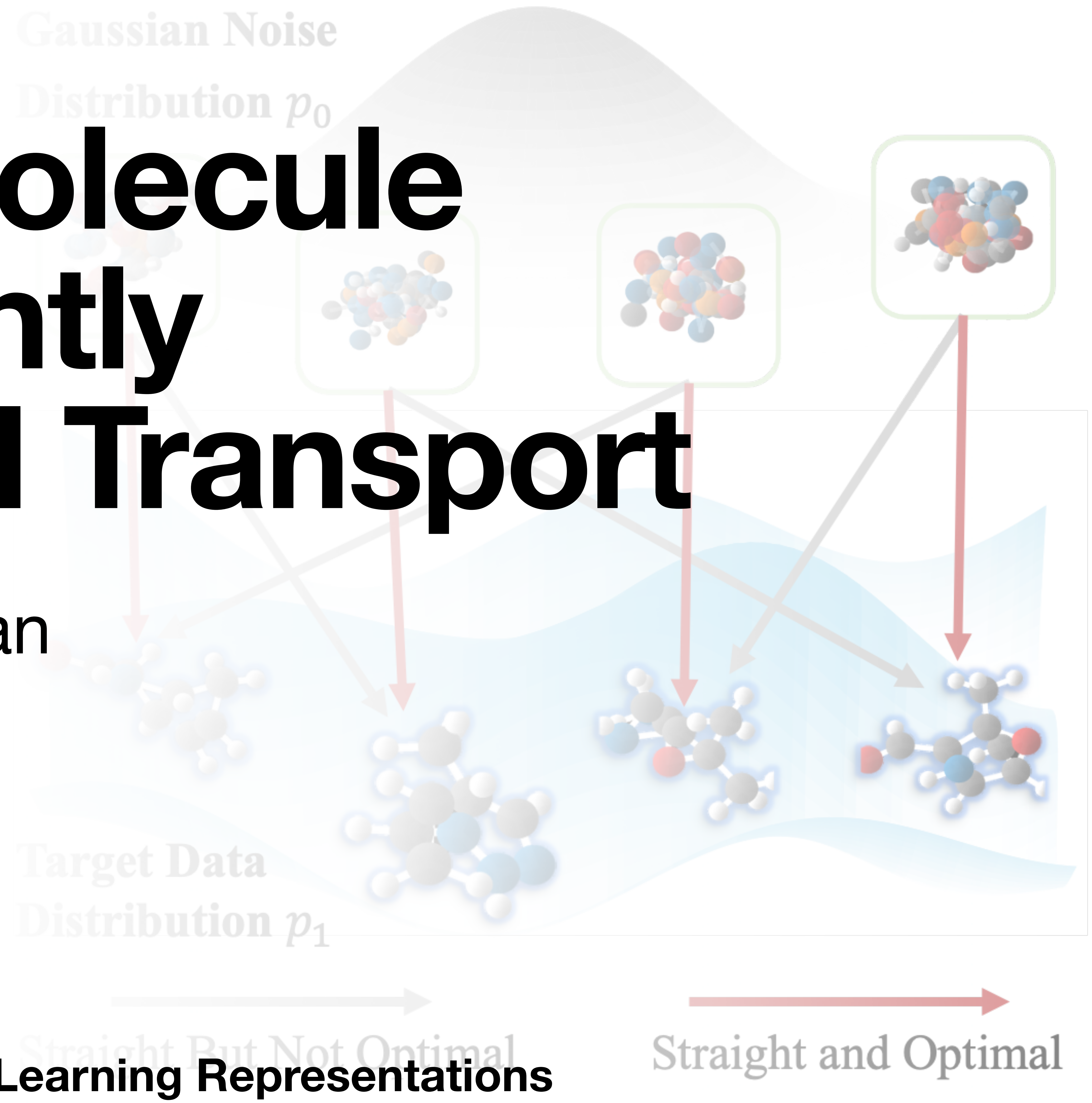
Accelerating 3D Molecule Generation via Jointly Geometric Optimal Transport

