Representation Learning and Super-Resolution Generation for Scientific Visualization

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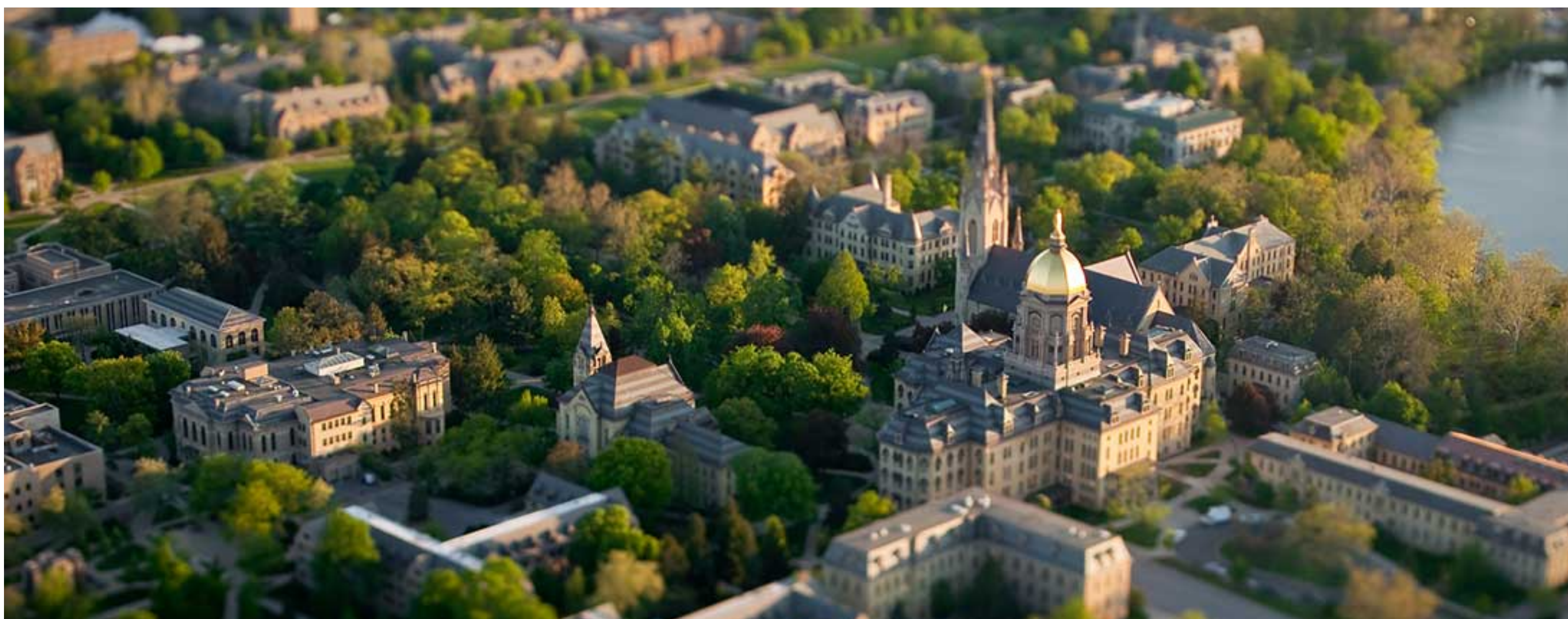
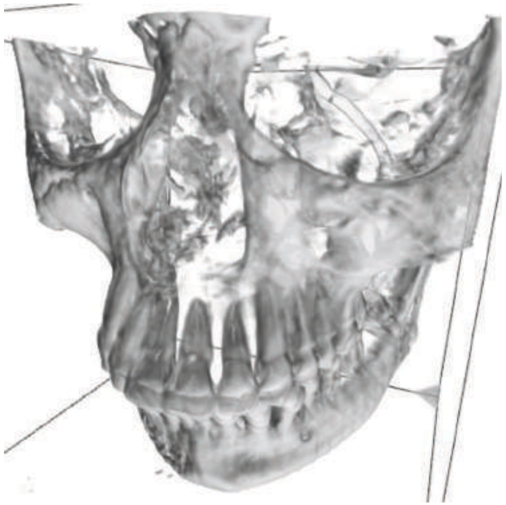


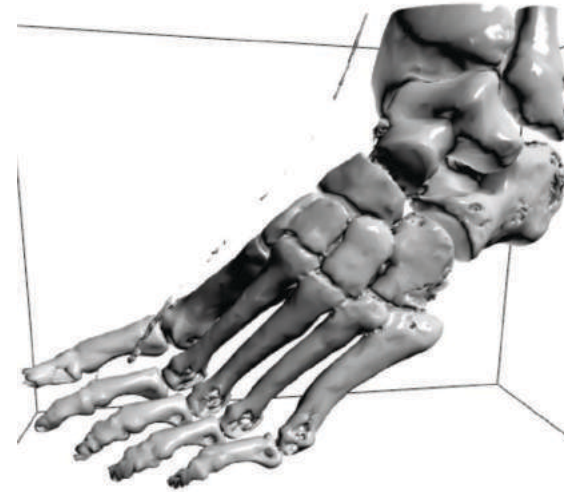
Outline of talk

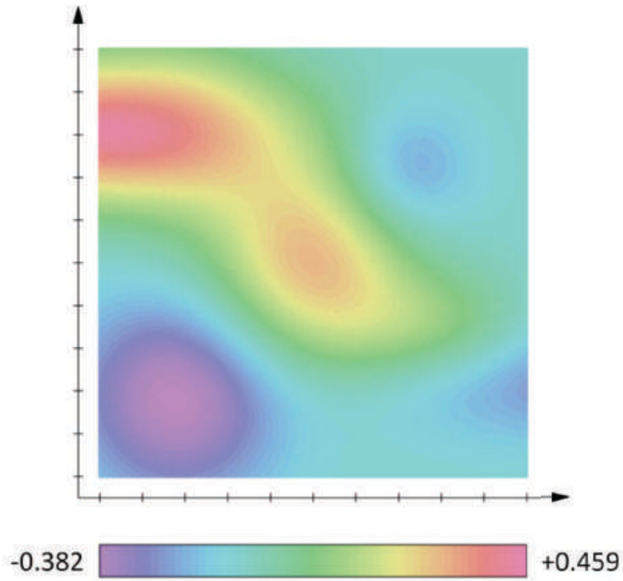
- Scientific visualization
- FlowNet for representation learning
- TSR-TVD for super-resolution generation
- Improvement and expansion
- Emerging directions for AI+VIS research

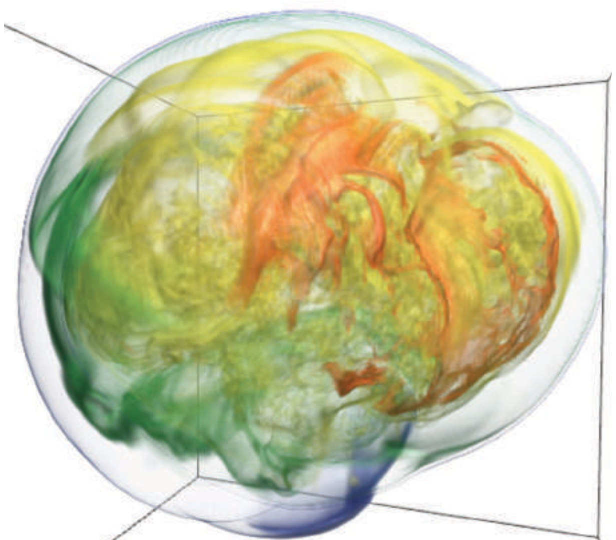
Scientific visualization

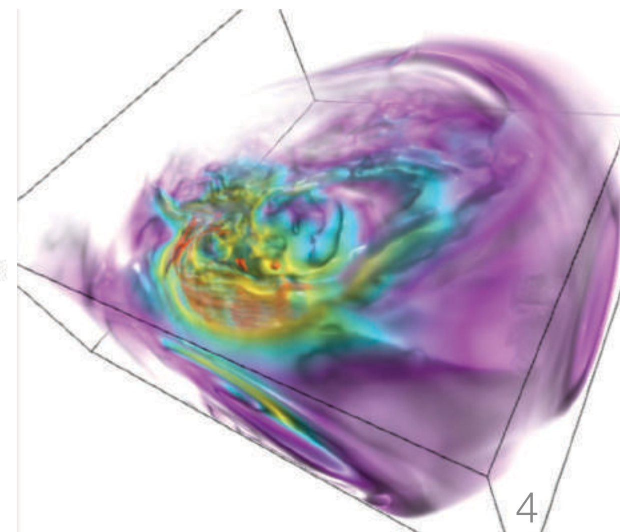
Scalar fields



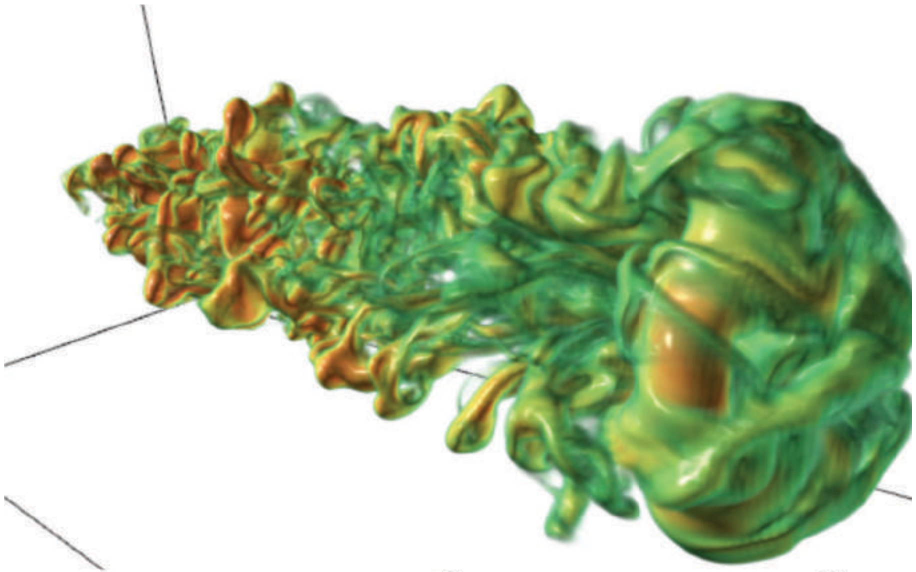


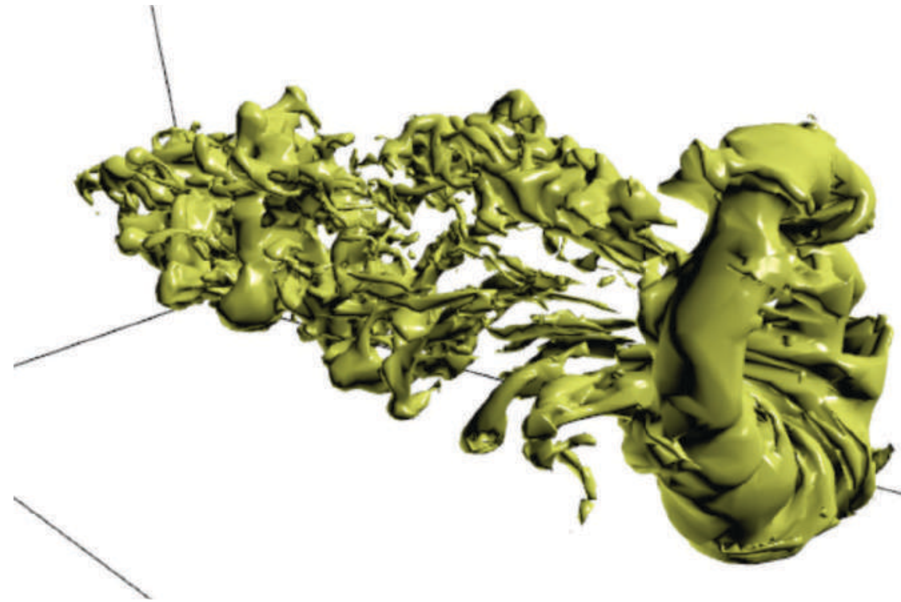


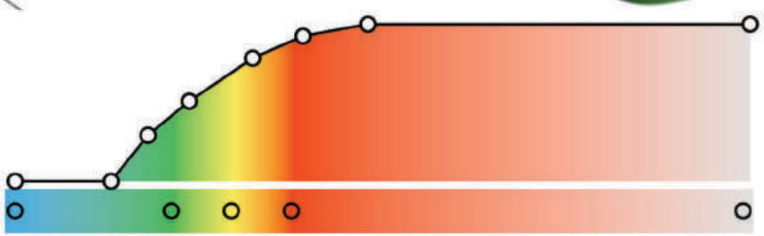




Direct volume rendering and isosurface rendering

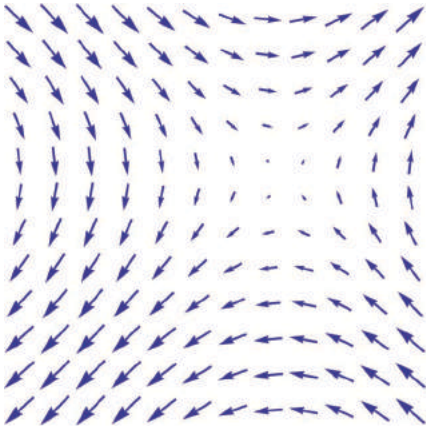


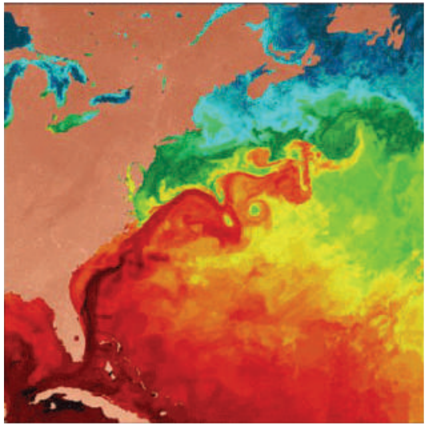
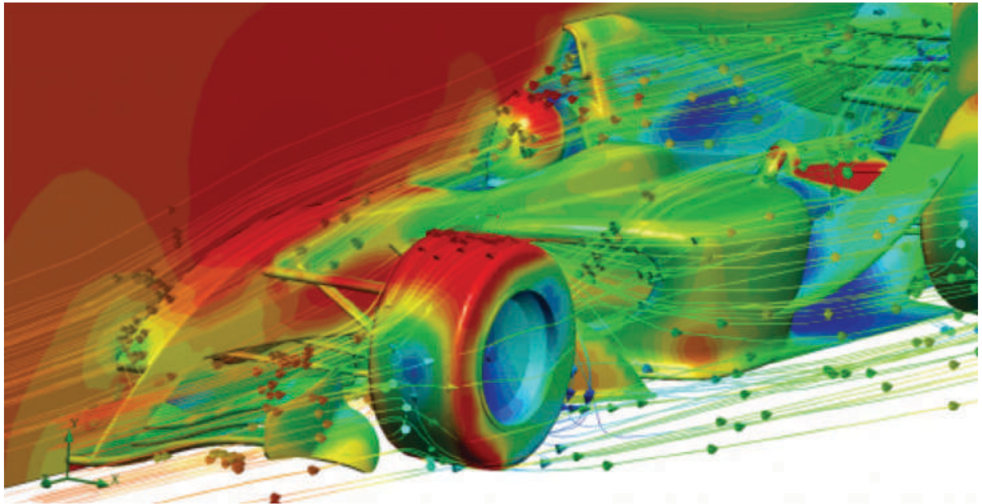




