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SSD: Shell-Guided *Spherical* Diffusion for Molecular Geometry Generation



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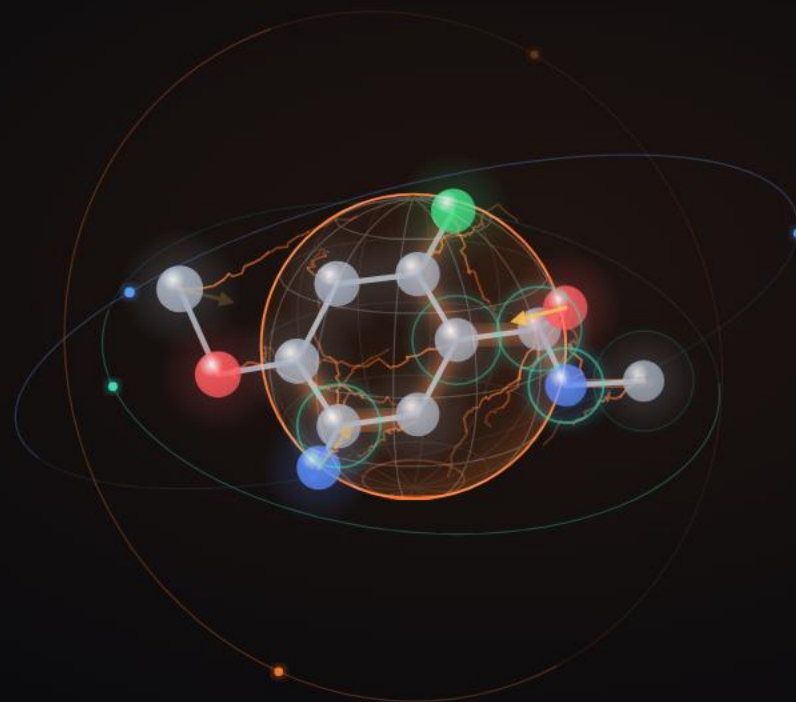
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Presented by **Yun-Yen Chuang**, CEO, Maxora AI

THE TASK

Generating 3D molecular geometry

Conditional generation

molecular graph $\rightarrow$ 3D conformations



Unconditional refinement

noisy 3D geometry $\rightarrow$ valid structure



Coordinate-space backbones:

GeoDiff

SubGDiff

EDM

MCF

SemlaFlow

THE HIDDEN ASSUMPTION

Every run starts from a Gaussian

$$\mathbf{x}_T \sim \mathcal{N}(0, \sigma_T^2 I_{3n})$$

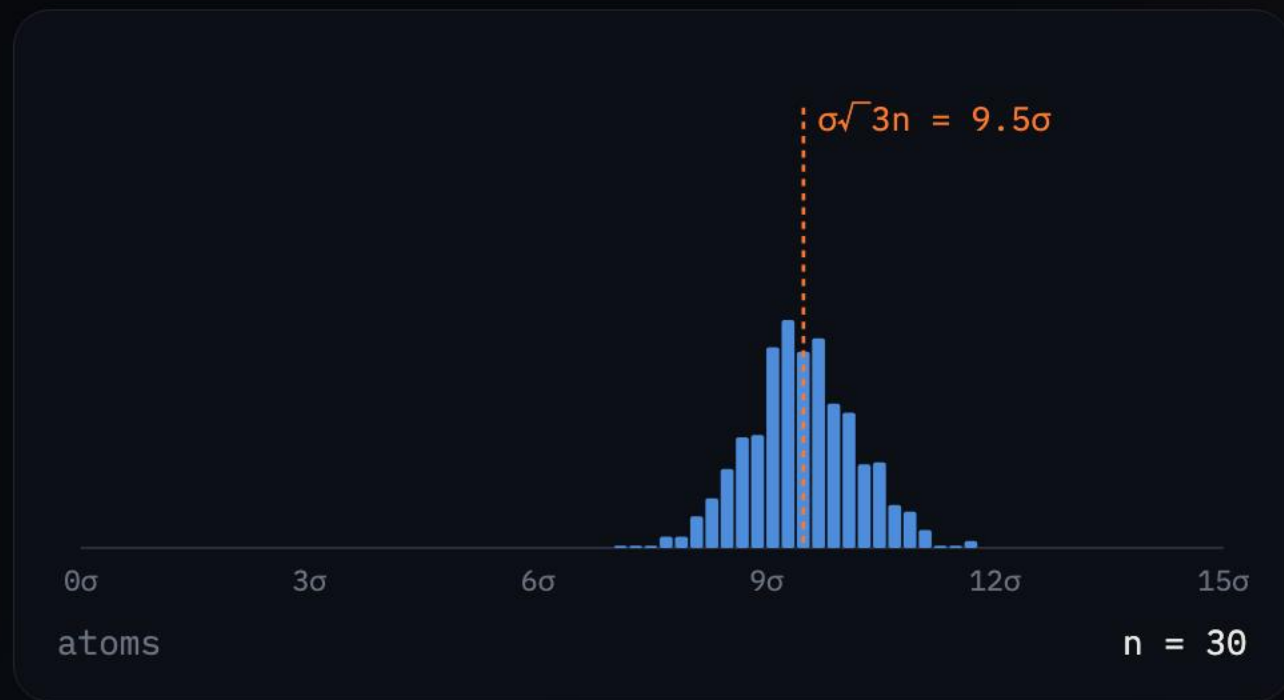
It looks like harmless noise. But a Gaussian in **3n** dimensions has a very specific geometry, and that geometry has **nothing to do with molecules**.

