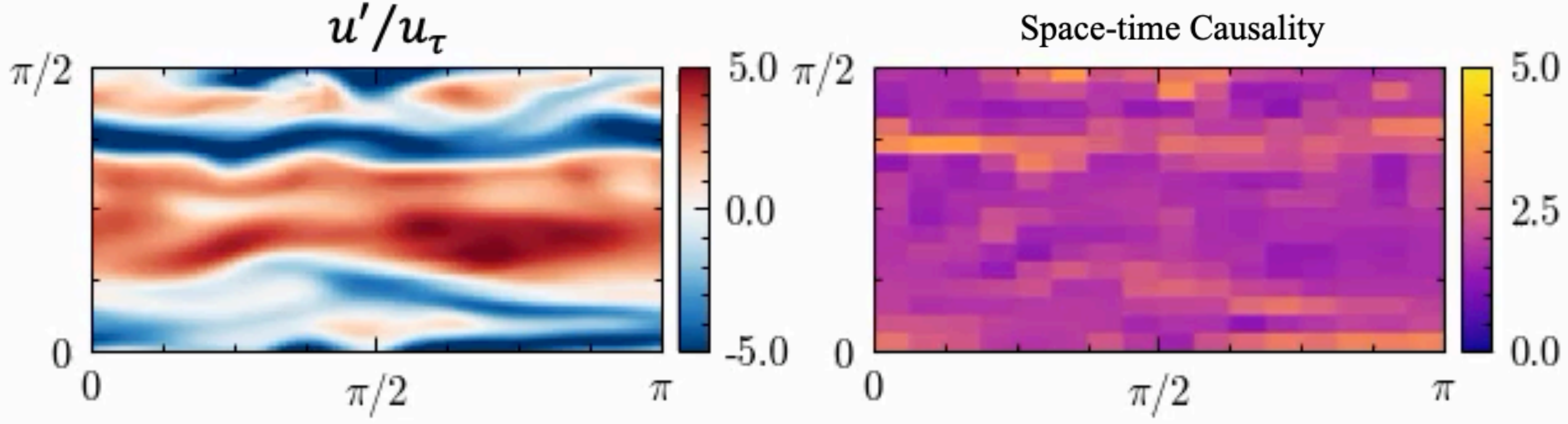
Question: When and where streamwise velocity is causal to the wall shear stress in the future?

Problem and Data:

- Turbulent Channel Flow
- DNS at $Re_\tau = 180$
- Wall-normal plane at $y^+ = 60$
- $u'(\boldsymbol{x}, t;\ y^+) \rightarrow \tau_x(\boldsymbol{x}, t + T)$
- T = 10 plus units