Transfer function

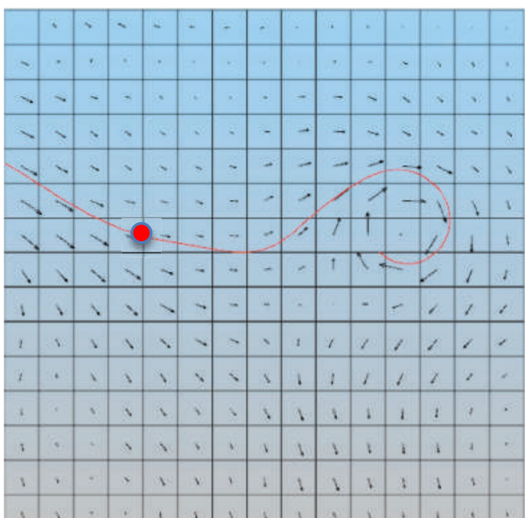
Vector fields

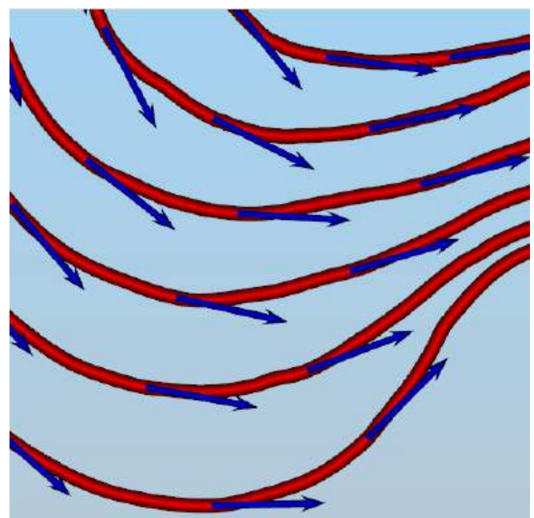


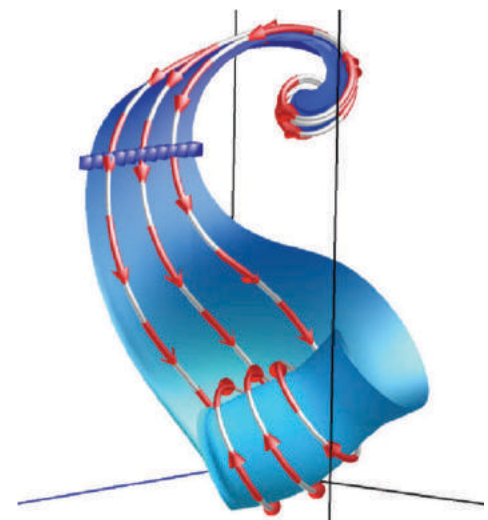




Streamlines and stream surfaces

- Streamlines are a family of curves that are instantaneously tangent to the velocity vector of the flow
- Show the trajectory a seed will travel in at any point in time
- Replace a seeding point with a seeding curve trace a stream surface

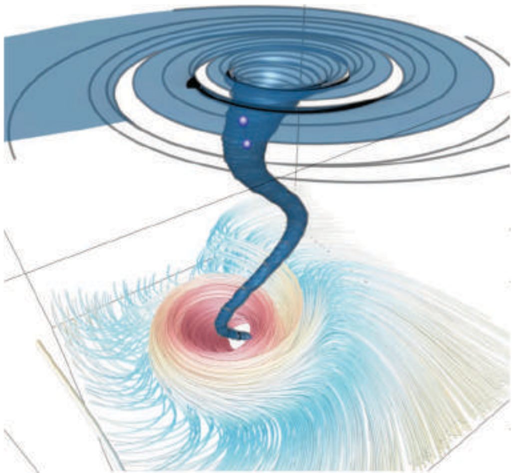


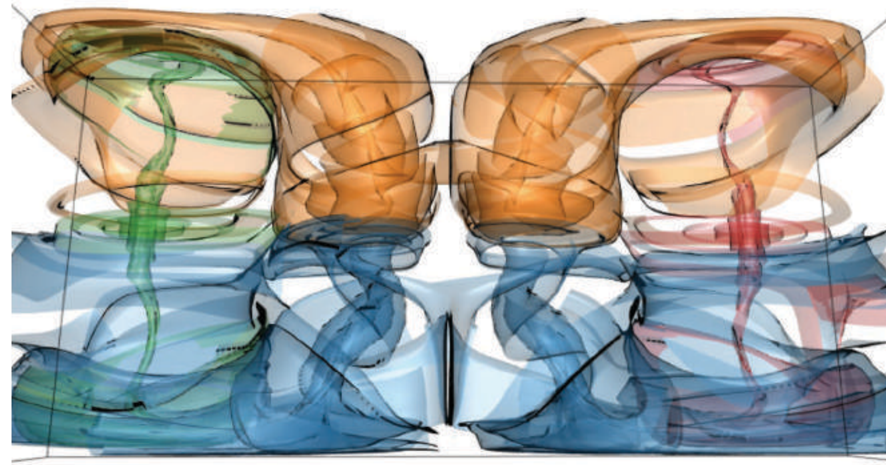


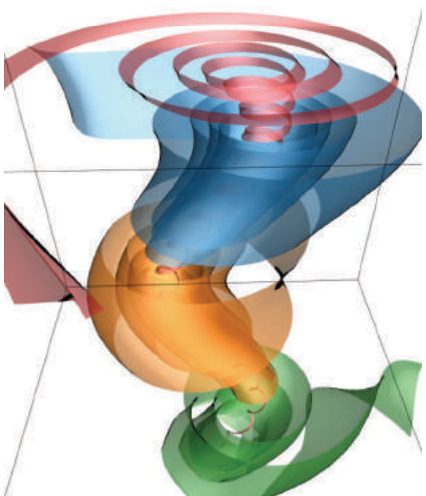


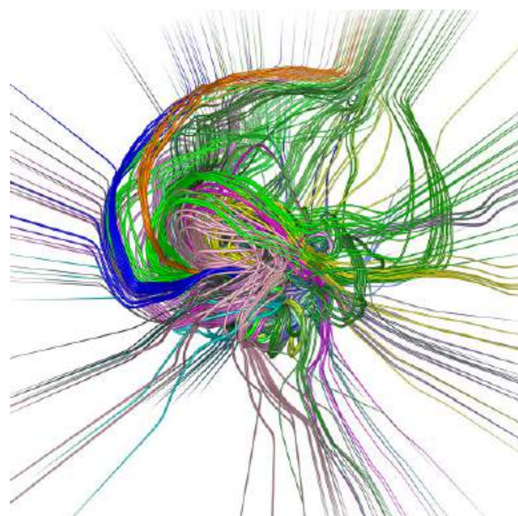
FlowVisual https://sites.nd.edu/chaoli-wang/flowvisual/

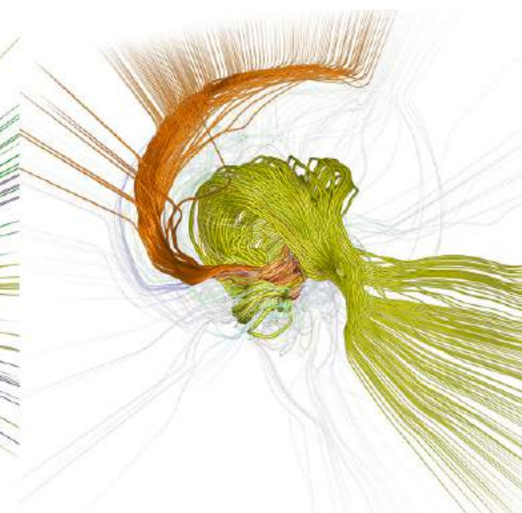
Examples of flow lines and surfaces



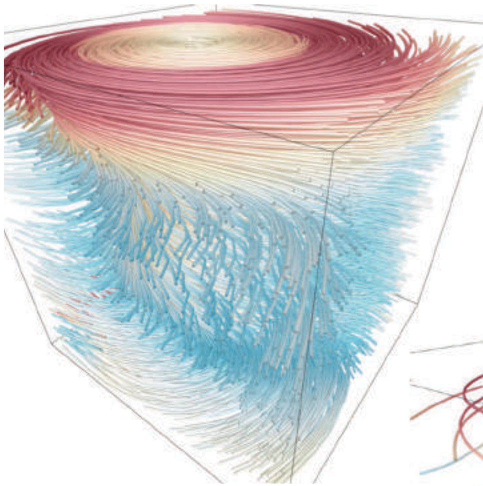


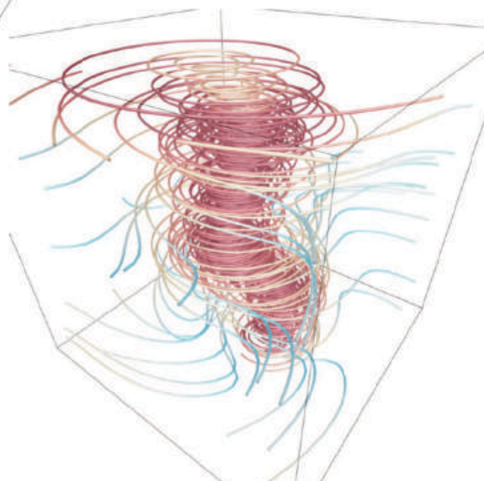


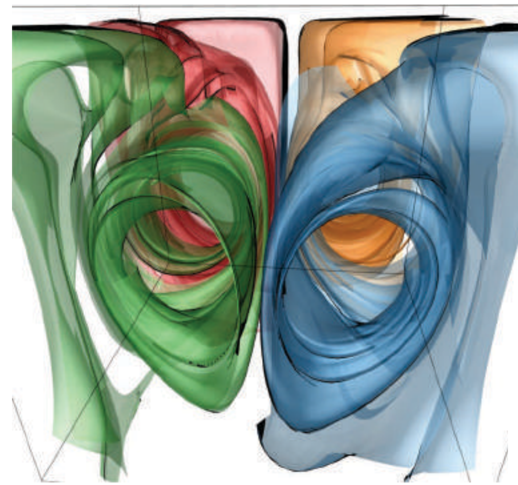




FlowNet





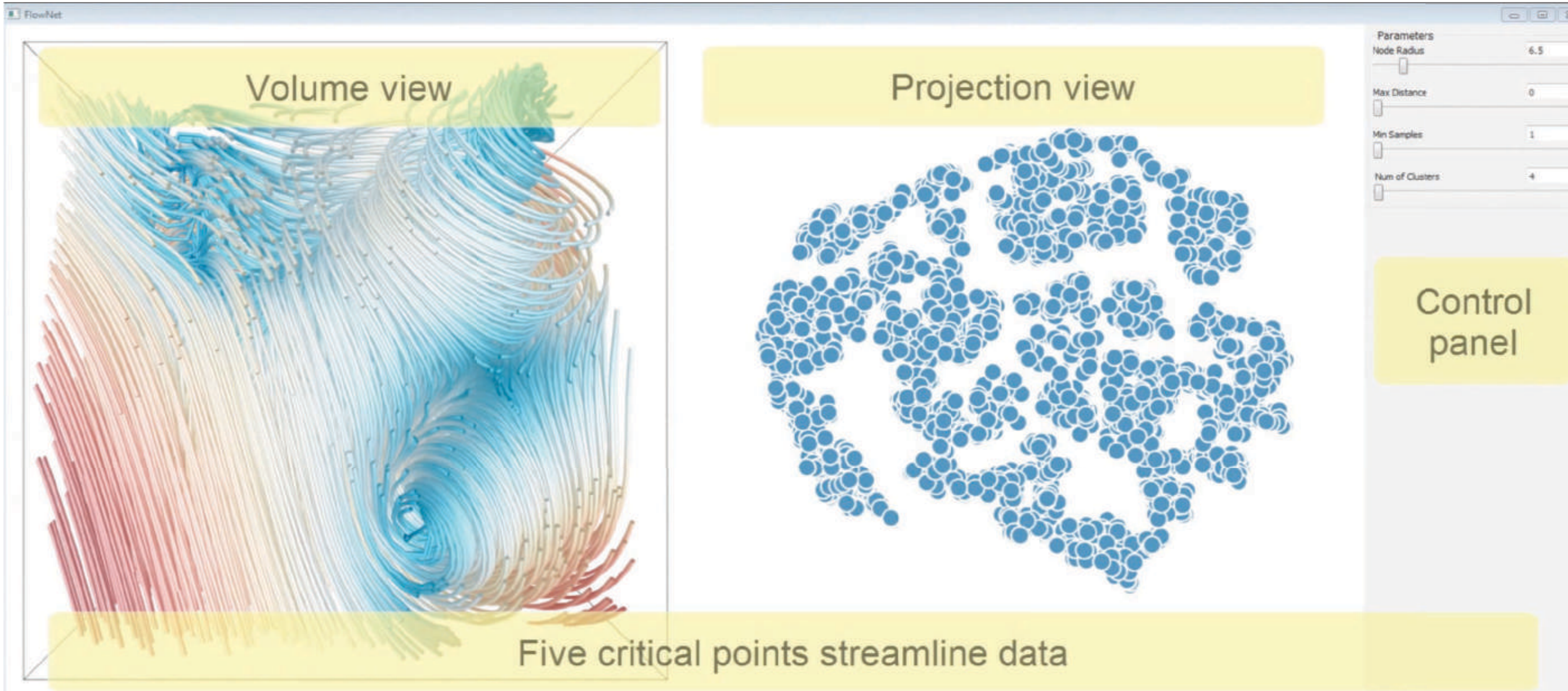


Jun Han, Jun Tao, and Chaoli Wang. FlowNet: A Deep Learning Framework for Clustering and Selection of Streamlines and Stream Surfaces. *IEEE Transactions on Visualization and Computer Graphics*, 26(4):1732-1744, 2020.