• Gaussian prior



GAUSSIAN ANNULUS THEOREM

The prior is a thin shell of radius $\sigma_T \sqrt{3n}$

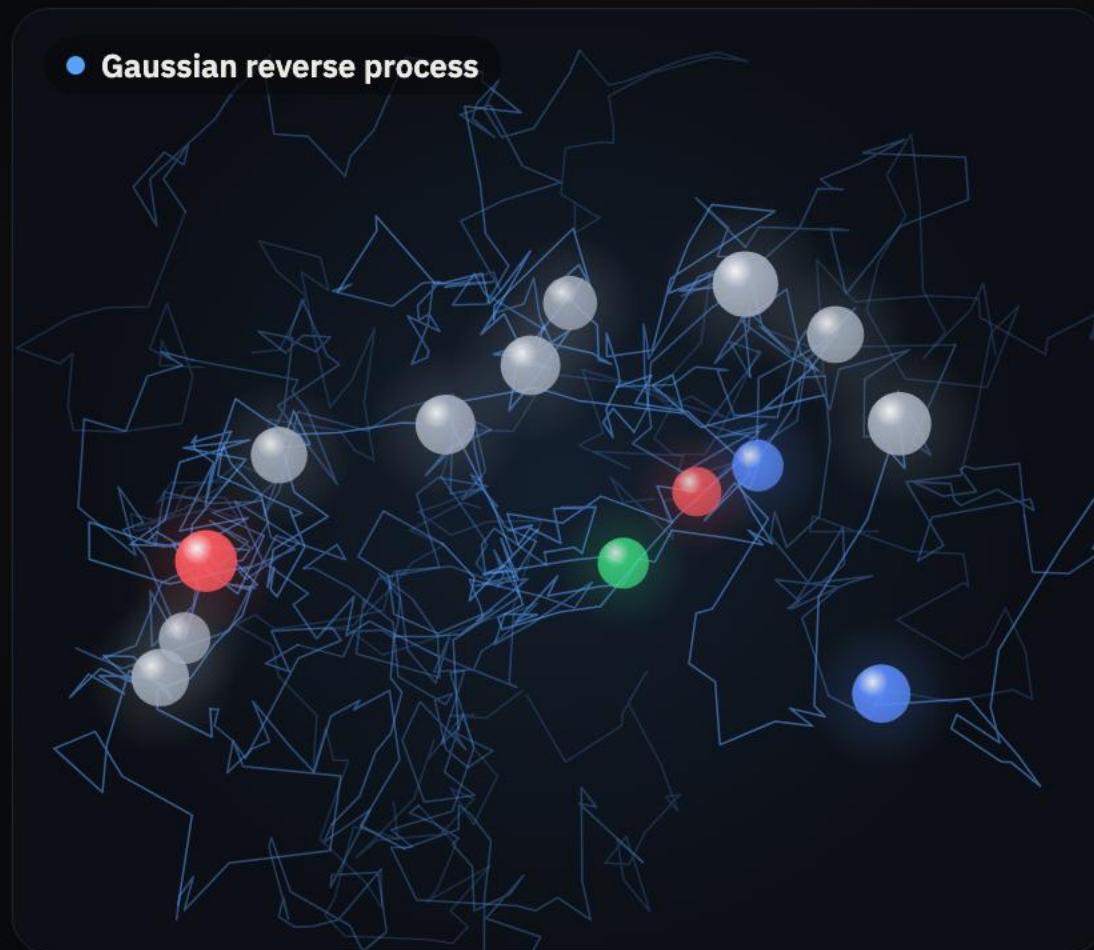


- As n grows, the shell moves outward
- Its width stays roughly the same
- The radius is set by **noise level** and **atom count**, **not chemistry**