Haokai Hong, Wanyu Lin, Kay Chen Tan
The Hong Kong Polytechnic University



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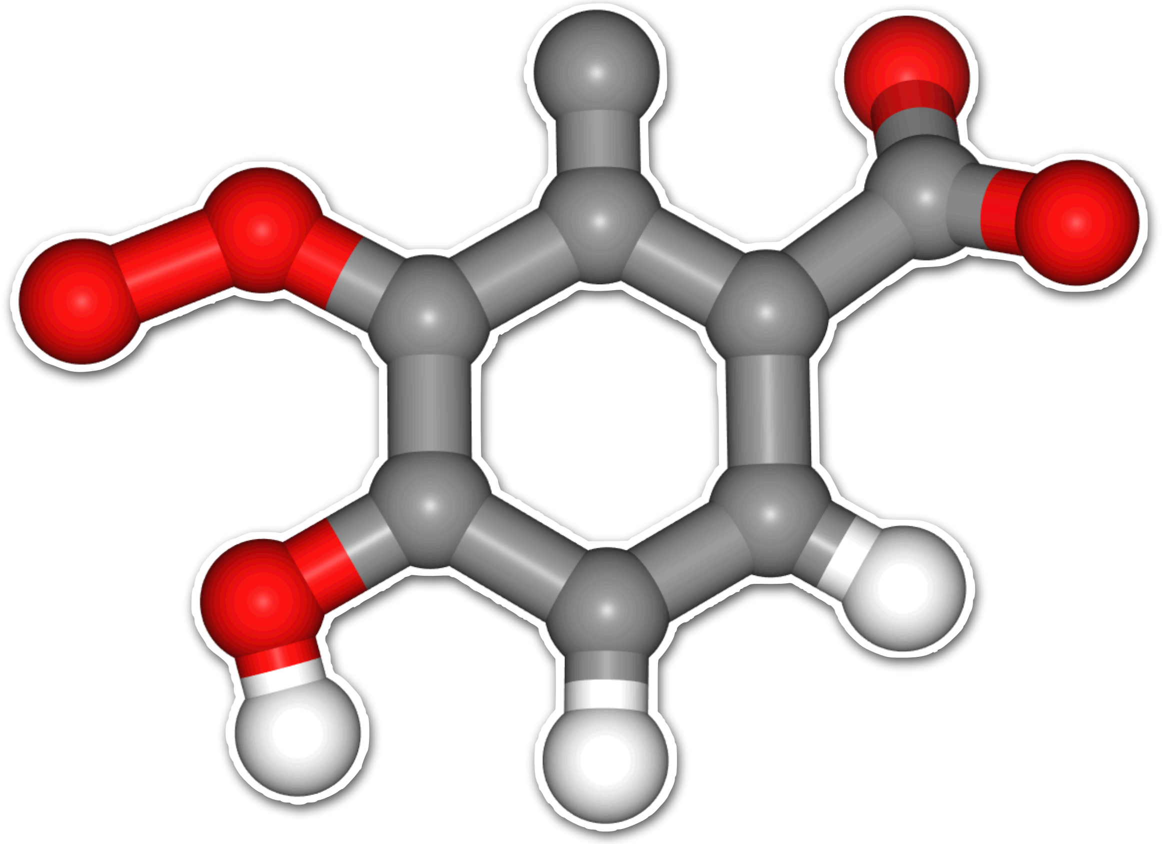
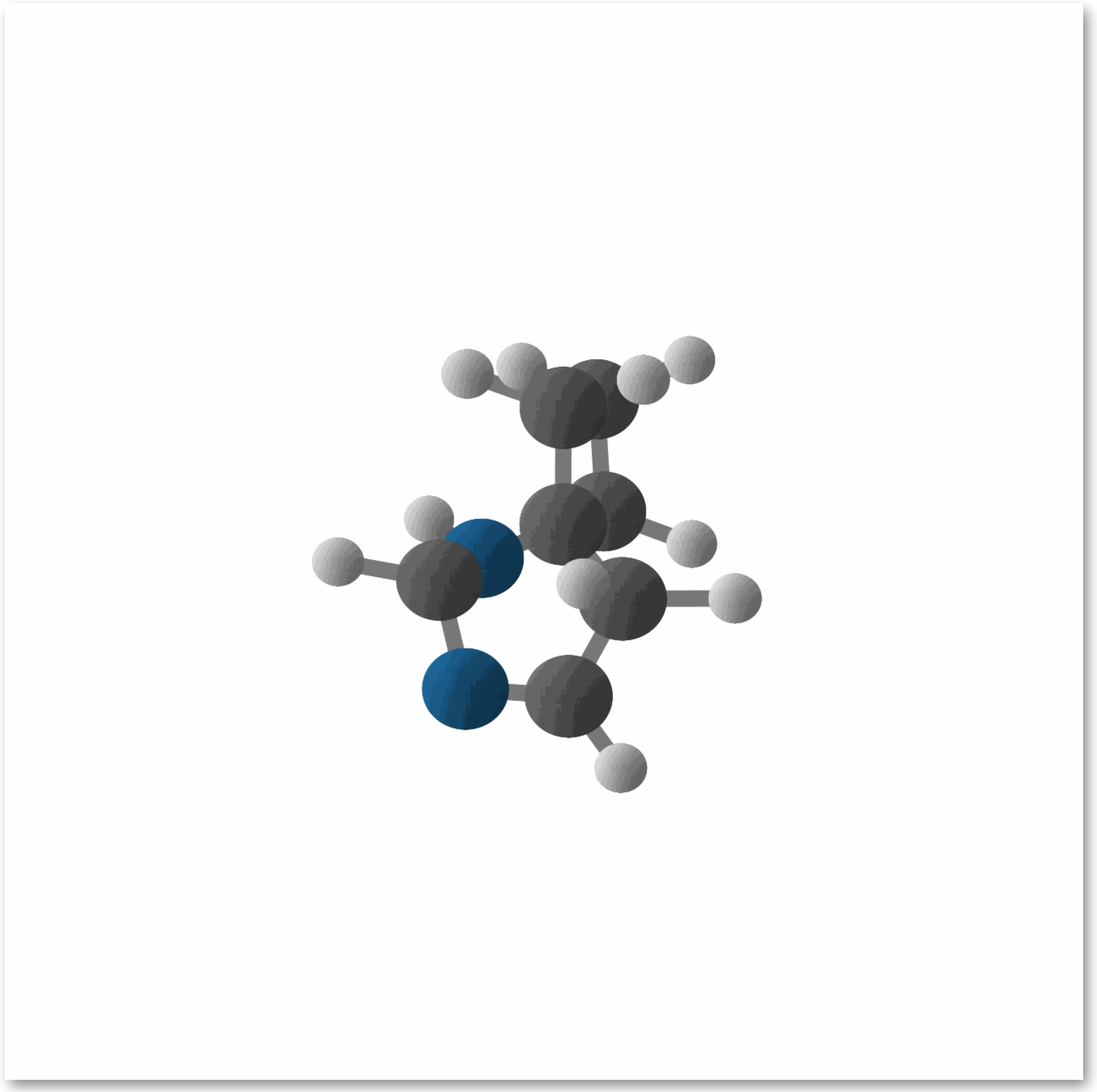
Background