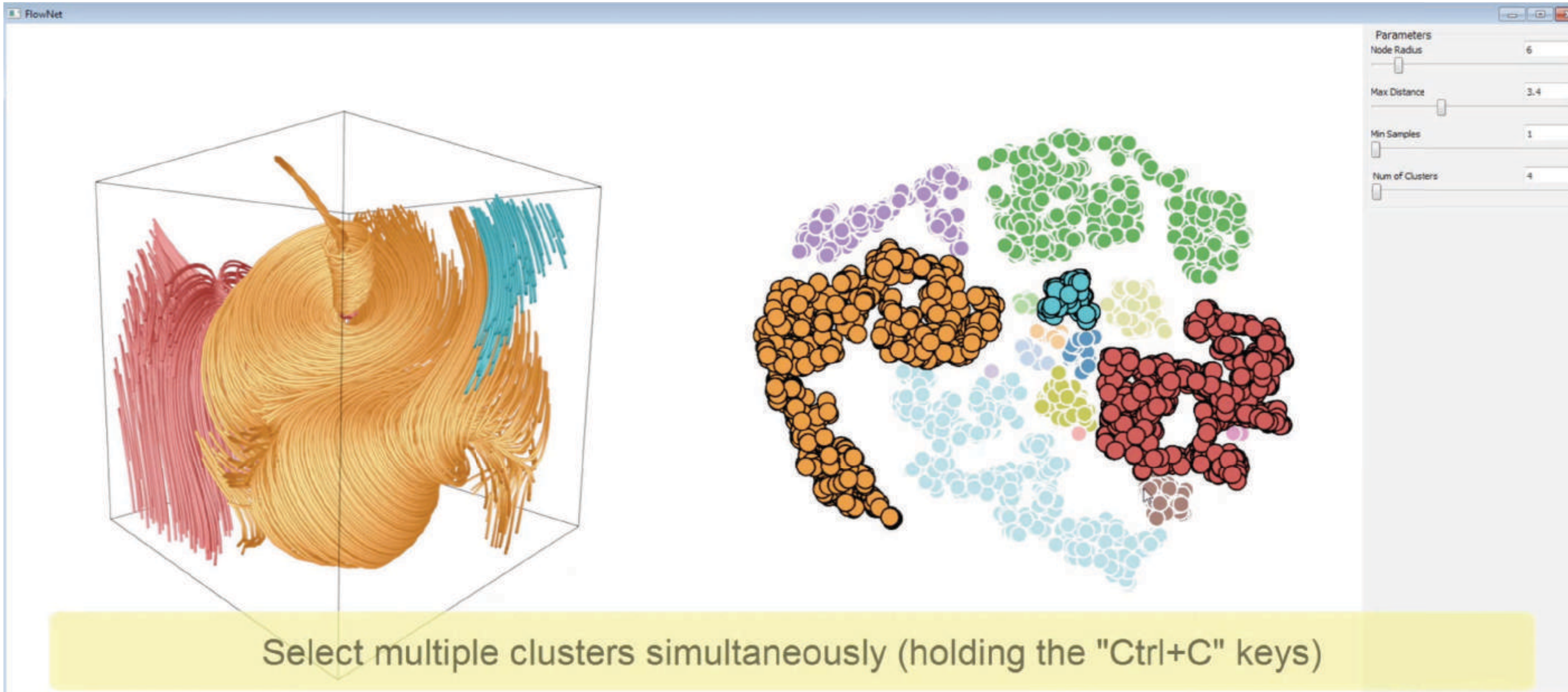
Outline of approach

- Goal
  - A single deep learning approach for identifying representative flow lines or flow surfaces
- Key ideas
  - Leverage an autoencoder to automatically learn line or surface feature descriptors
  - Apply dimensionality reduction and interactive clustering for exploration and selection

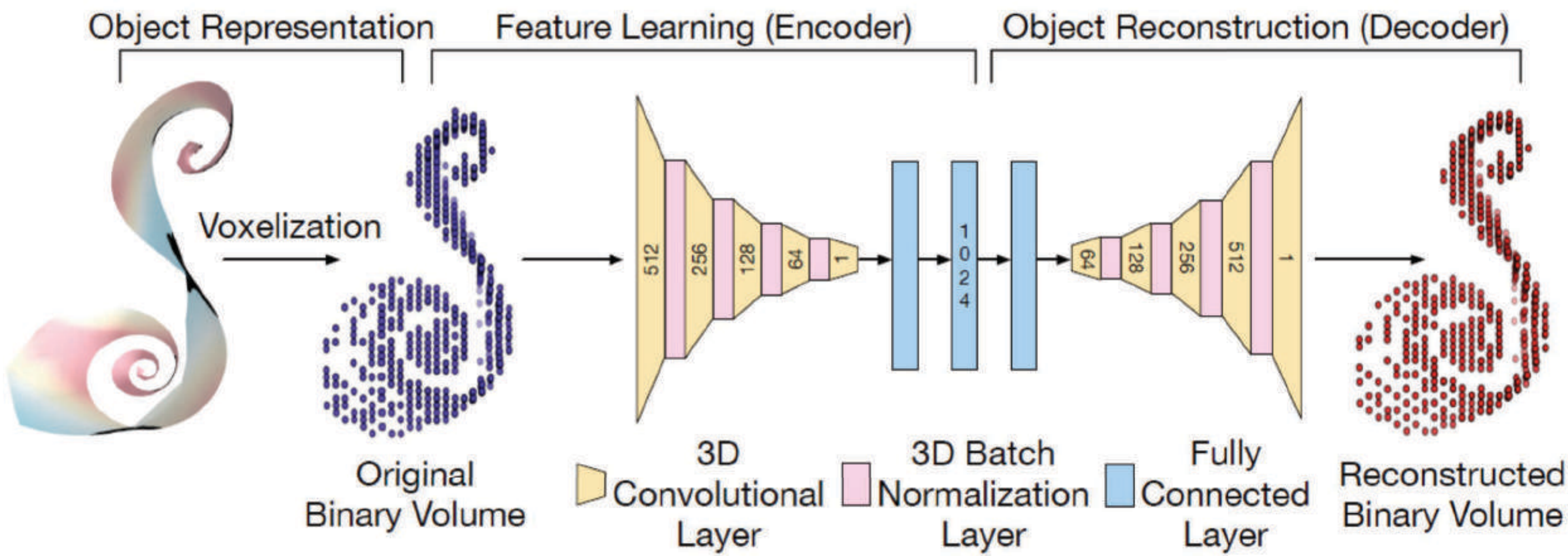
FlowNet user interface



Video demo


FlowNet
Parameters
Node Radius
6
Max Distance
3.4
Min Samples
1
Num of Clusters
4
Select multiple clusters simultaneously (holding the "Ctrl+C" keys)

FlowNet architecture

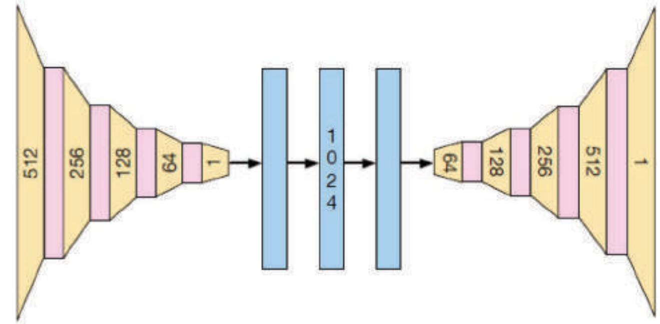


- Encoder-decoder framework
- 3D voxel-based binary representation as input
- Feature descriptor learning in the latent space

Why voxel-based approach?

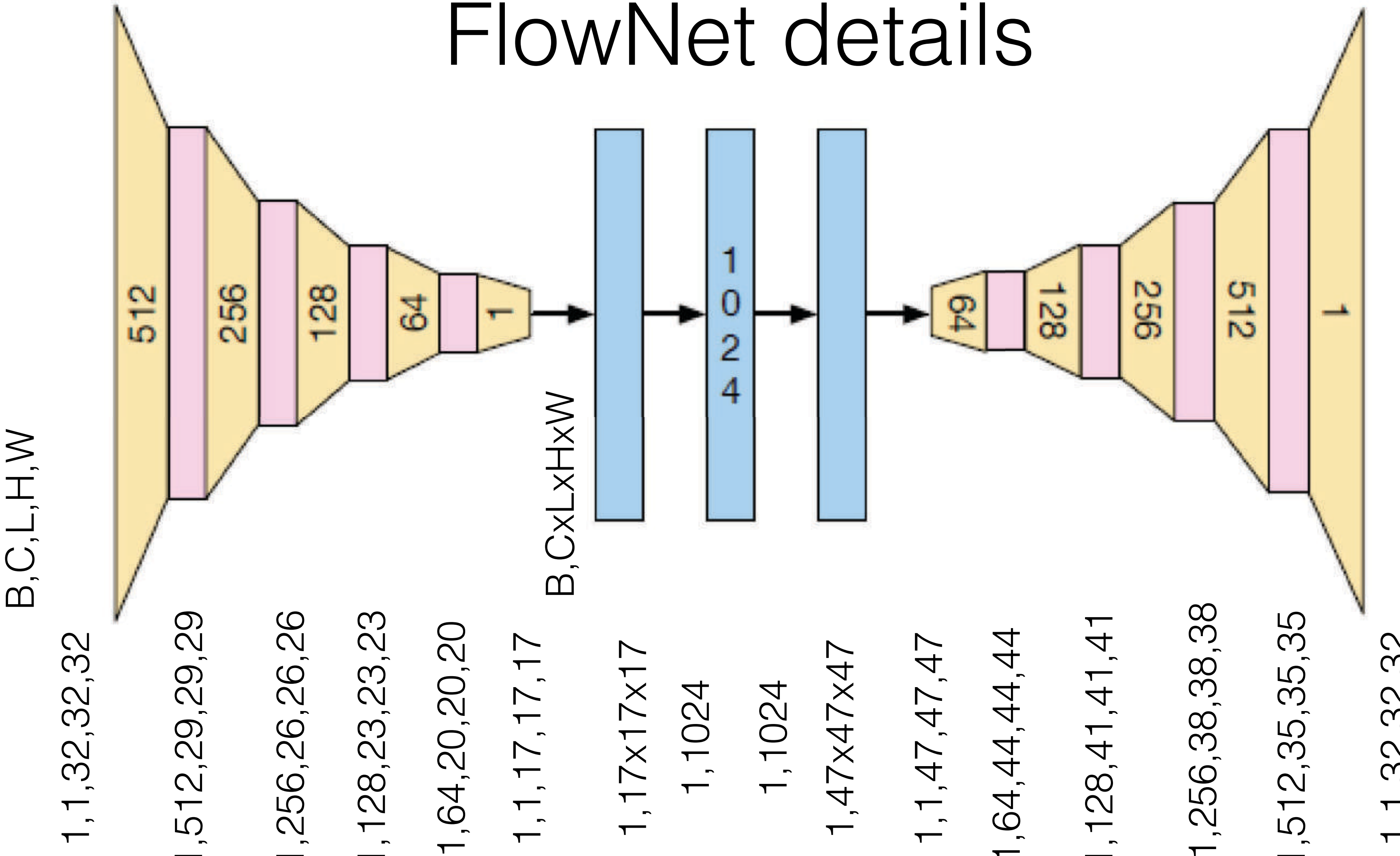
- Manifold-based
  - Suitable for 3D mesh manifold (genus zero or higher genus surface)
  - Does not work for flow lines or surfaces (non-closed)
- Multiview-based
  - Represent 3D shape with images rendered from different views
  - Flow surfaces could be severely self-occluded
- Voxel-based
  - No precise line or surface is required for loss function computation and reconstruction quality evaluation
  - Currently limited to a low resolution (e.g., 128^3)
  - Encode any 3D volumetric information (line, surface, volume)

FlowNet details



- The encoder consists of four convolutional (CONV) layers with batch normalization (BN) added in between, one CONV layer w/o BN, followed by two fully-connected layers
- The decoder consists of five CONV layers and four BN layers
- Apply the rectified linear unit (ReLU) at the hidden layers and the sigmoid function at the output layer
- Consider three loss functions: binary cross entropy, mean squared error (MSE), and Dice loss

FlowNet details



Dimensionality reduction and object clustering

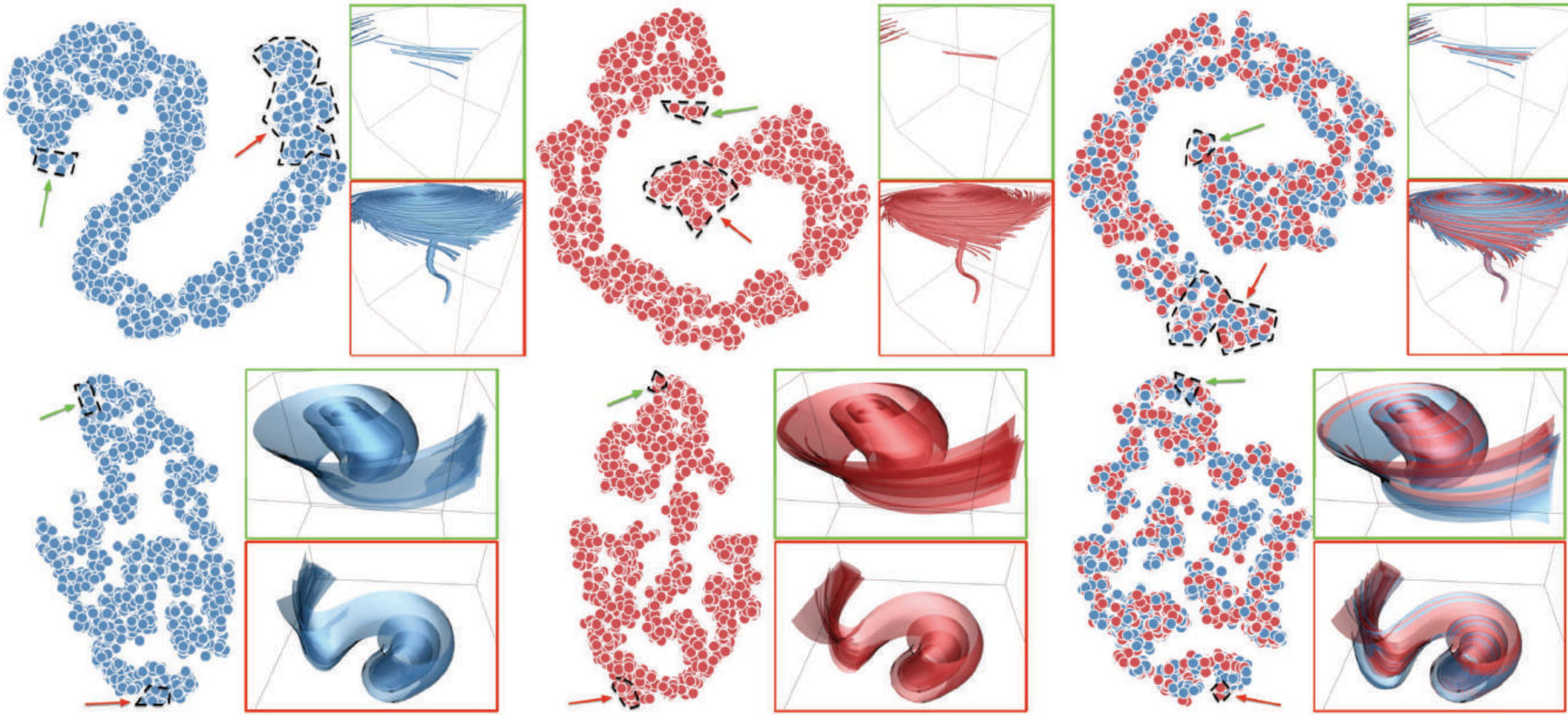
- Consider three dimensionality reduction methods: t-SNE (*neighborhood-preserving*), MDS and Isomap (*distance-preserving*)
- Consider three clustering methods: DBSCAN (*density-based*), k-means (*partition-based*), and agglomerative clustering (*hierarchy-based*)
- Finally choose t-SNE + DBSCAN
- Compare three distance measures: FlowNet feature Euclidean distance, streamline MCP distance, and streamline Hausdorff distance

Parameter setting and performance

Data Set	Original Dimension	Downsampled Dimension	Kernel Size	Training # Lines	Training F_1 Score	Testing # Lines	Testing F_1 Score
ABC	$51 \times 51 \times 51$	$51 \times 51 \times 51$	$3 \times 3 \times 3$	3,000	0.91	3,000	0.82
Bénard flow	$128 \times 32 \times 64$	$64 \times 16 \times 32$	$4 \times 1 \times 2$	3,000	0.87	3,000	0.80
car flow	$368 \times 234 \times 60$	$92 \times 59 \times 15$	$6 \times 4 \times 1$	3,000	0.81	3,000	0.69
computer room	$417 \times 345 \times 60$	$105 \times 87 \times 15$	$8 \times 6 \times 2$	3,000	0.74	3,000	0.68
crayfish	$322 \times 162 \times 119$	$81 \times 40 \times 30$	$4 \times 2 \times 2$	3,000	0.86	3,000	0.78
five critical pts	$51 \times 51 \times 51$	$51 \times 51 \times 51$	$3 \times 3 \times 3$	3,000	0.96	3,000	0.72
solar plume	$126 \times 126 \times 512$	$32 \times 32 \times 128$	$2 \times 2 \times 8$	4,000	0.83	4,000	0.76
square cylinder	$192 \times 64 \times 48$	$96 \times 32 \times 24$	$8 \times 3 \times 2$	3,000	0.84	3,000	0.72
supernova	$100 \times 100 \times 100$	$50 \times 50 \times 50$	$2 \times 2 \times 2$	3,000	0.86	3,000	0.75
tornado	$64 \times 64 \times 64$	$50 \times 50 \times 50$	$3 \times 3 \times 3$	3,000	0.91	3,000	0.76
two swirls	$64 \times 64 \times 64$	$32 \times 32 \times 32$	$4 \times 4 \times 4$	3,000	0.88	3,000	0.75