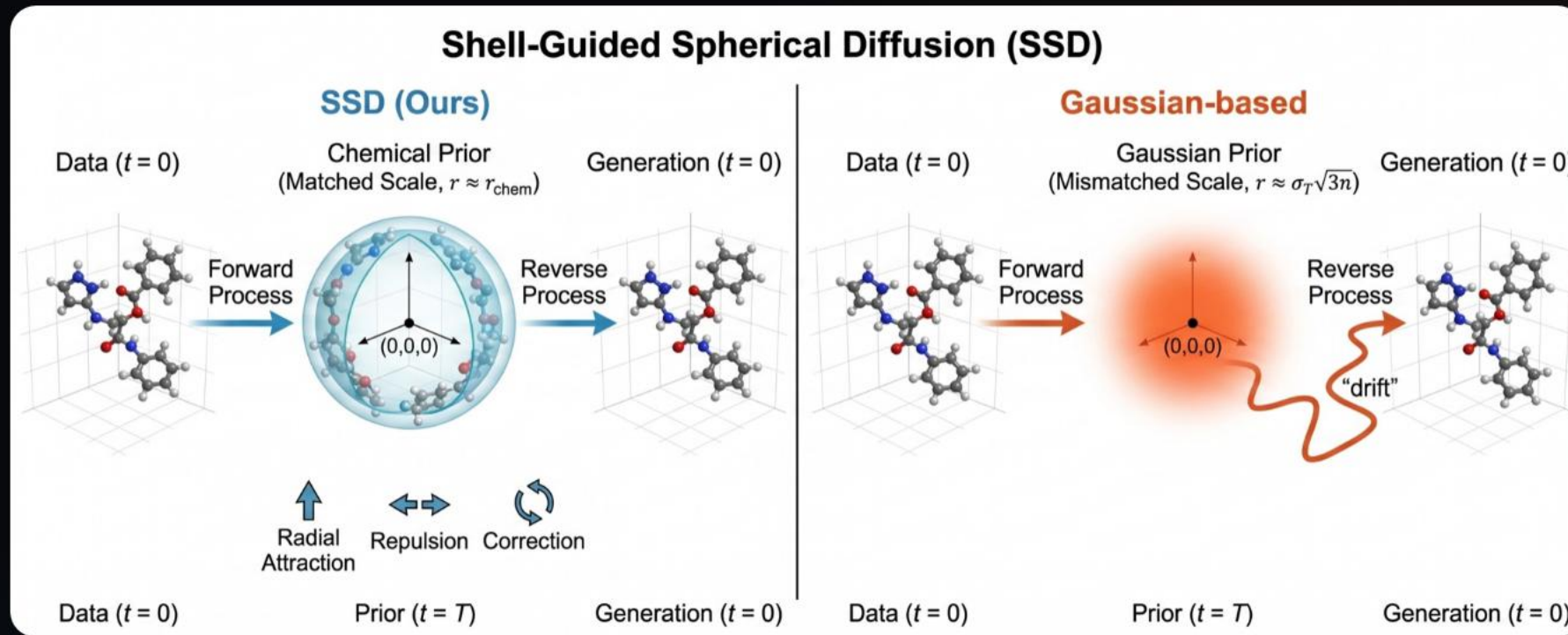
WHY IT MATTERS

A scale mismatch with real costs

- Distorted score magnitudes
- High spatial entropy: long, unstable early trajectories
- Worse as molecules grow, where Gaussian baselines degrade most