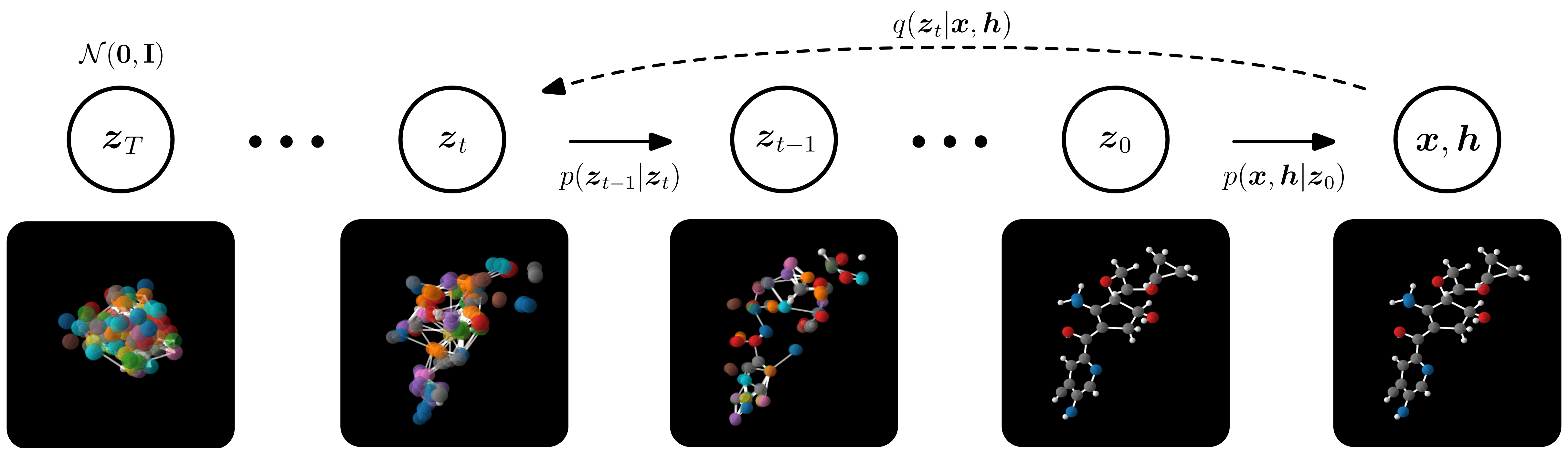
- Molecules as atomic geometric graphs
  - Atom coordinates: (x, y, z);
  - Atom type: $\mathbf{H}, \mathbf{O}, \mathbf{F}, \ldots$
- Generation
  - 3D coordinates and atom types.