Data Set	Original Dimension	Downsampled Dimension	Kernel Size	Training # Surfaces	Training F_1 Score	Testing # Surfaces	Testing F_1 Score
ABC	$51 \times 51 \times 51$	$51 \times 51 \times 51$	$3 \times 3 \times 3$	2,000	0.84	2,000	0.71
Bénard flow	$128 \times 32 \times 64$	$64 \times 16 \times 32$	$4 \times 1 \times 2$	2,000	0.84	2,000	0.79
car flow	$368 \times 234 \times 60$	$92 \times 59 \times 15$	$6 \times 4 \times 1$				
computer room	$417 \times 345 \times 60$	$105 \times 87 \times 15$	$8 \times 6 \times 2$	2,000	0.83	2,000	0.59
crayfish	$322 \times 162 \times 119$	$81 \times 40 \times 30$	$4 \times 2 \times 2$				
five critical pts	$51 \times 51 \times 51$	$51 \times 51 \times 51$	$3 \times 3 \times 3$	2,000	0.72	2,000	0.57
solar plume	$126 \times 126 \times 512$	$32 \times 32 \times 128$	$2 \times 2 \times 8$	1,000	0.84	1,000	0.57
square cylinder	$192 \times 64 \times 48$	$96 \times 32 \times 24$	$8 \times 3 \times 2$	2,000	0.91	2,000	0.86
supernova	$100 \times 100 \times 100$	$50 \times 50 \times 50$	$2 \times 2 \times 2$				
tornado	$64 \times 64 \times 64$	$50 \times 50 \times 50$	$3 \times 3 \times 3$	2,000	0.88	2,000	0.78
two swirls	$64 \times 64 \times 64$	$32 \times 32 \times 32$	$4 \times 4 \times 4$	2,000	0.91	2,000	0.81

Qualitative evaluation


Training set only　　Test set only　　Training set + test set

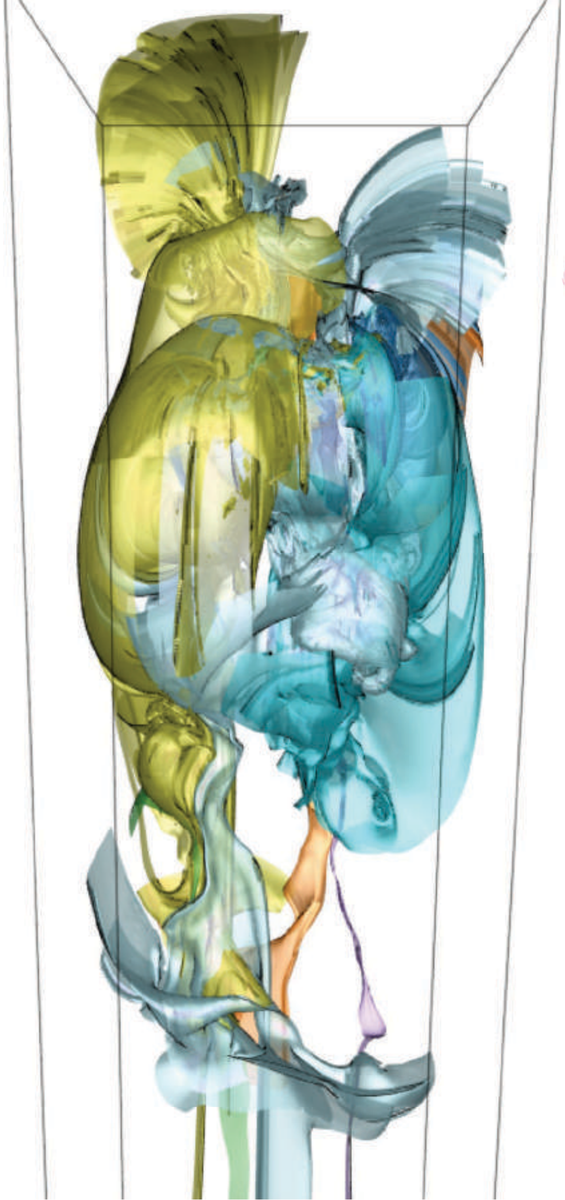
Quantitative evaluation

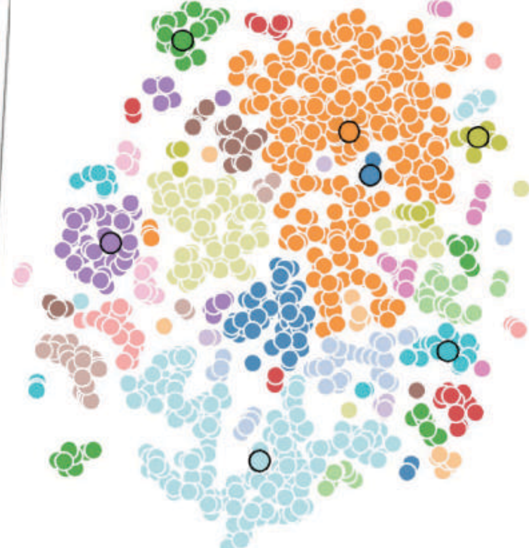
Data Set	# Lines	PSNR (db)				
		Ours	$p(s)$	$I(s;V)$	REP	Xu's
crayfish	70	**30.94**	30.84	30.91	30.02	28.97
solar plume	100	30.68	30.37	30.07	**30.75**	15.78
five critical pts	140	**26.25**	21.23	21.13	25.50	20.16
tornado	60	**29.74**	28.12	29.44	29.13	28.30
two swirls	80	**36.35**	36.30	34.55	36.21	27.72

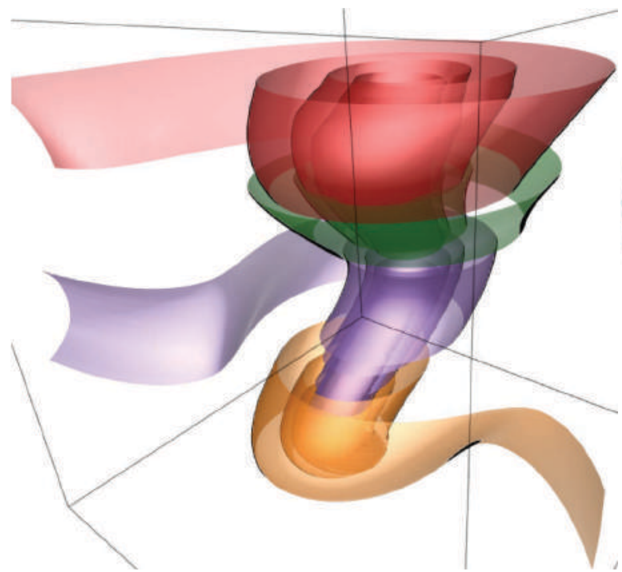
Data Set	# Lines	AAD				
		Ours	$p(s)$	$I(s;V)$	REP	Xu's
crayfish	70	**0.102**	0.105	0.103	0.116	0.144
solar plume	100	0.283	0.309	0.286	**0.280**	0.303
five critical pts	140	**0.023**	0.031	0.036	0.026	0.031
tornado	60	**0.080**	0.167	0.116	0.105	0.101
two swirls	80	**0.065**	0.066	0.079	0.070	0.071

- Use representative streamlines to reconstruct the vector field using gradient vector flow (GVF)