Start diffusion where molecules *actually live*



① Spherical-shell initialization

radius calibrated to chemistry

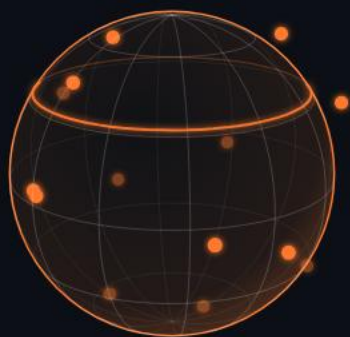
② Shell-aware dynamics

in the forward and reverse processes

① INITIALIZATION

Draw the shell, then sample x_T on it

● SSD



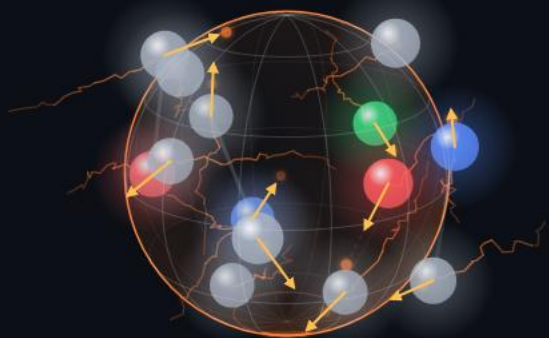
● Gaussian



- Centre every state at zero CoM
- r_{SSD} = mean radius of centred training conformations: **6.37 Å** QM9, **21.16 Å** Drugs
- A fixed, dataset-level constant
- $x_T^{(i)} = r \cdot v^{(i)} / \|v^{(i)}\|$, $v^{(i)} \sim N(0, I)$, then re-centre

Molecule $\rightarrow$ shell, at uniform speed

● SSD



● Gaussian

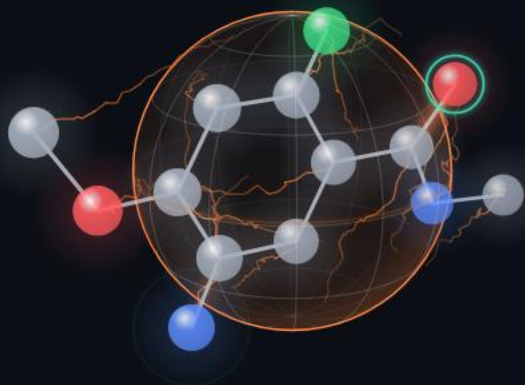


$$f^{(i)}(\mathbf{x}_t, t) = \alpha_t \frac{\mathbf{x}_T^{(\pi(i))} - \mathbf{x}_t^{(i)}}{\|\mathbf{x}_T^{(\pi(i))} - \mathbf{x}_t^{(i)}\|}$$

- Random permutation π , resampled every trajectory
- Distance shrinks **linearly**, independent of start; atoms stop on arrival
- Unlike OU's exponential pull with long tails

Shell $\rightarrow$ molecule with three drifts

● SSD



● Gaussian



$$d\mathbf{x}_t^{(i)} = [\mathbf{v}_{\text{rad}} + \mathbf{v}_{\text{rep}} + \mathbf{v}_{\text{score}}] dt + \sigma_t d\mathbf{w}_t^{(i)}$$

● $\mathbf{v}_{\text{rad}} = -\alpha_t \mathbf{x} / \|\mathbf{x}\|$ · toward the centre

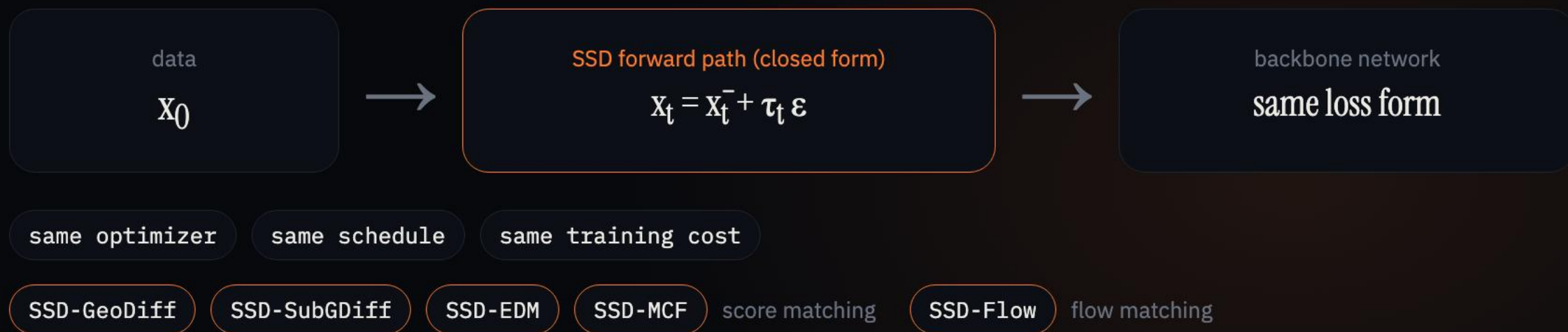
● $\mathbf{v}_{\text{rep}}$ · keeps atoms $\geq d_{\text{min}}$ apart