Space-time causality: Application



Outline

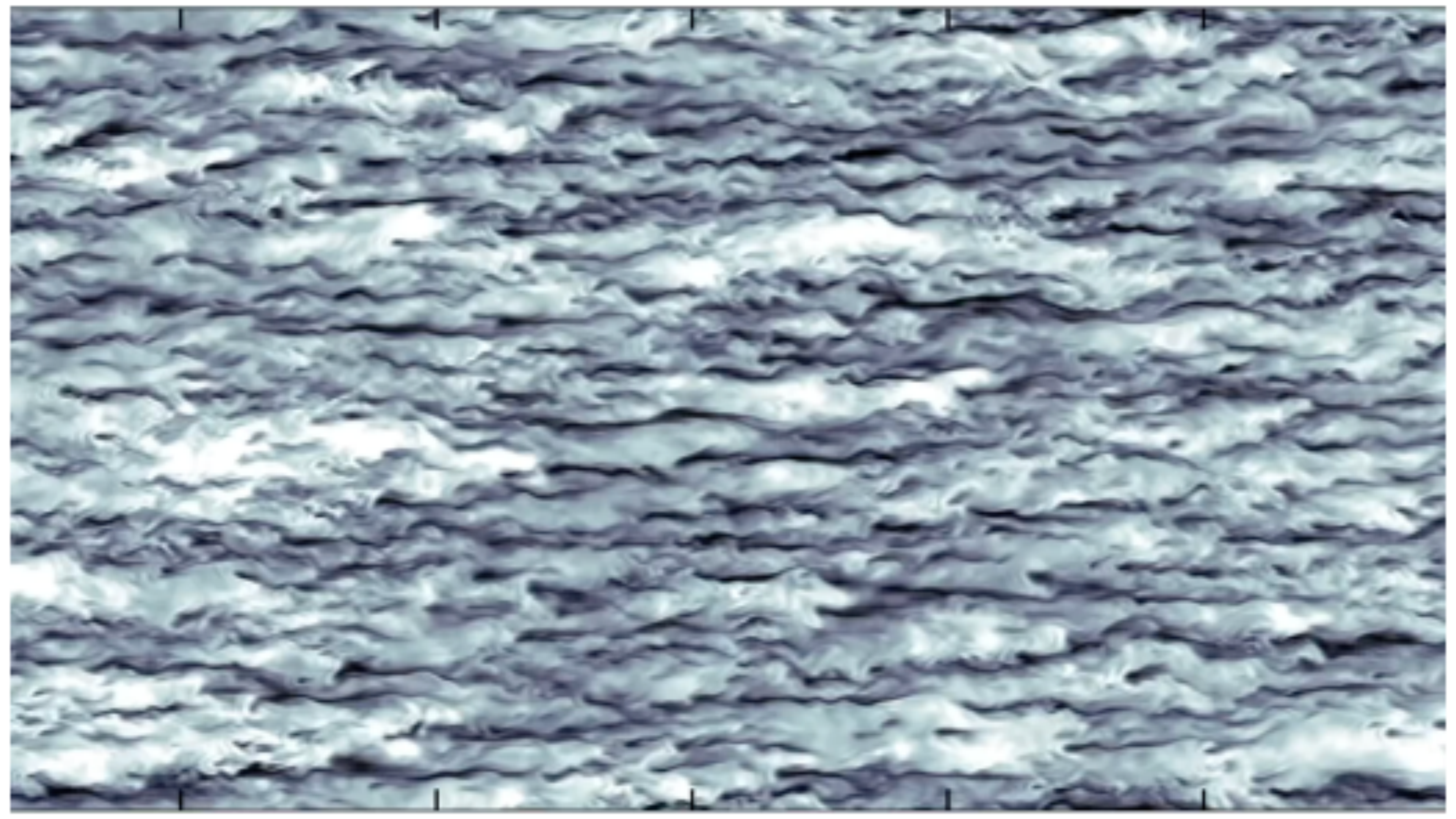
- **What is causality?**
- **Frameworks for causal inference**
  - Interventional vs. observational
- **Three level of causality**
  - Average causality
  - State-dependent causality
  - Space-time causality
- **Limitations**