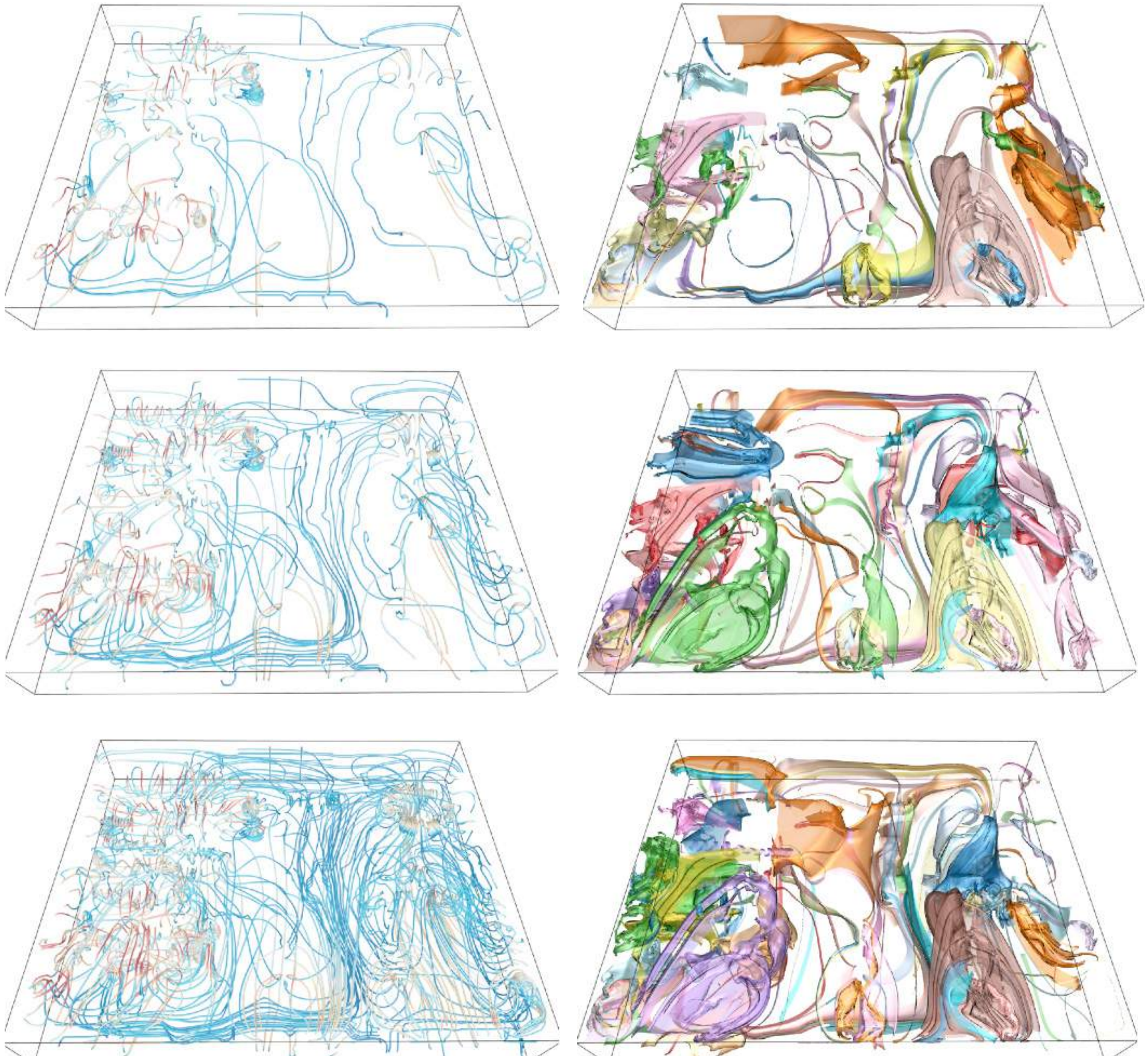
FlowNet results

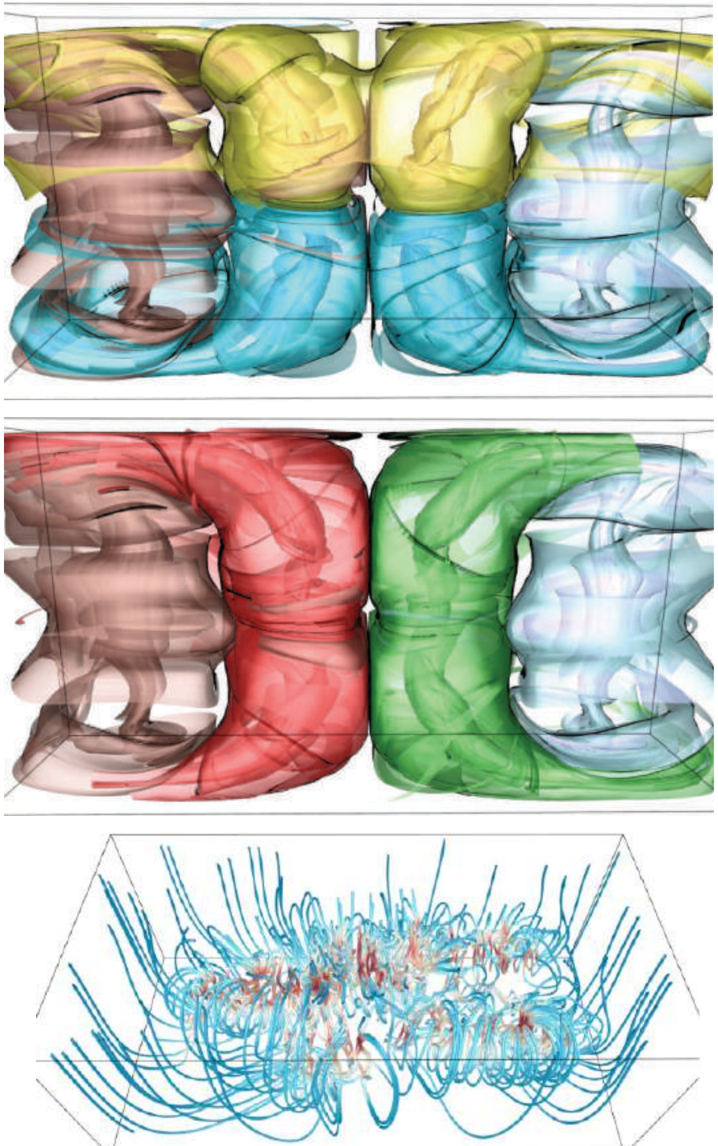




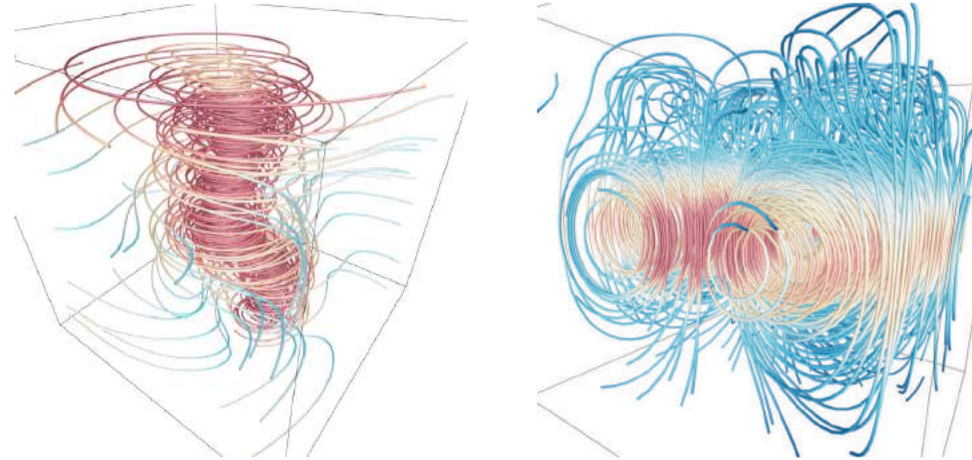


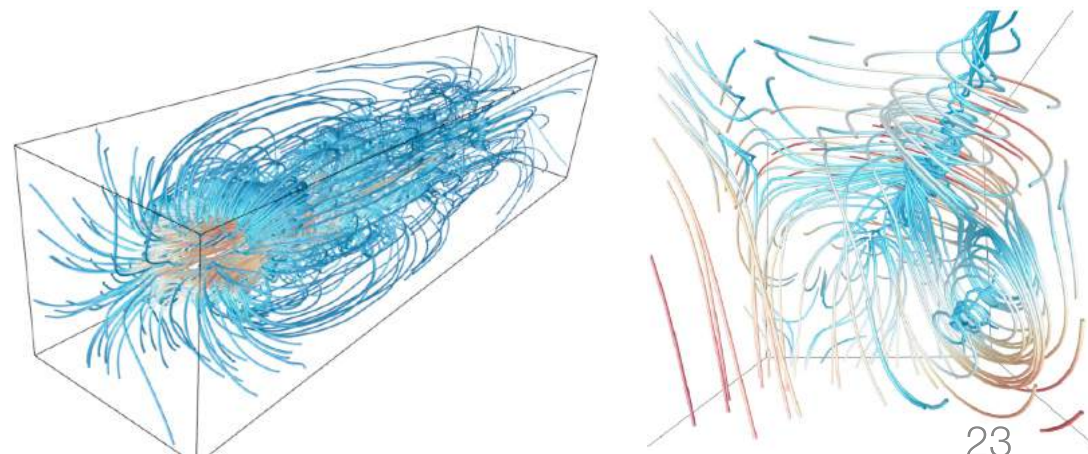
FlowNet results



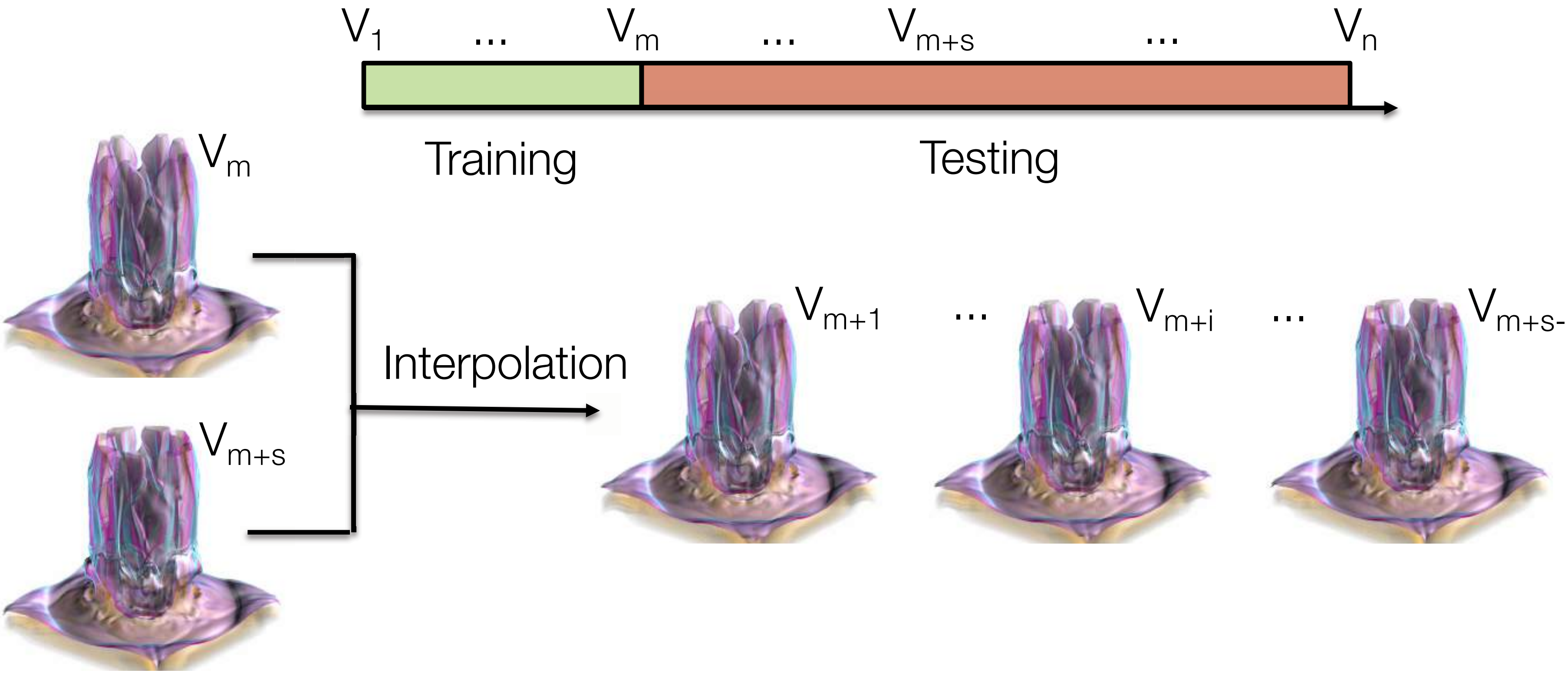


FlowNet results





TSR-TVD

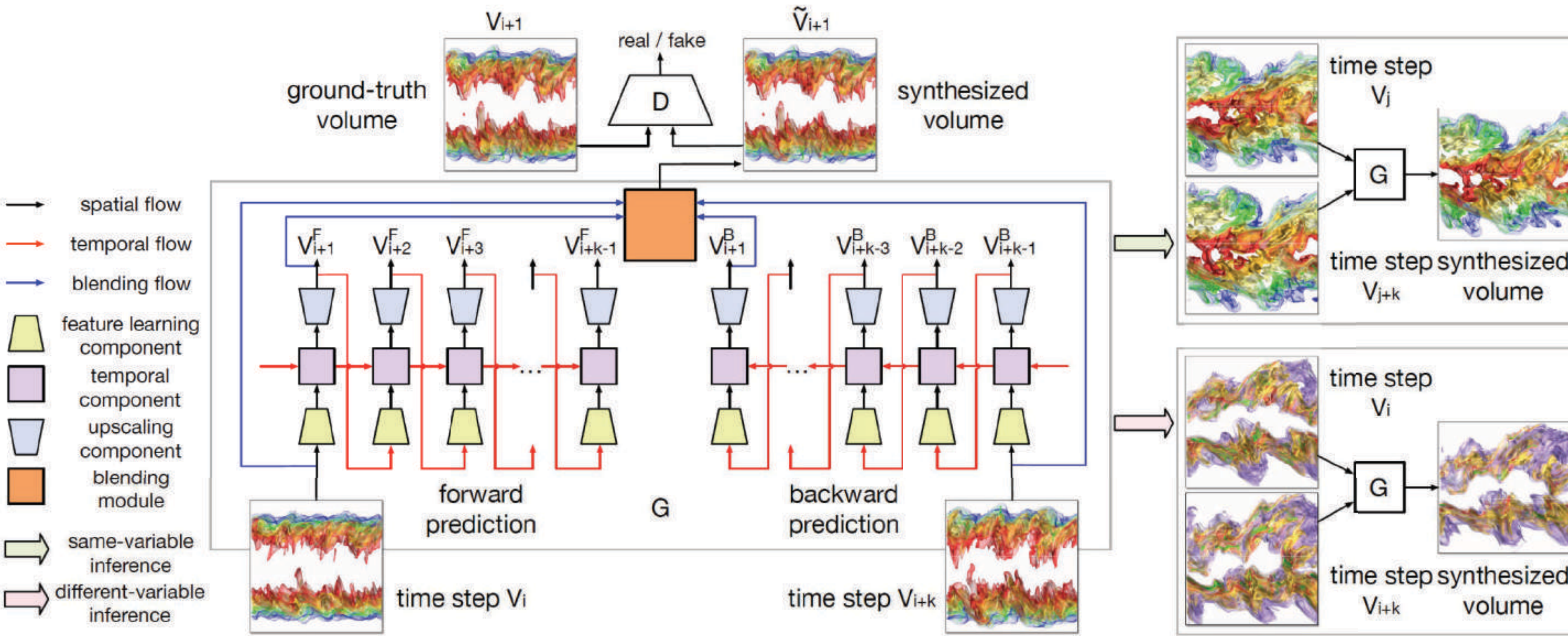


Jun Han and Chaoli Wang. TSR-TVD: Temporal Super-Resolution for Time-Varying Data Analysis and Visualization. *IEEE Transactions on Visualization and Computer Graphics*, 26(1):205-215, 2020.

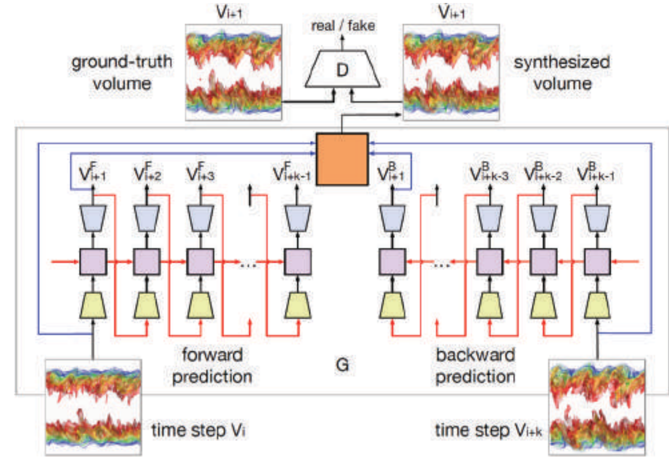
Outline of approach

- Goal
  - Generation of temporal super-resolution (TSR) of time-varying data (TVD)
- Key idea
  - Leverage a recurrent generative network, a combination of recurrent neural network (RNN) and generative adversarial network (GAN) to generate temporal high-resolution volume sequences

TSR-TVD architecture

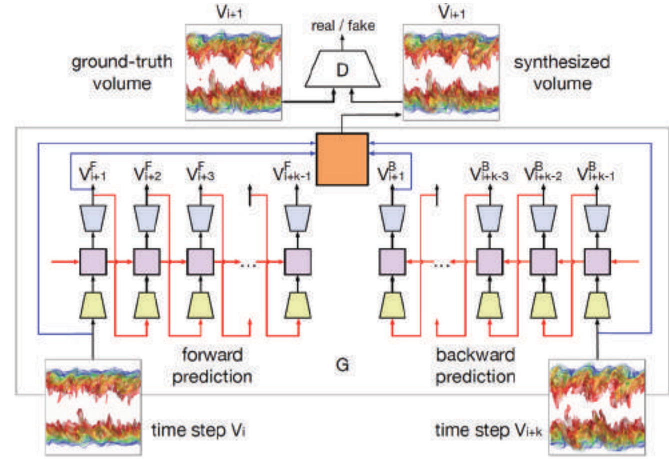


Generator and discriminator

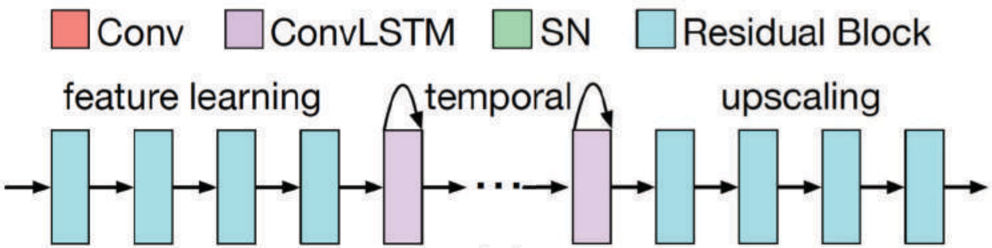


- Generator *G* consists of the predicting and blending modules
  - Predicting module produces a forward prediction V^F through V_i and a backward prediction V^B through V_{i+k}
  - Blending module takes V_i, V_{i+k}, V^F, and V^B that share the same time step as input and outputs the synthesized volume
- Discriminator *D* distinguishes the synthesized volume from the ground-truth volume

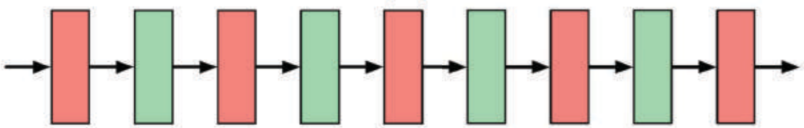
Architecture details



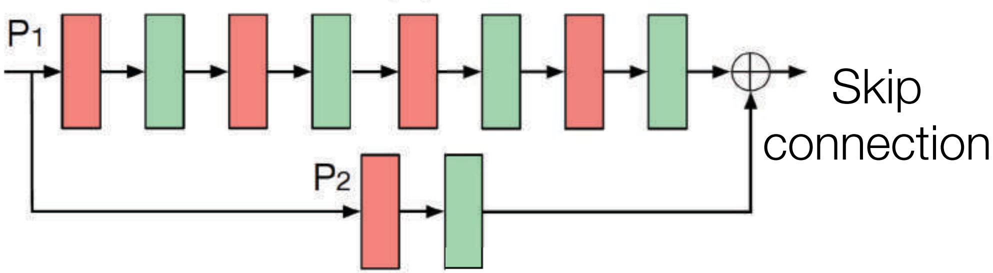
Predicting module in *G*



(a)


(b)

Network architecture of *D*



(c)

Residual block

Loss function

- Adversarial loss that trains *G* with the goal of fooling *D*
- Volumetric loss that mixes the adversarial loss with a more traditional loss, such as L_2 distance
- Feature loss that constrains *G* to produce natural statics at multiple scales

Quantitative evaluation

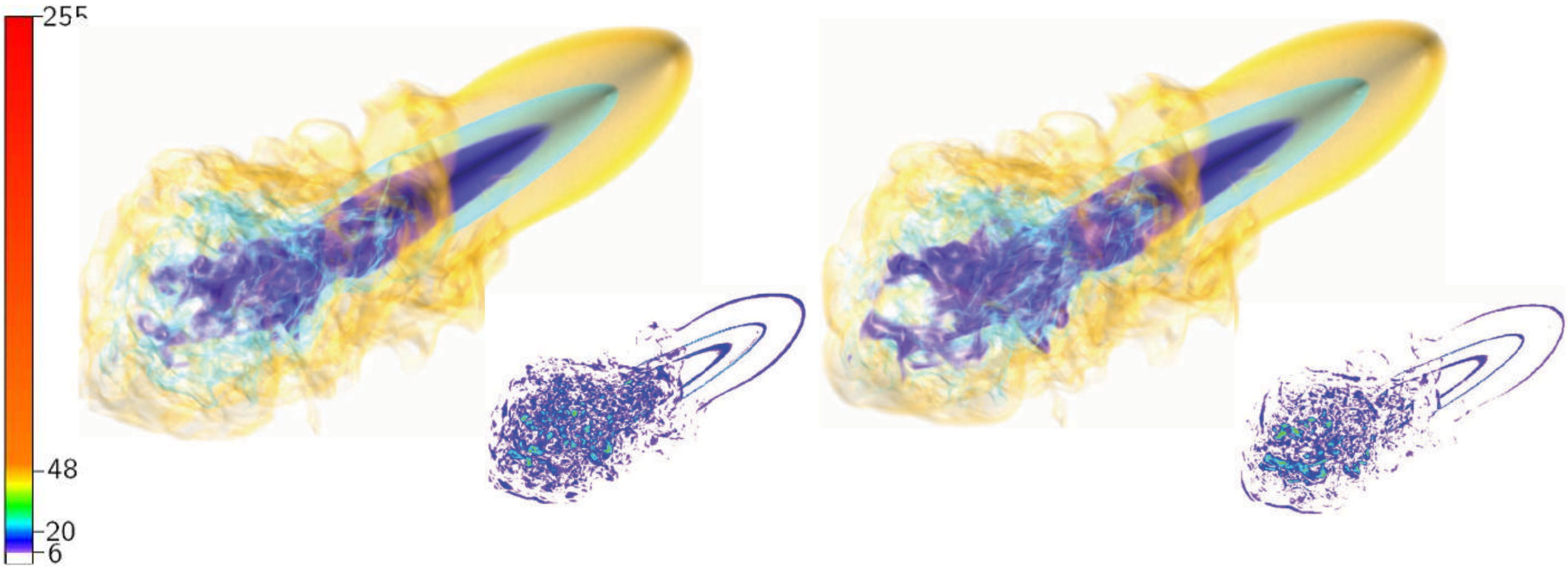
data set (variable)	LERP	PSNR (dB) RNN	CNN	TSR	LERP	SSIM RNN	CNN	TSR
combustion (HR)	25.61	**26.13**	25.72	25.81	0.66	0.70	0.69	**0.72**
combustion (MF)	25.12	**25.86**	25.43	25.62	0.71	0.73	0.73	**0.74**
supernova (E)	22.34	**24.31**	23.81	23.74	0.61	0.64	0.63	**0.66**
vortex	26.62	**27.42**	26.85	26.90	0.73	0.75	0.75	**0.75**

Table 3. Comparison of average IS values at selected isovalues.