● $\mathbf{v}_{\text{score}} = \sigma_t^2 s_\theta$ · backbone's SE(3) network

A shell-aware hybrid sampler, not an exact time reversal · SE(3)-equivariant by construction

TRAINING

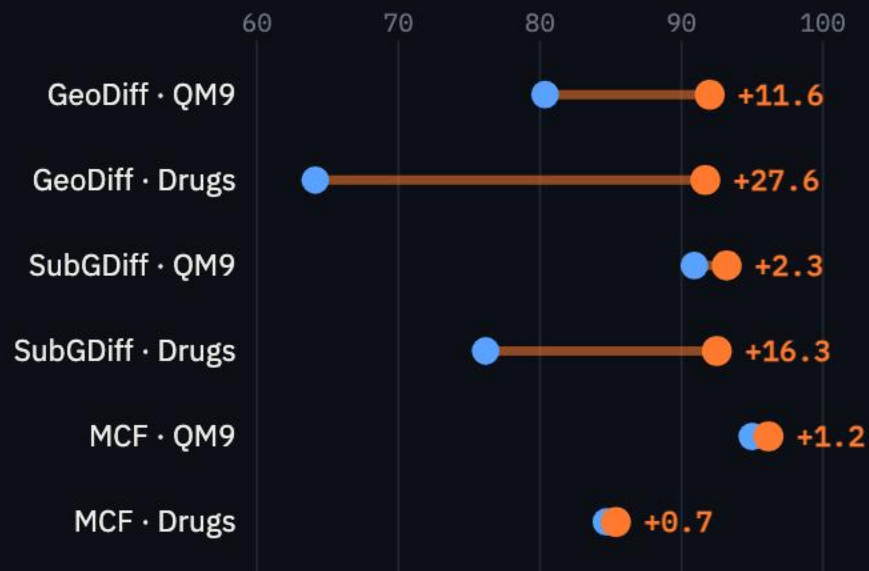
Still trained, inside each backbone's own pipeline



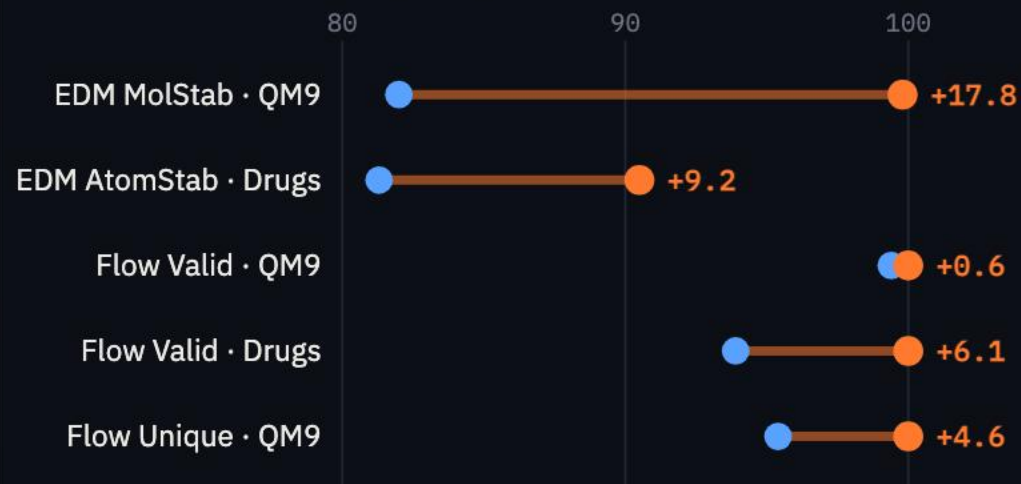
MAIN RESULTS · EACH BACKBONE UNDER ITS OWN PROTOCOL