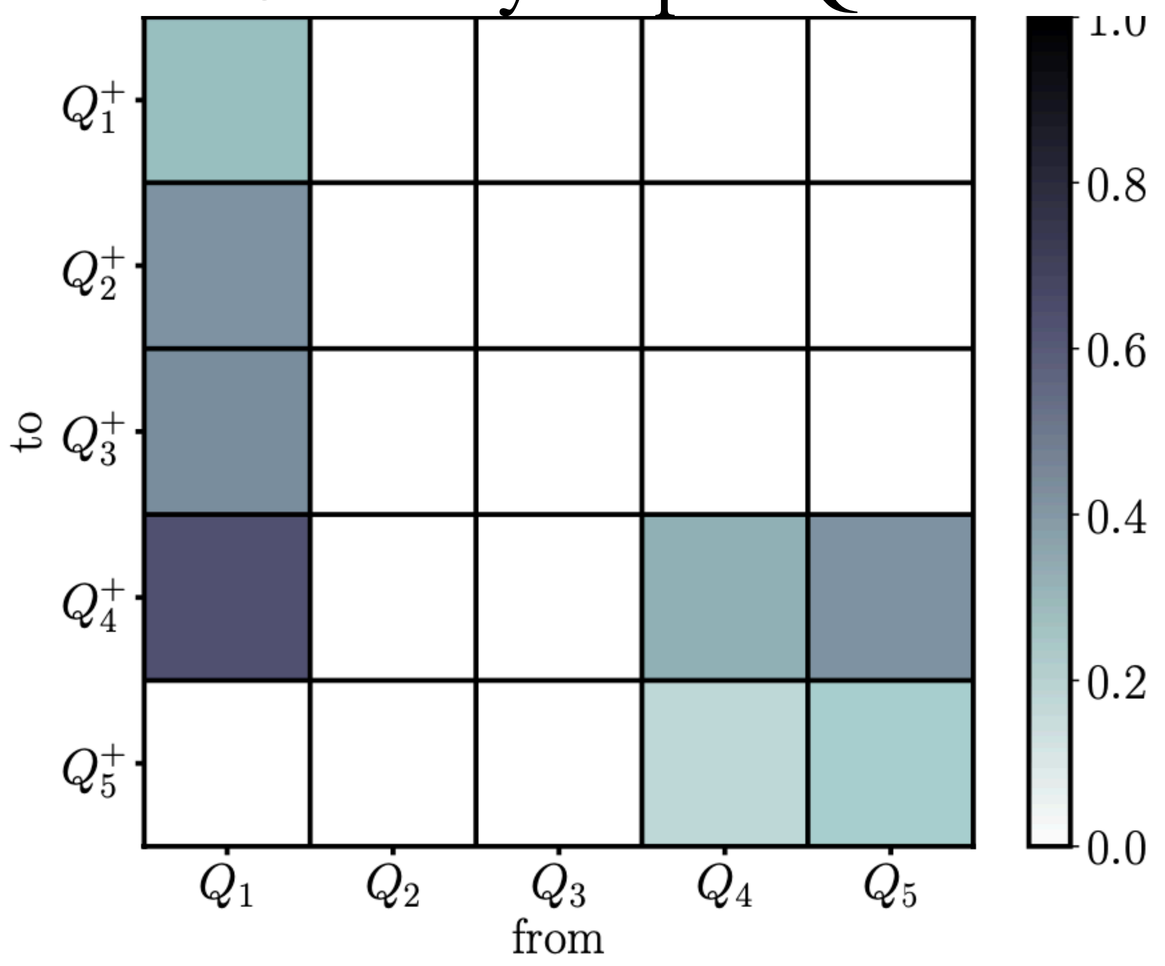
Some limitations

- Causal inference is just a tool. It might help to get the correct answers if the correct questions are asked
- The best definition of causality might depend on goal/application
- Some properties might be partially lost when unobserved variables play a key role in the causal network
- Only applicable to time-varying variables (not to constants/parameters of the system)
- The method are data-hungry
- …

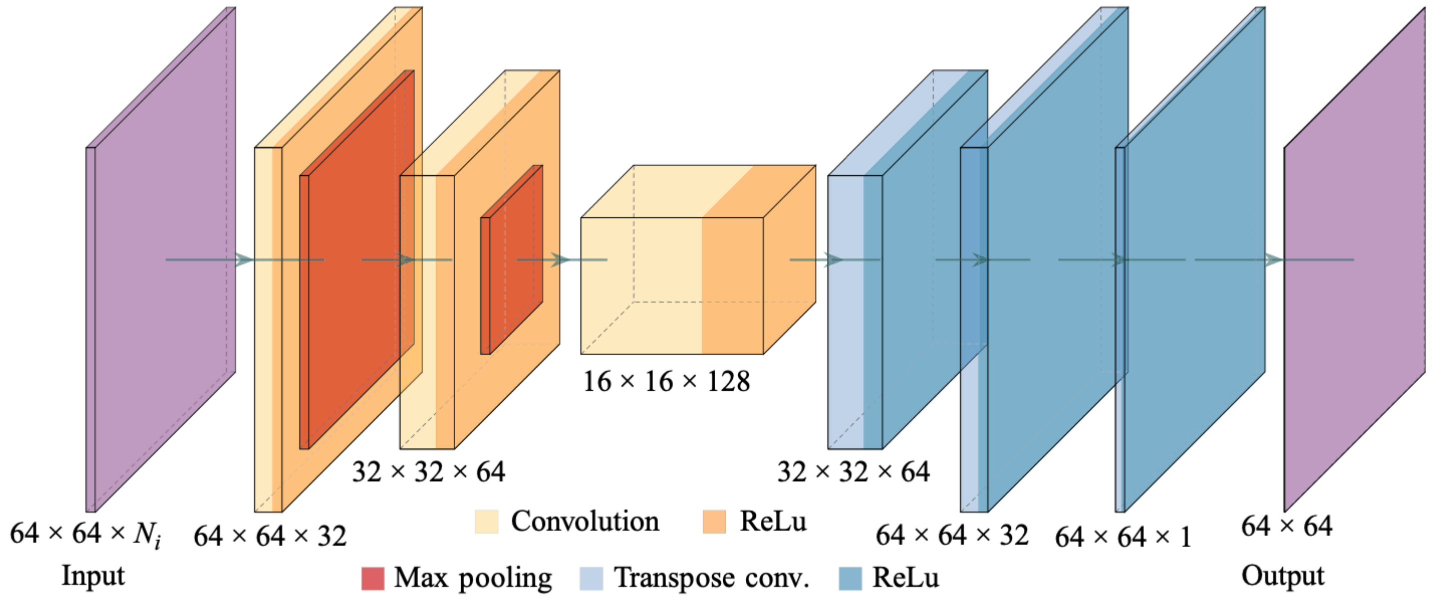
Why causal analysis in fluid dynamics?