	LERP		TSR-TVD	
data set (variable)	$v = 0$	$v = 0.176$	$v = 0$	$v = 0.176$
supernova (E)	0.56	0.24	**0.71**	**0.68**
	$v = 0.255$	$v = 0.569$	$v = 0.255$	$v = 0.569$
combustion (HR)	0.65	0.59	**0.73**	**0.72**

- PNSR at data-level, SSIM at image-level, and IS at feature-level

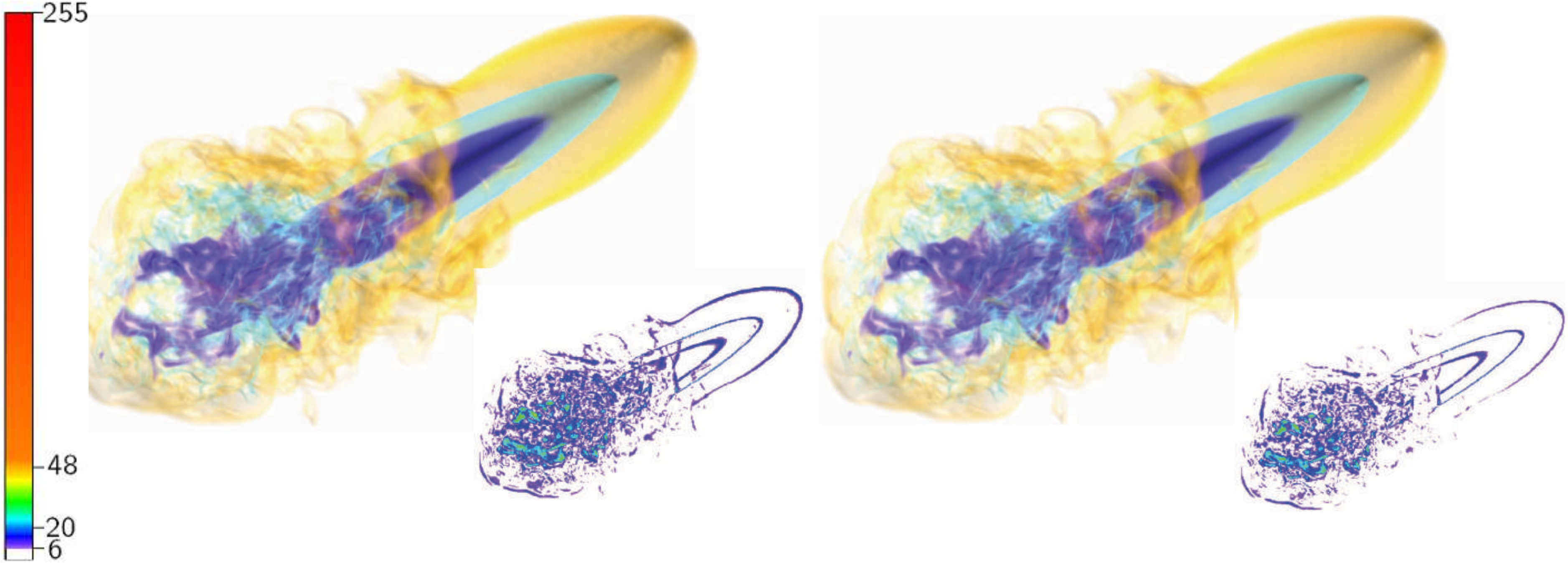
Qualitative analysis (solar plume)



Linear interpolation

TSR-TVD

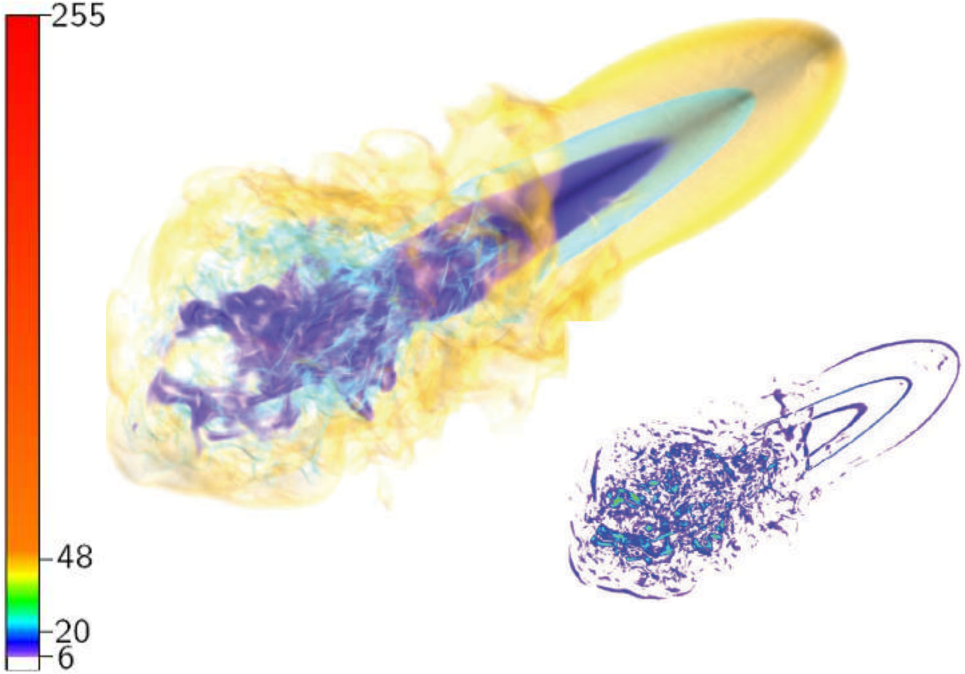
Qualitative analysis (solar plume)



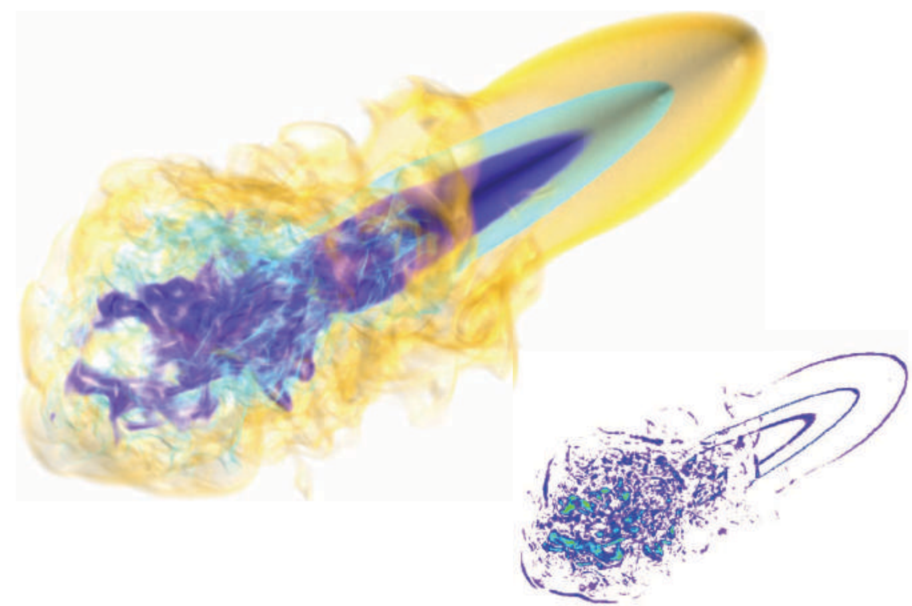
RNN

TSR-TVD

Qualitative analysis (solar plume)

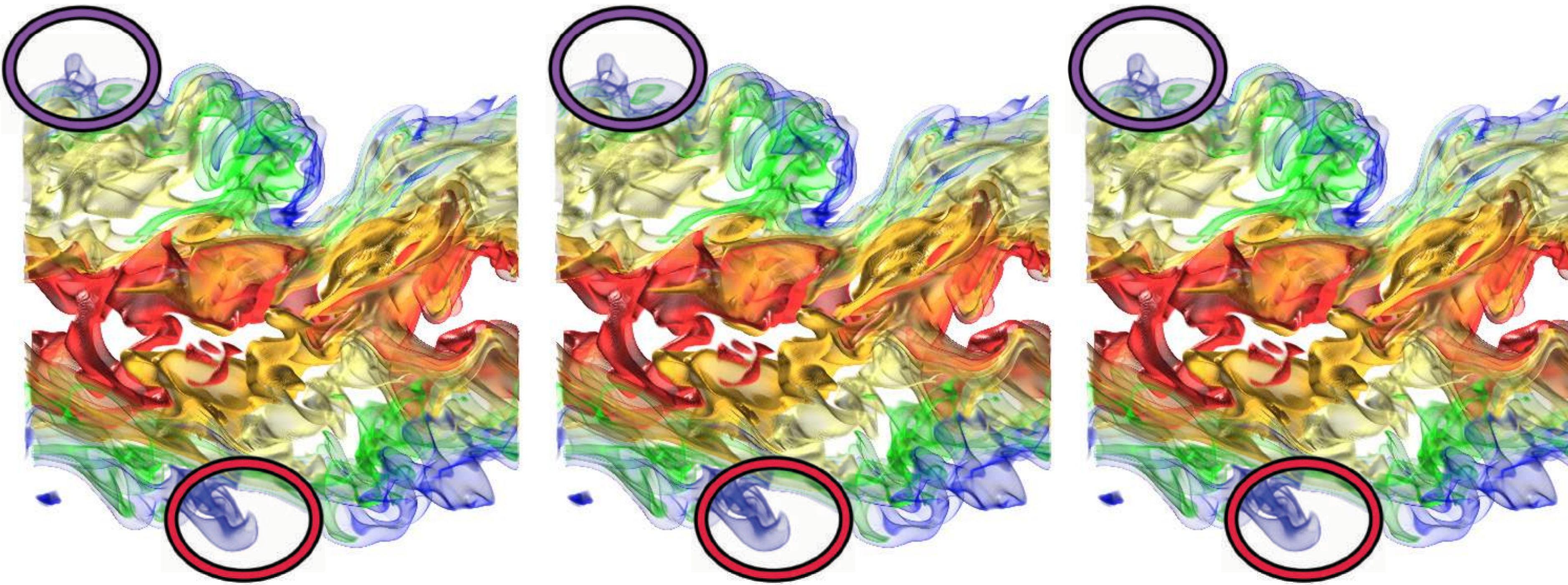


CNN



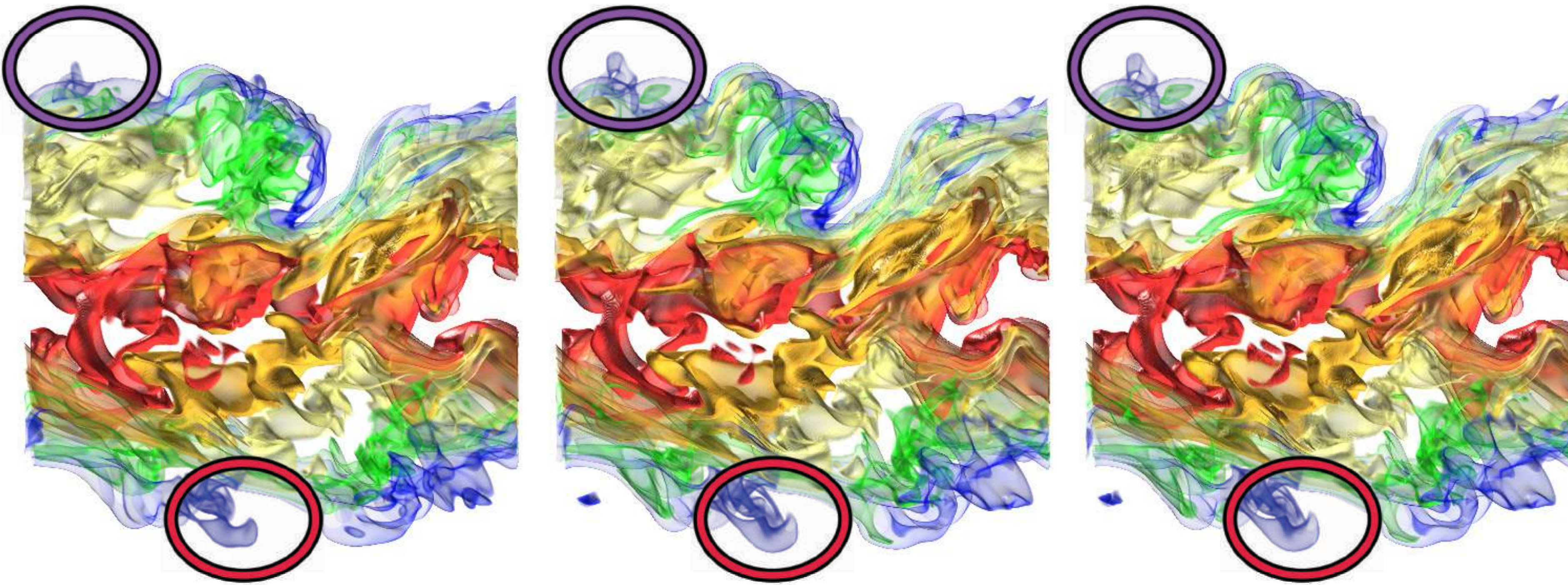
TSR-TVD

Qualitative analysis (combustion, MF)



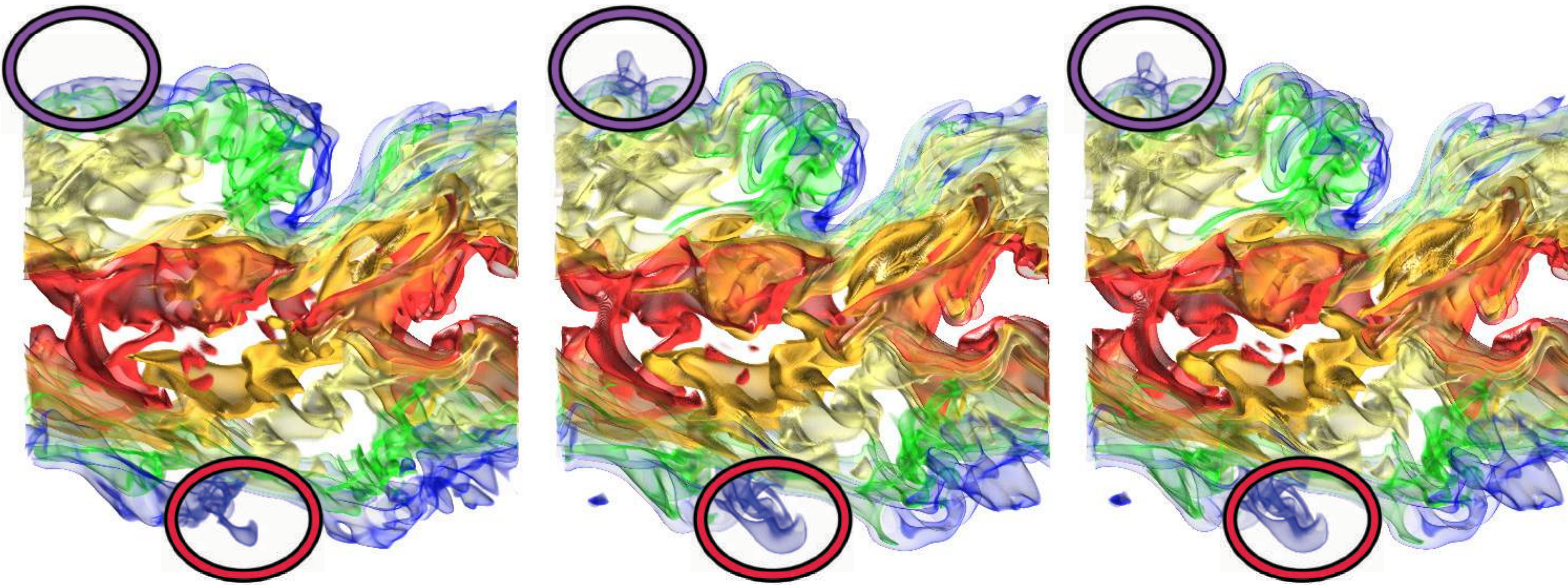
Linear interpolation | Ground truth | TSR-TVD