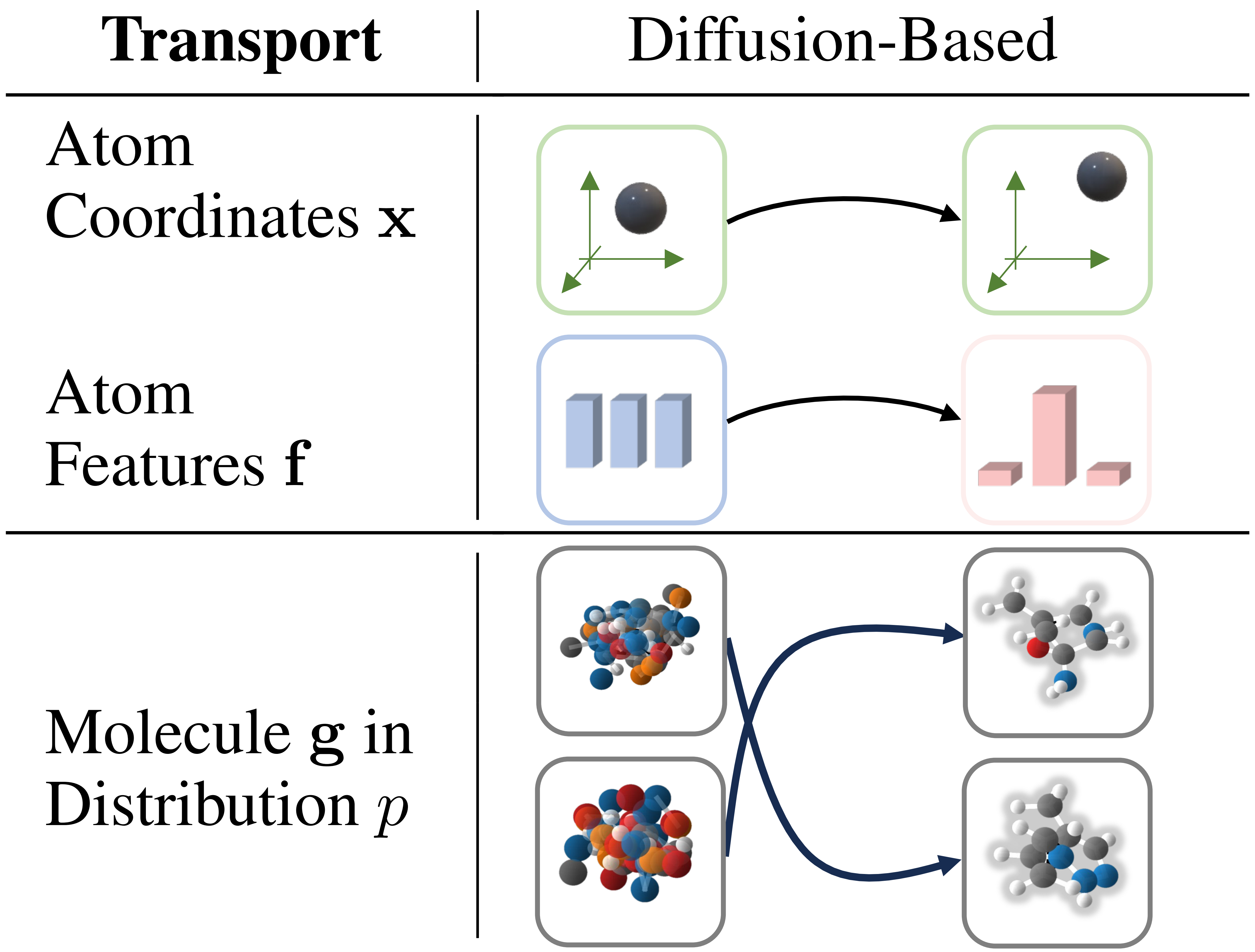




Existing Methods: Diffusion Model

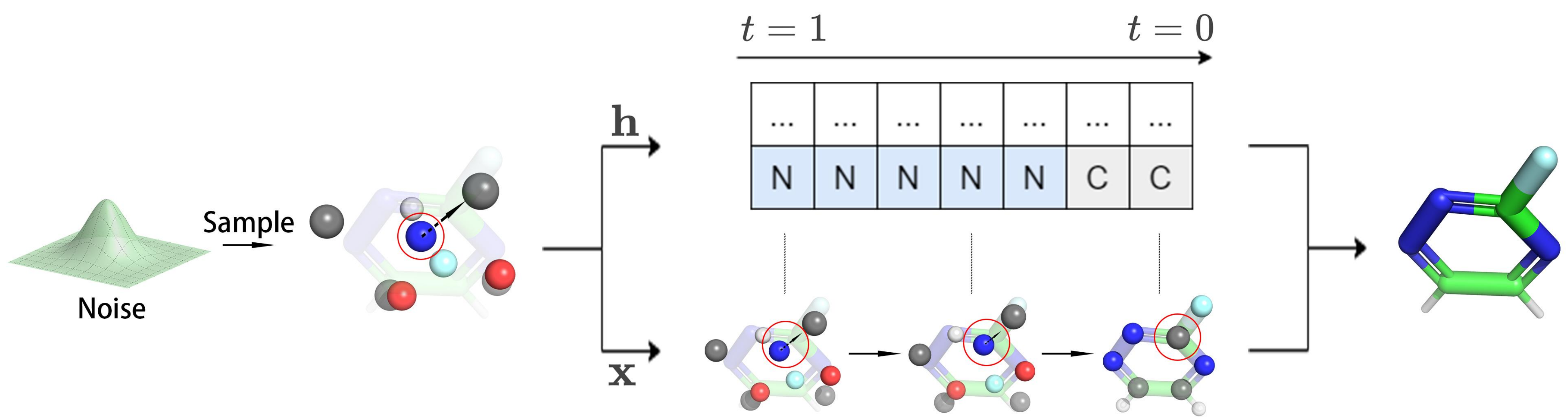
- Superior molecule generation results
- Slow inference: ~1,000 sampling steps
- High cost for large-scale inference