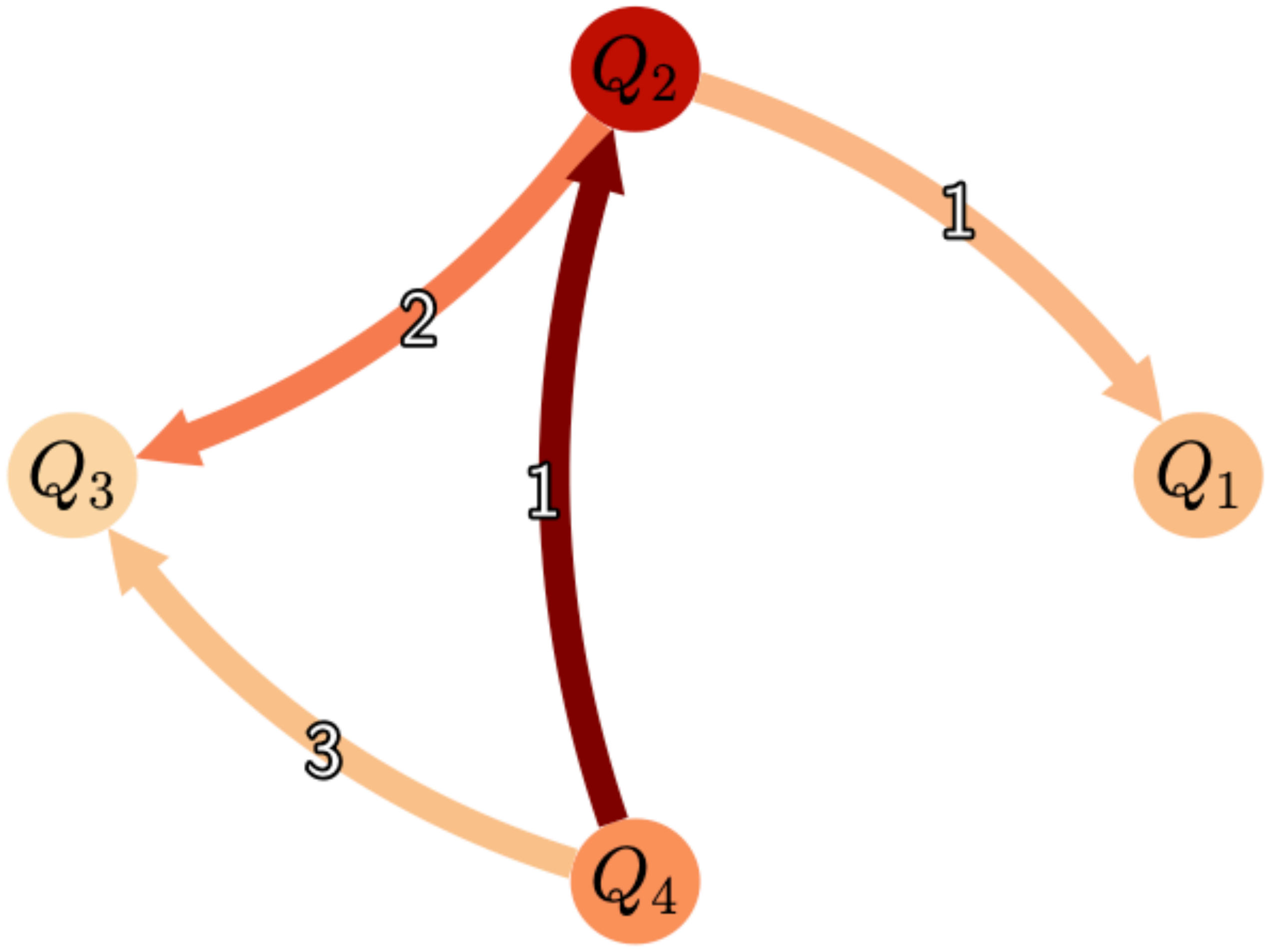
Physical insight





Causality-preserving reduced-order models





Causality-driven control