Qualitative analysis (combustion, MF)



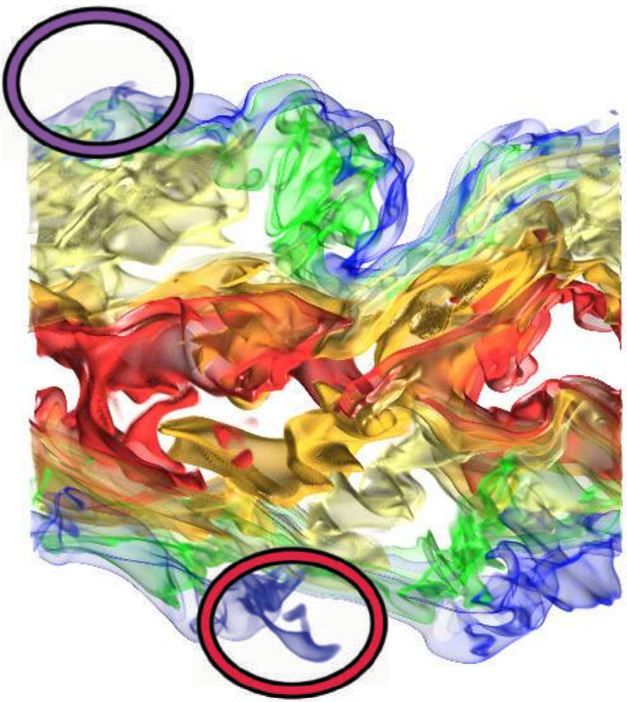
Linear interpolation | Ground truth | TSR-TVD

Qualitative analysis (combustion, MF)

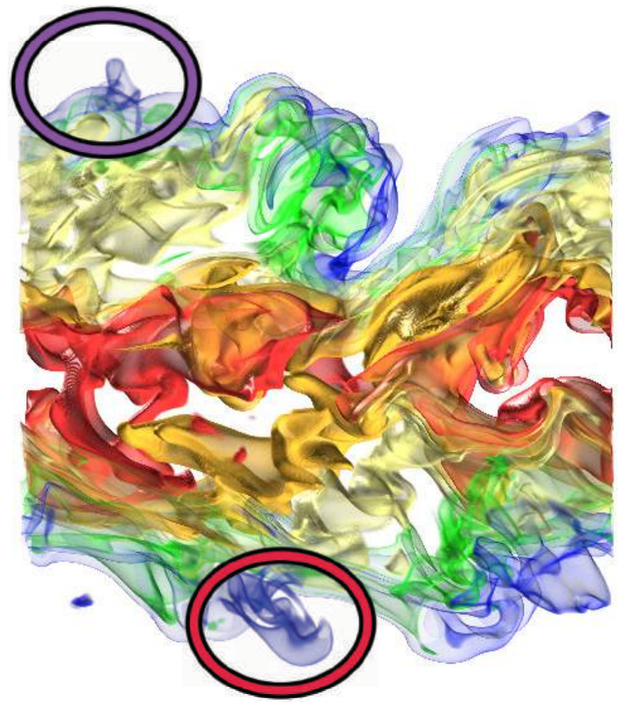


Linear interpolation　　Ground truth　　TSR-TVD

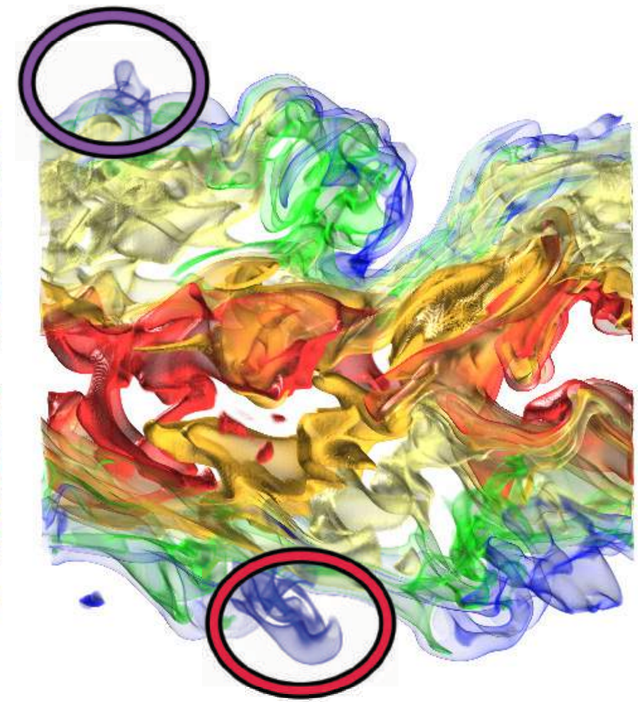
Qualitative analysis (combustion, MF)



Linear interpolation

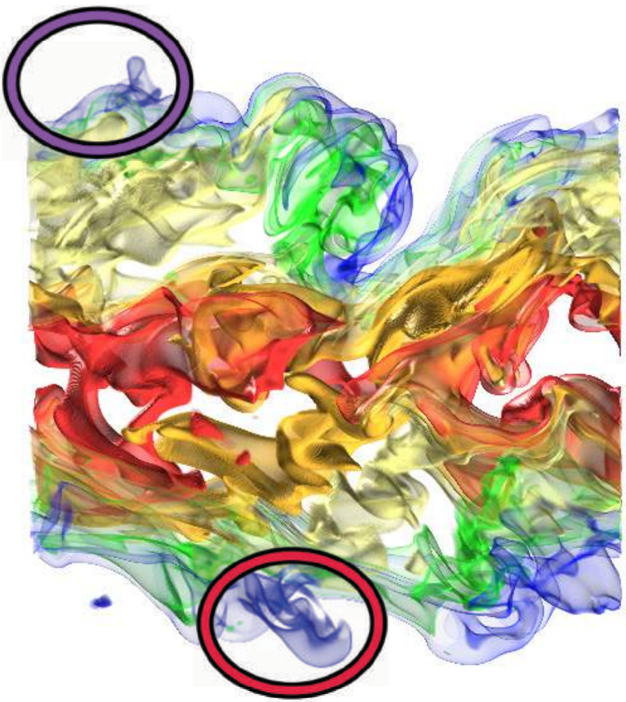


Ground truth

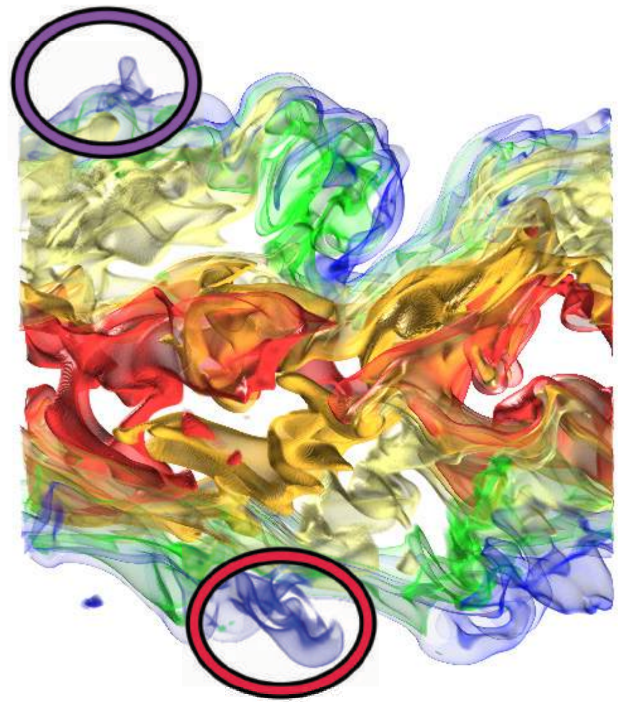


TSR-TVD

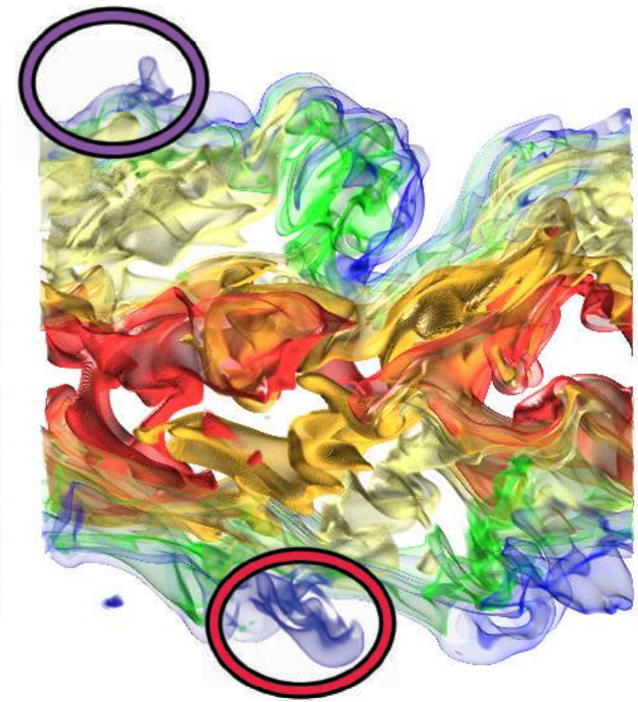
Qualitative analysis (combustion, MF)



Linear interpolation

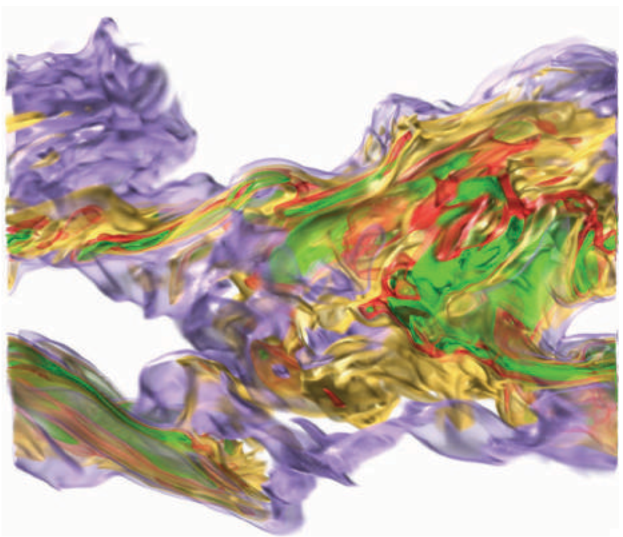


Ground truth

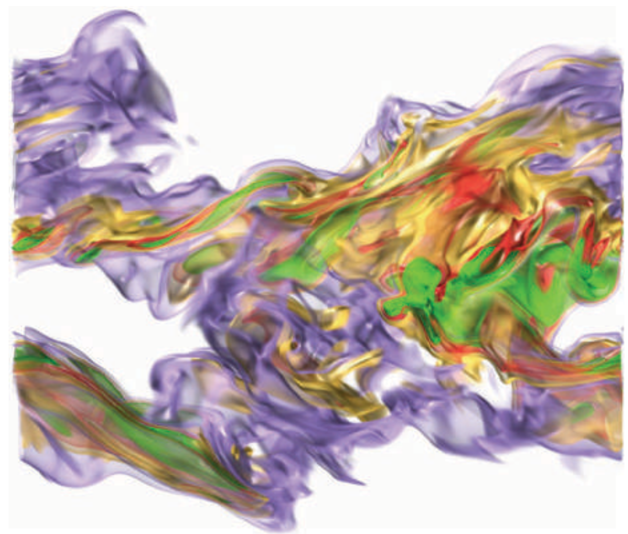


TSR-TVD

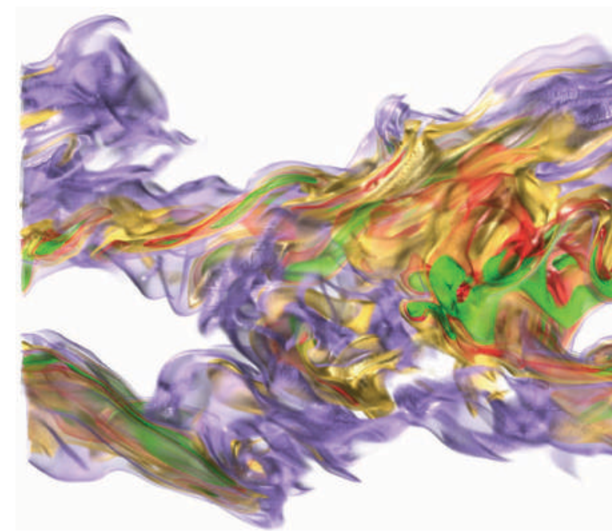
Qualitative analysis (combustion, MF→HR)



Linear interpolation



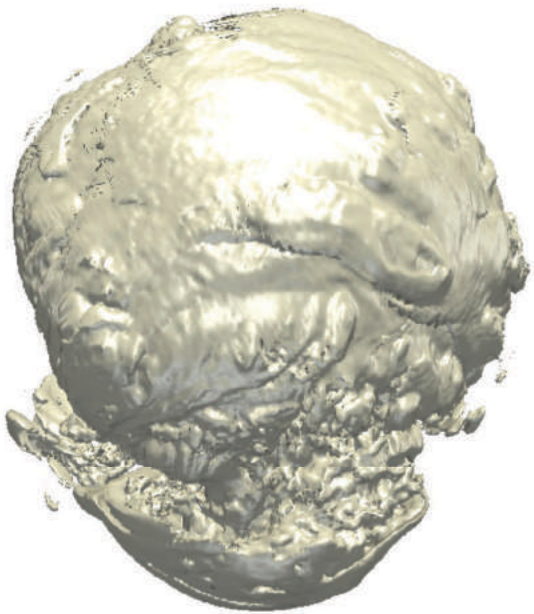
Ground truth



TSR-TVD

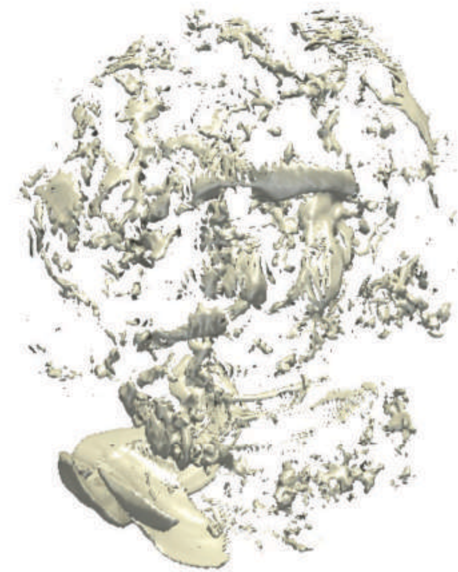
Comparison of LERP and TSR-TVD of volueme rendering
using the combustion data set.