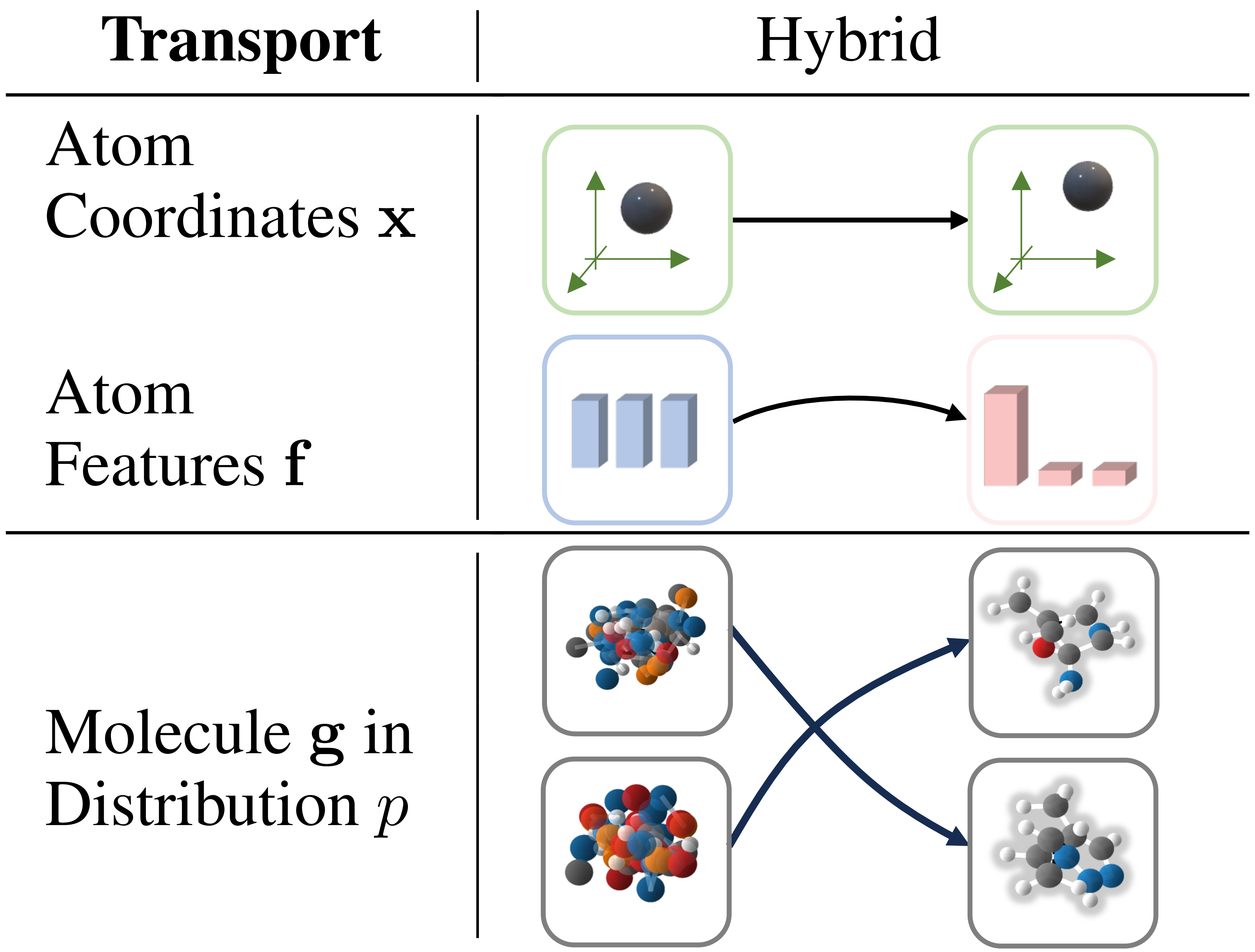




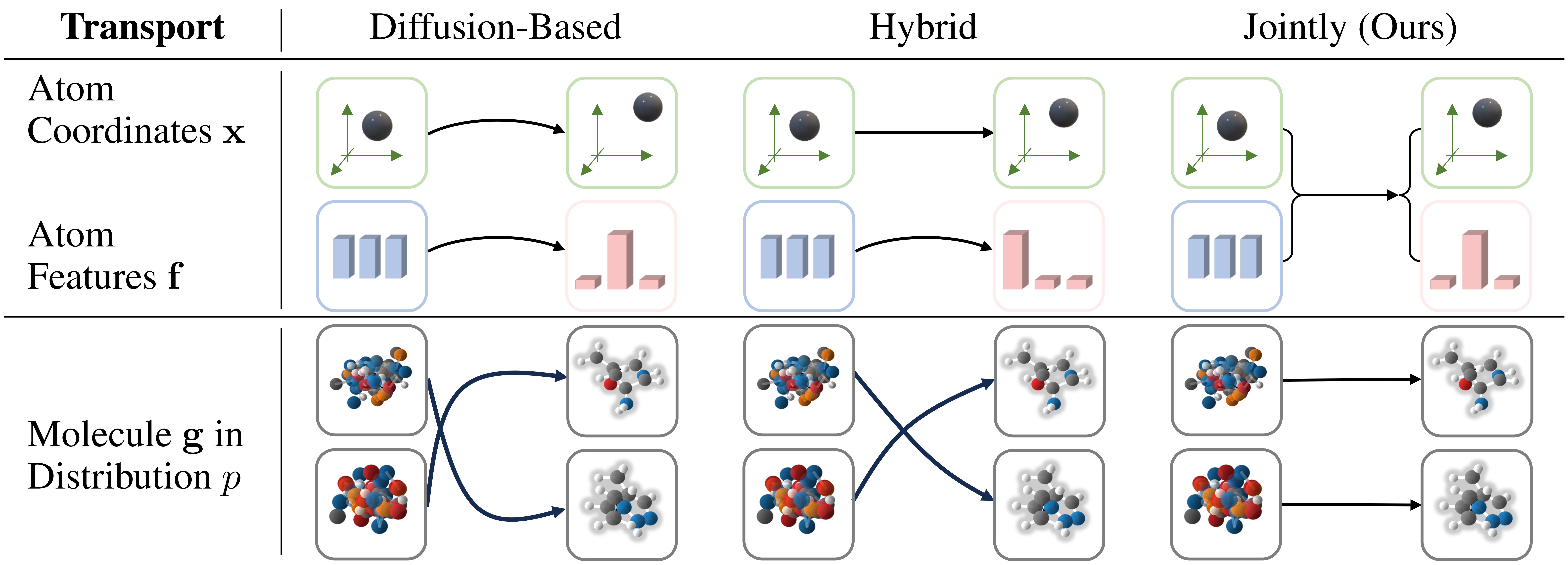
Existing Methods: Flow Matching

- Simulation-free training paradigm
- Faster molecule generation
- Non-optimal transport