Consistent gains across five backbones

Conditional · COV-R (%) ↑



Unconditional · QM9 / Drugs ↑



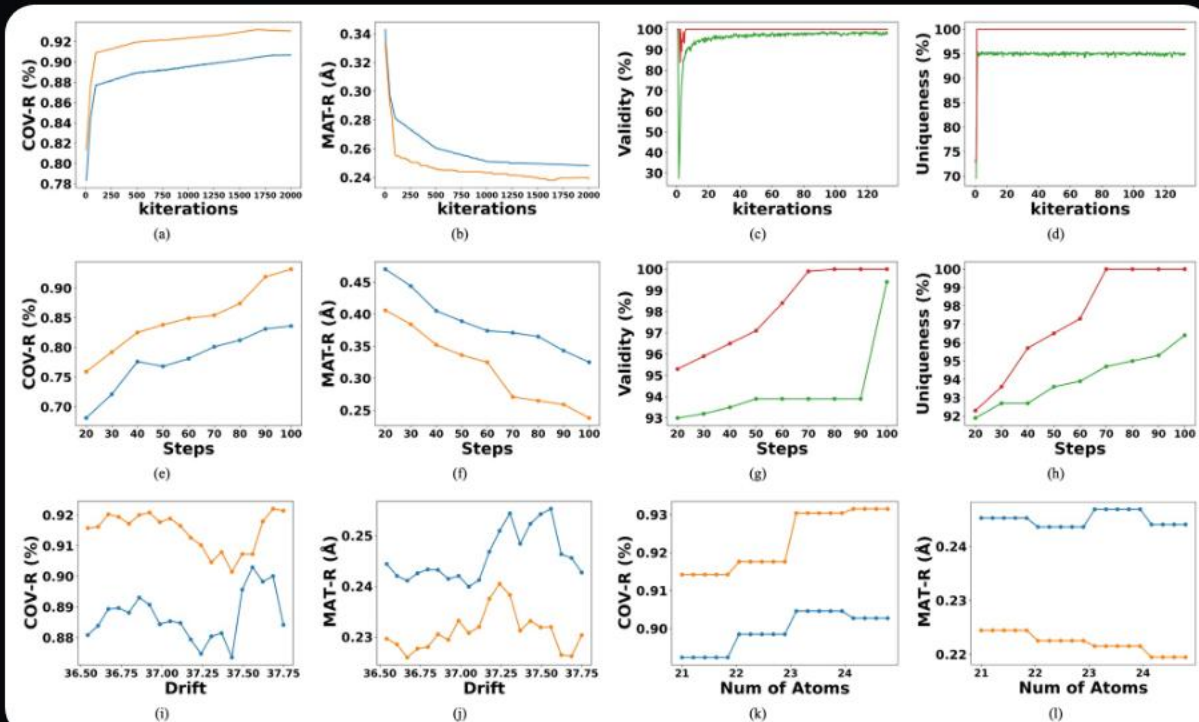
● Backbone ● + SSD

MCF · Drugs gain is not statistically significant · three seeds confirm the SubGDiff, EDM and Flow gains

Shell *and* dynamics are both required

COV-P (%) ↑





TRAINING & SAMPLING

Faster convergence, robust,
scales with size

- Converges faster during training
- Ahead from 20 to 100 sampling steps
- Wins once drift $> 36.6 \text{ \AA}$ or $n > 21$

+32.5 COV-R on GEOM-Drugs molecules with
 ≥ 50 atoms

Paths stay on the shell and run straighter

Radial deviation (Å) ↓

0.45 → 0.18

SDE · SubGDiff → SSD-SubGDiff

0.21 → 0.11

ODE · SemlaFlow → SSD-Flow

Path excess (path length / $\|x_T - x_0\|$) ↓

1.29 → 1.11

ODE, like-for-like · SemlaFlow → SSD-Flow

246.91 → 1.71

SDE · gap also reflects SSD's smaller thin-shell noise

TAKEAWAYS

- The Gaussian prior's radius is a **non-chemical artifact**
- SSD: a chemically scaled shell + shell-aware dynamics
- Plugs into 5 backbones, keeps their loss form and training cost
- Converges faster and generates better, especially for large molecules



project page

shelldiffusion.github.io/SSD-ShellDiffusion
code · data · checkpoints released

Thank you