Qualitative analysis (supernova, entropy, v=0.176)



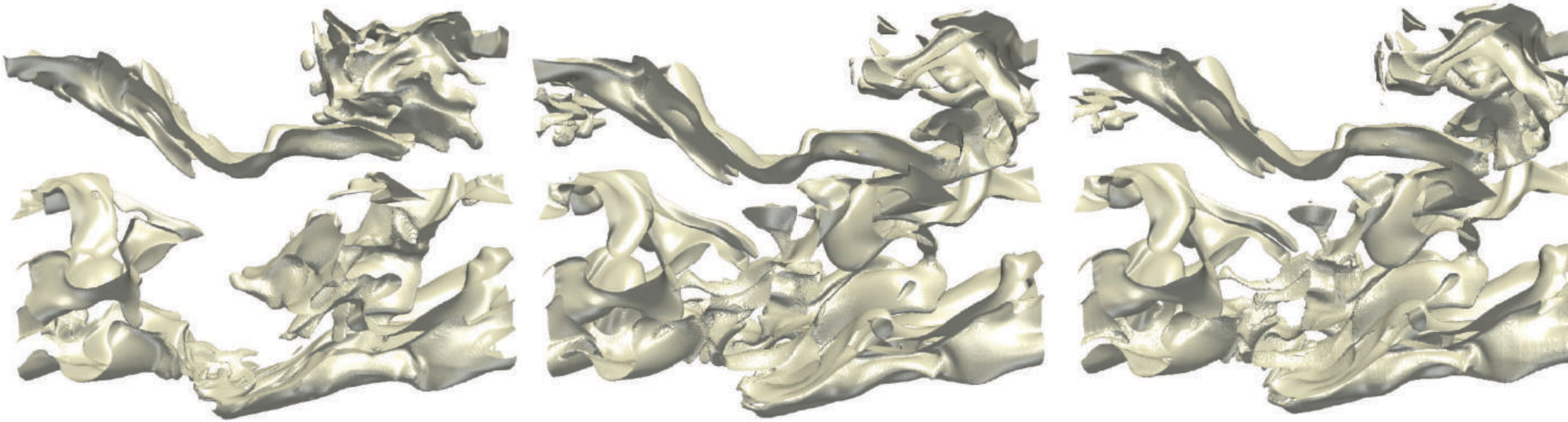
Linear interpolation

Ground truth



TSR-TVD

Qualitative analysis (combustion, HR, v=0.569)

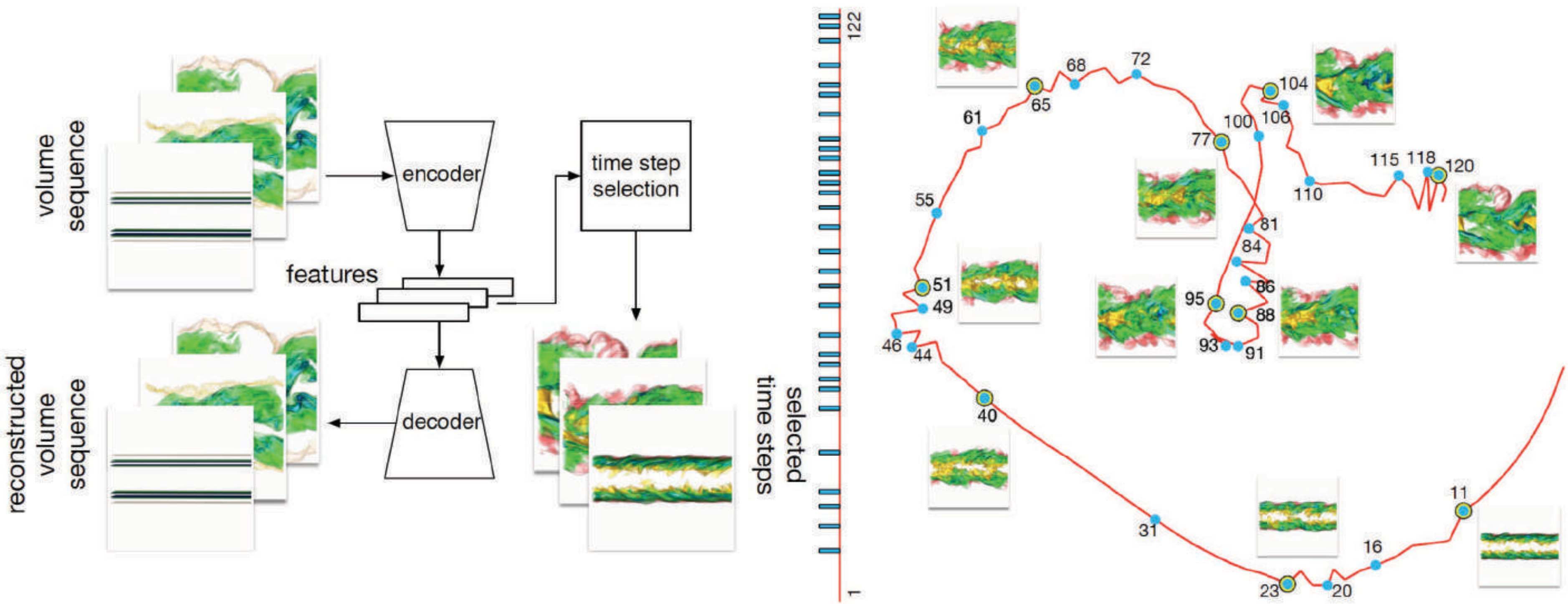


Linear interpolation Ground truth TSR-TVD

Comparison of LERP and TSR-TVD of isosurface rendering using the combustion (heat release) data set.

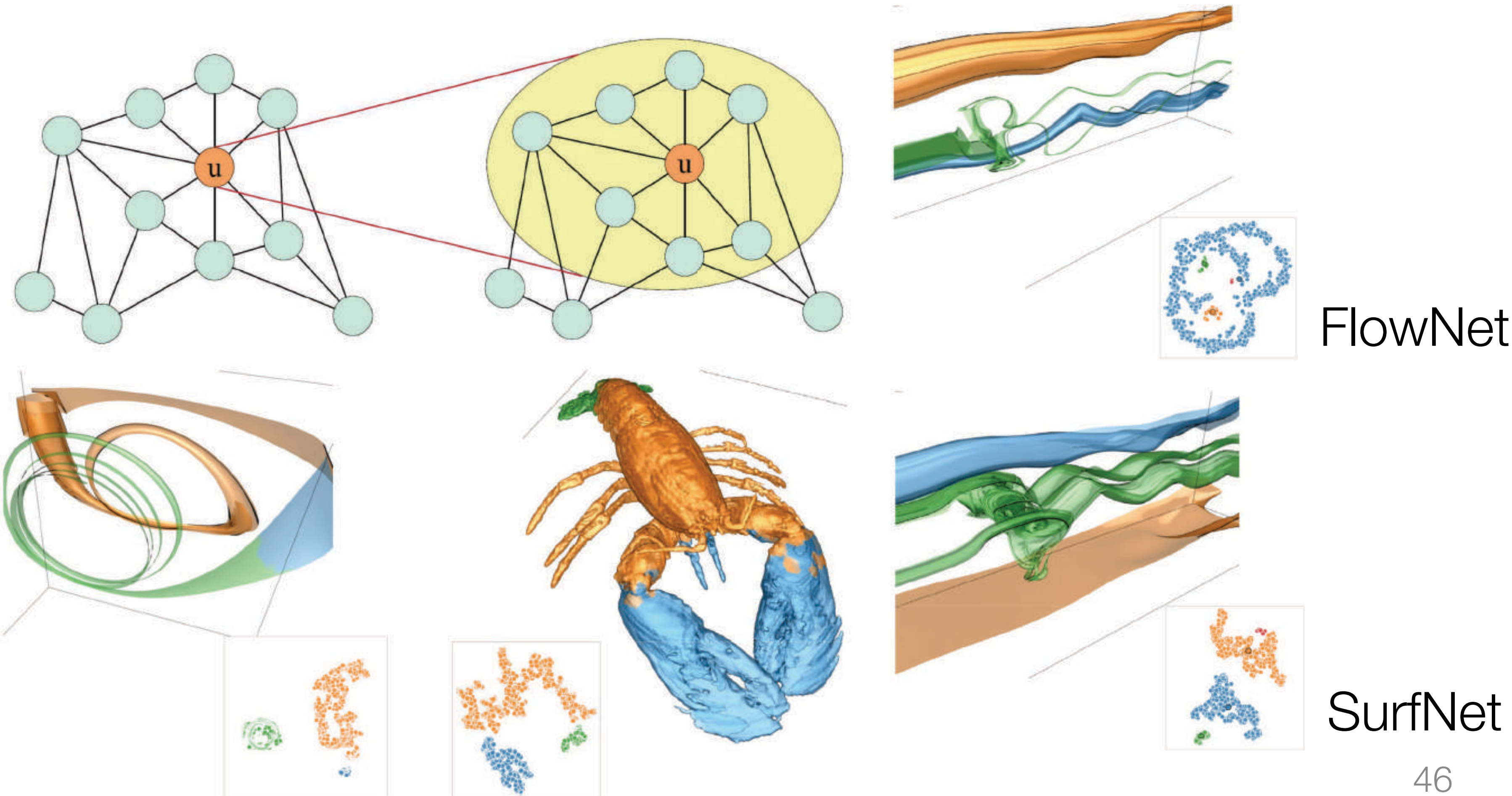
Future research directions

Representation learning for volumes

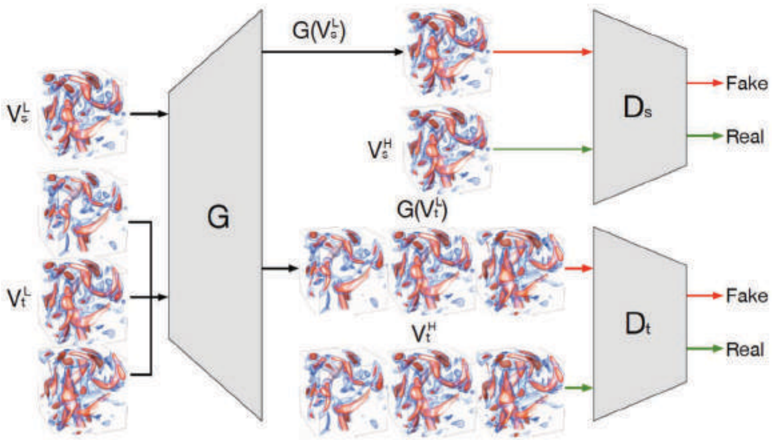


William P. Porter, Yunhao Xing, Blaise R. von Ohlen, Jun Han, and Chaoli Wang. A Deep Learning Approach to Selecting Representative Time Steps for Time-Varying Multivariate Data. In *Proceedings of IEEE VIS Conference (Short Papers)*, pages 131-135, 2019.

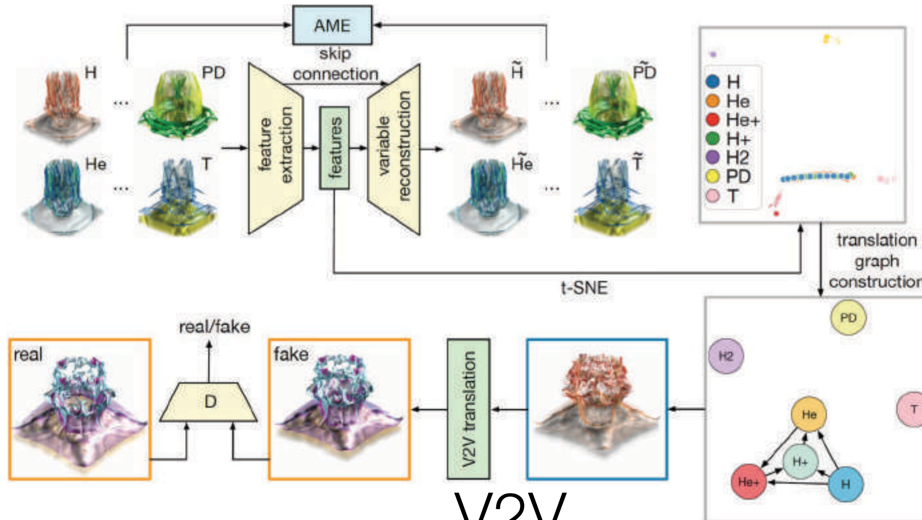
From voxel to graph representation



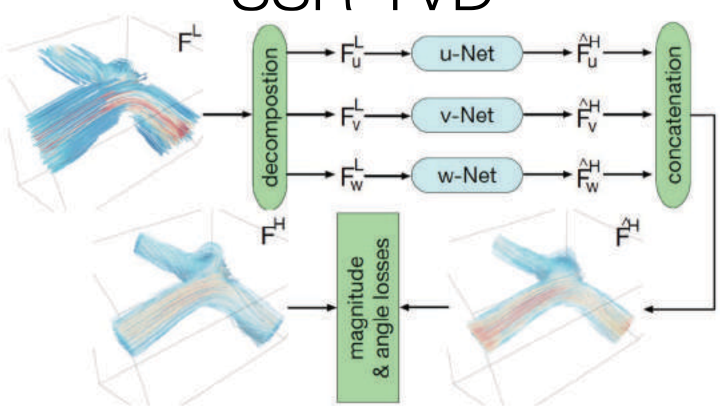
Other super-resolution works



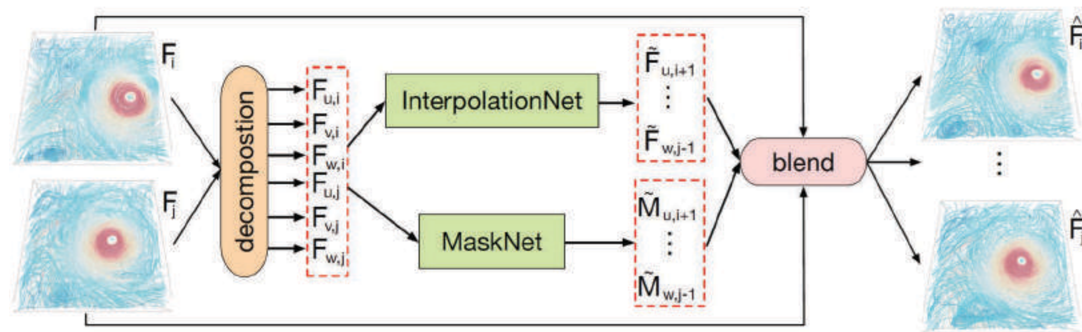
SSR-TVD



V2V



SSR-VFD



TSR-VFD

Key concerns

- Training time
  – May take hours to a few days on a single GPU
- Synthesized details
  – Largely avoid fake details by using observation-driven instead of noise-driven GAN
- Ground truth
  – Possible to generate super-resolution w/o the presence of the original high-resolution data
- Model generalization
  – Could apply the trained model to different sequences or ensemble runs of the same or similar simulations

Emerging directions in AI+VIS

- VIS for AI
  - Interpreting or explaining the inner working of neural nets
  - Network model debugging, improvement, comparison, and selection
  - Teaching and learning deep learning concepts

Fred Hohman, Minsuk Kahng, Robert Pienta, and Duen Horng Chau. Visual Analytics in Deep Learning: An Interrogative Survey for the Next Frontiers. *IEEE Transactions on Visualization and Computer Graphics*, 25(8):2674-2693, 2019.

- AI for VIS
  - Representation learning for clustering and selection
  - Data generation and augmentation
  - Replacing the traditional visualization pipeline
  - Simulation parameter space exploration
  - Parallel and in situ workflow optimization
  - Physics-informed deep learning

Acknowledgements

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  - Graduate students: Jun Han, Hao Zheng, Martin Imre
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  - Exchange students: Yunhao Xing (Columbia), Yihong Ma (Notre Dame)
  - iSURE students: Li Guo (CMU), Shaojie Ye (UW-Madison)
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Thank you!

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