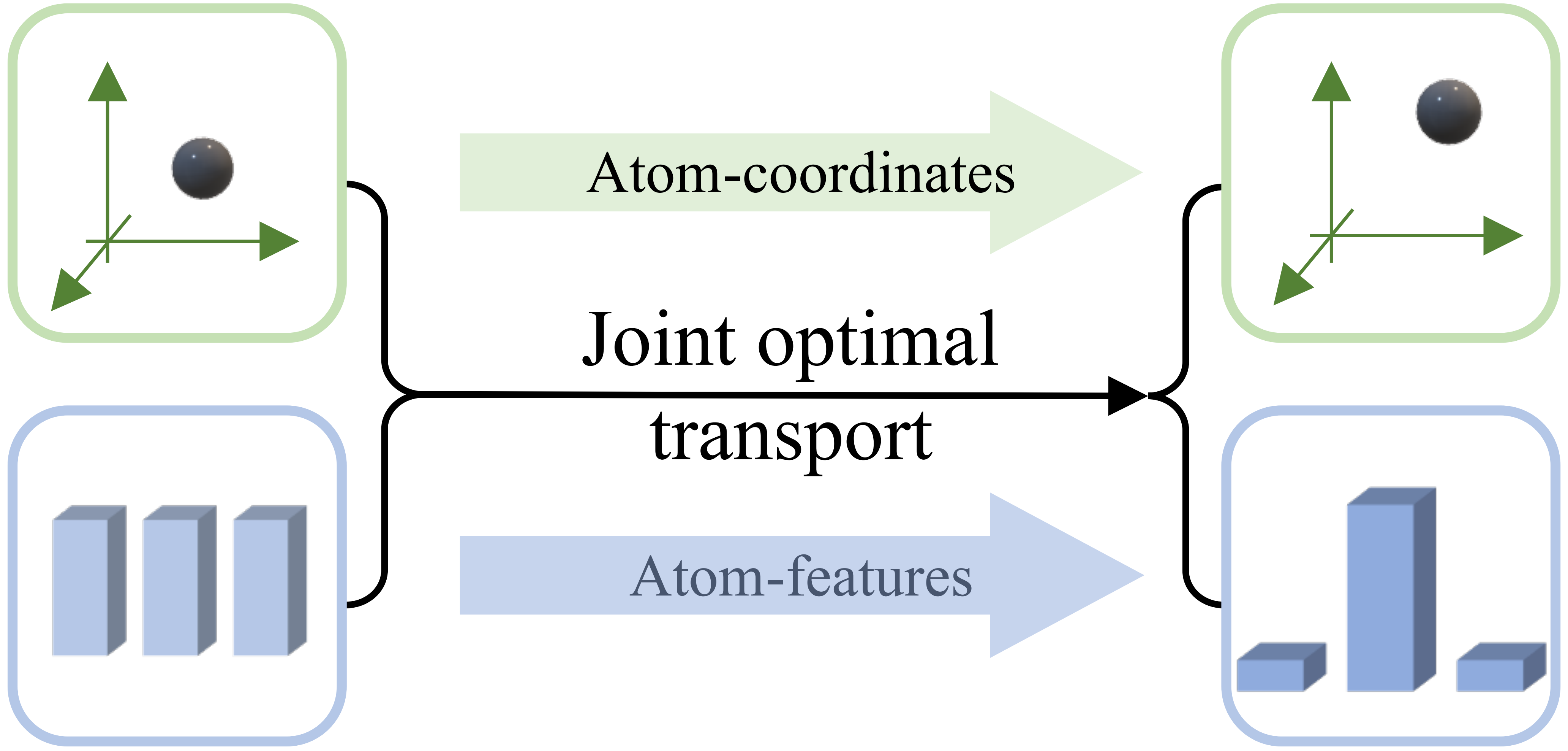
Motivation



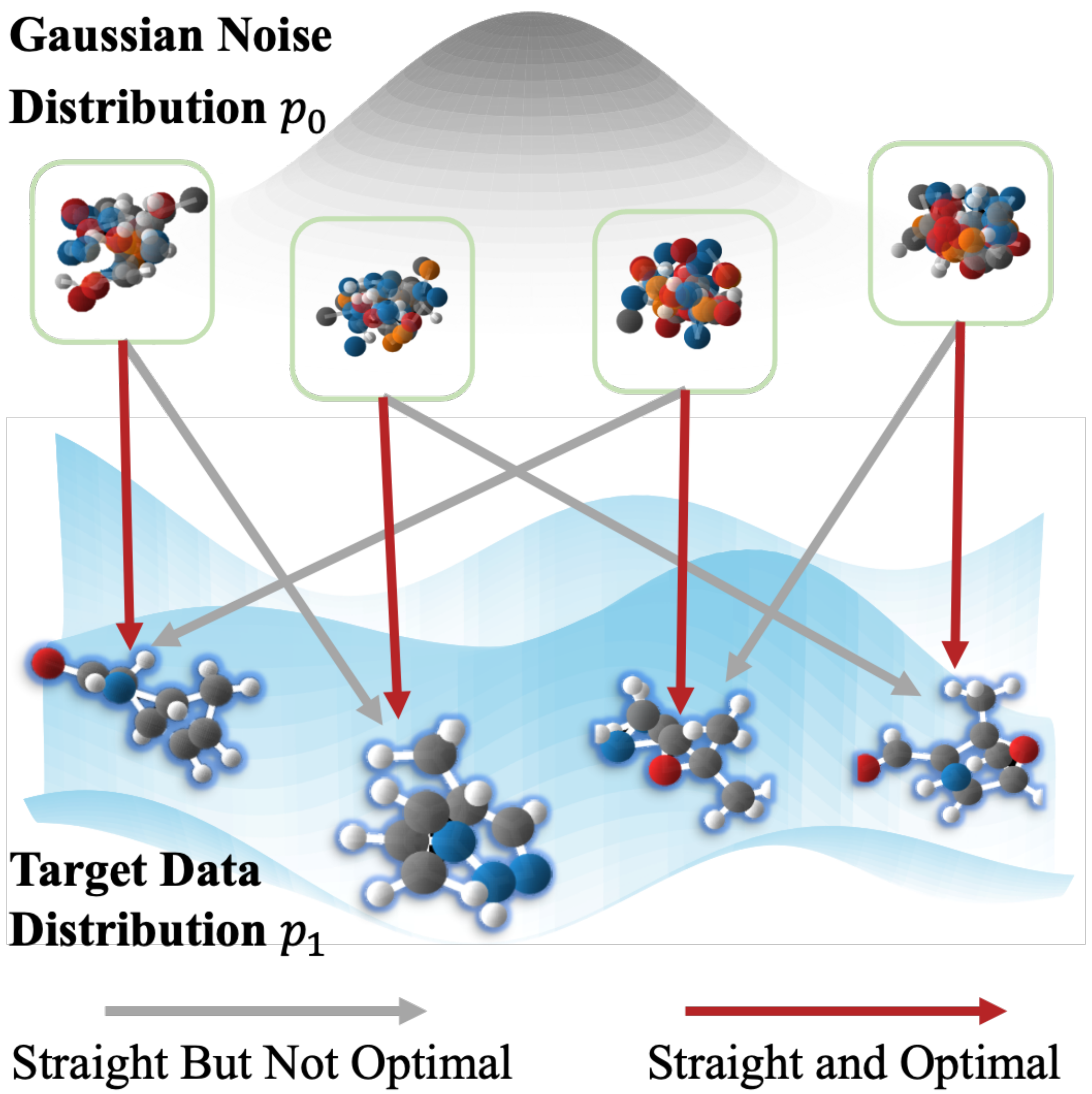
Transport
Diffusion-Based
Hybrid
Jointly (Ours)
Atom Coordinates $\mathbf{x}$
Atom Features $\mathbf{f}$
Molecule $\mathbf{g}$ in Distribution p

Our Method: GOAT

- **Optimal Molecule Transport**



- **Optimal Distribution Transport**



Our Method: GOAT

- **Geometric transport cost:**

$$\min_{\Gamma} \mathbb{E}[\hat{c}_g(\mathbf{g}_0, \mathbf{g}_1)],$$

$$\textbf{s. t.} \quad (\mathbf{g}_0, \mathbf{g}_1) \in \Gamma(p_0, p_1),$$

$$\hat{c}_g(\mathbf{g}_0, \mathbf{g}_1) = \lambda \min_{\mathbf{R},\mathbf{t},\pi} \|\pi(\mathbf{R}\mathbf{x}_1^1 + \mathbf{t}, \mathbf{R}\mathbf{x}_1^2 + \mathbf{t}, \ldots, \mathbf{R}\mathbf{x}_1^N + \mathbf{t}) - (\mathbf{x}_0^1, \mathbf{x}_0^2, \ldots, \mathbf{x}_0^N)\|_2$$

$$+(1-\lambda) \min_{\pi} \|\pi(\mathbf{h}_1^1, \mathbf{h}_1^2, \ldots, \mathbf{h}_1^N) - (\mathbf{h}_0^1, \mathbf{h}_0^2, \ldots, \mathbf{h}_0^N)\|_2, \forall \pi, \mathbf{R}, \text{ and } \mathbf{t}$$

Experiments on QM9 Dataset

QM9	Quality (↑)					Efficiency (↓)	
Metrics	Atom Sta	Valid	Uniqueness	Novelty	Significance	Steps	S-Time
Data	99.0	97.7	100.0	-	-	-	-
ENF	85.0	40.2	98.0	-	-	-	-
G-Schnet	95.7	85.5	93.9	-	-	-	-
GDM-aug	97.6	90.4	**99.0**	74.6	66.8	1000	1.50
EDM	98.7	91.9	98.7	65.7	59.6	1000	1.68
EDM-Bridge	98.8	92.0	98.6	-	-	1000	-
GeoLDM	98.9	93.8	98.8	58.1	53.9	1000	1.86
GeoBFN	98.6	93.0	98.4	70.3	64.4	100	0.16
EquiFM	98.9	**94.7**	98.7	57.4	53.7	200	0.37
GOAT (Ours)	**99.2**	92.9	**99.0**	**78.6**	**72.3**	**90**	**0.12**

SOTA Generation Quality

Fastest Generation Efficiency

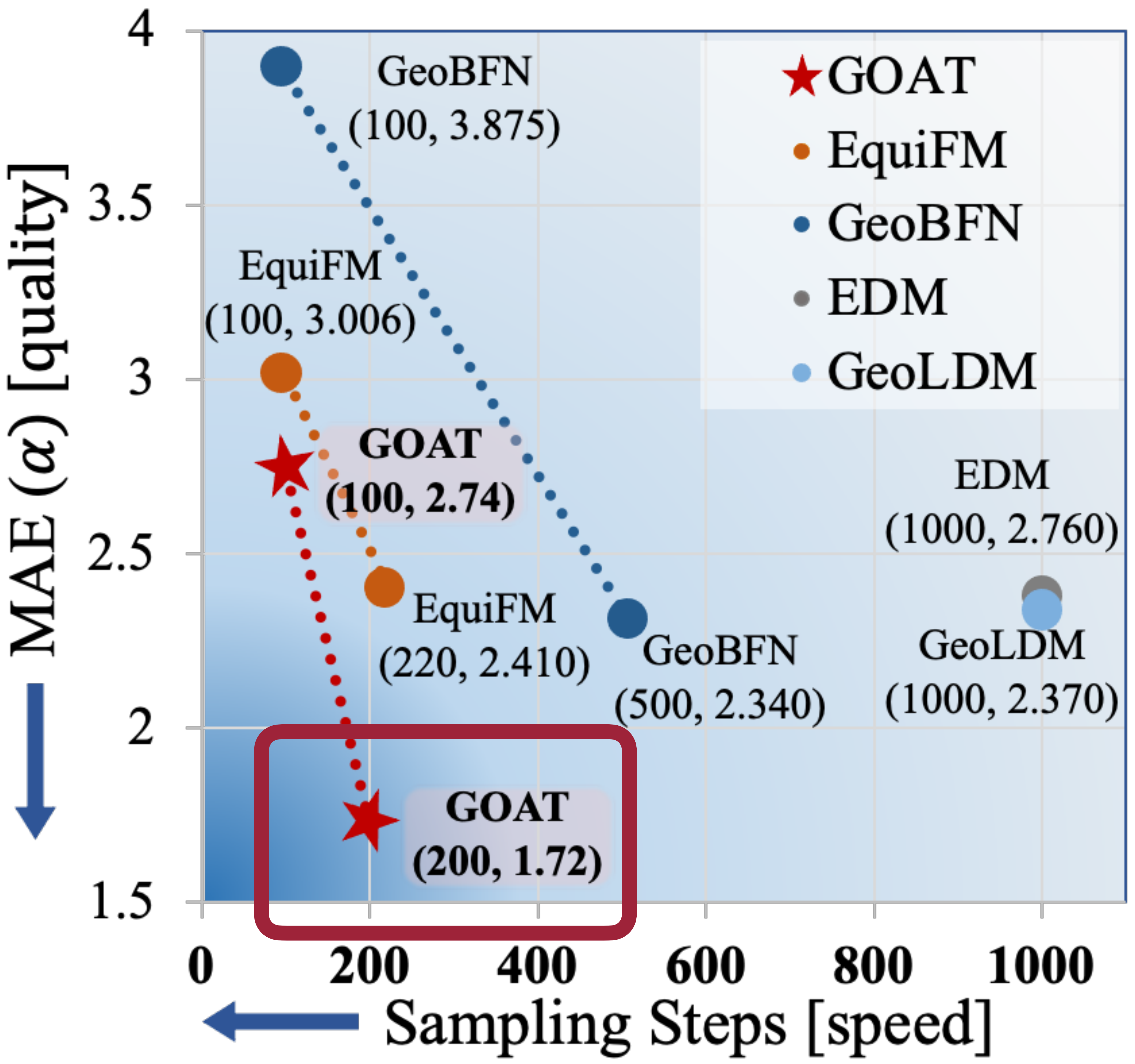
Experiments on GEOM-DRUG

GEOM-DRUG	Quality (↑)		Efficiency (↓)	
Metrics	Atom Sta	Valid	Steps	S-Time
Data	86.5	99.9	-	-
GDM-aug	77.7	91.8	1000	-
EDM	81.3	92.6	1000	14.88
EDM-Bridge	82.4	92.8	1000	-
GeoLDM	84.4	**99.3**	1000	12.84
GeoBFN	78.9	93.1	100	1.27
EquiFM	84.1	98.9	200	2.02
GOAT (Ours)	**84.8**	96.2	**90**	**0.94**

SOTA Performance on Large-Scale Dataset

Experiments on Conditional Generation

A New Trade-off Between Effectiveness and Efficiency



Takeaways

We developed a geometric optimal transport framework to accelerate 3D molecule generation

We achieves the fastest high-quality generation via addressing optimal molecule transport and optimal distribution transport