# Periodic Bayesian Flow Networks with Additive Accuracy


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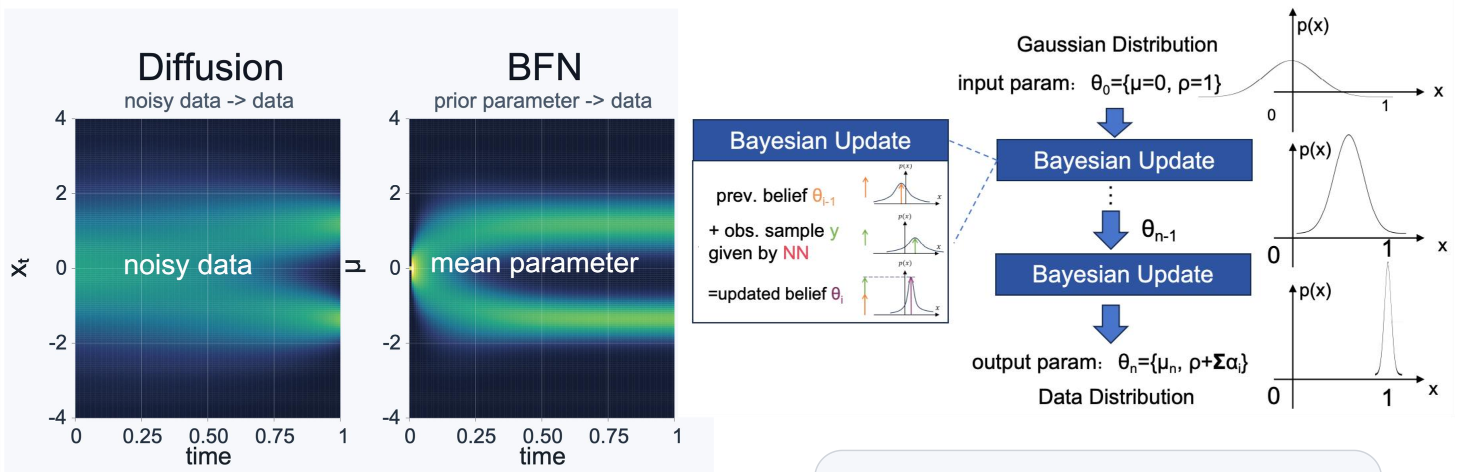
## ① BFN: Distribution-Centric

- Diffusion denoises noisy $x_t$; BFN denoises belief means $\mu_t$.
- Means average observations, so the network sees cleaner inputs.

**Cleaner inputs → smoother target → easier convergence**

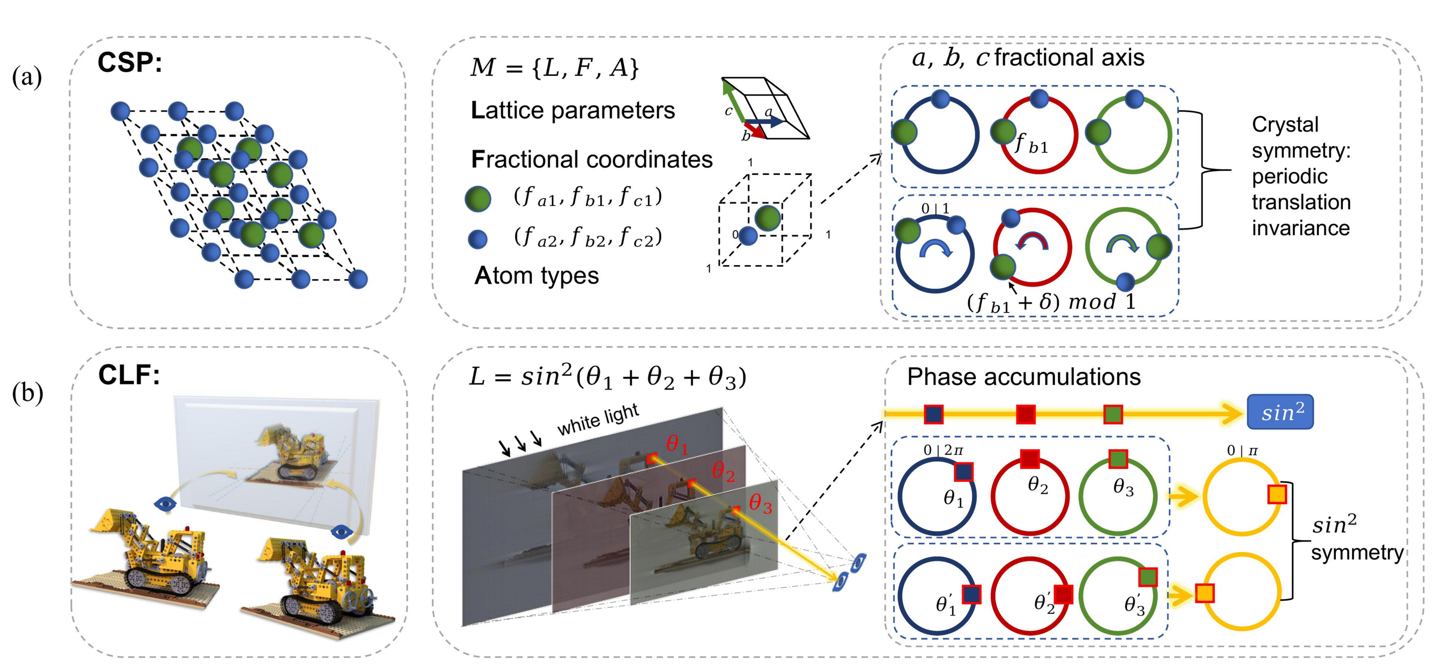



**data point path** **belief mean path**

BFN moves the posterior belief toward data; the net works on a compressed state.

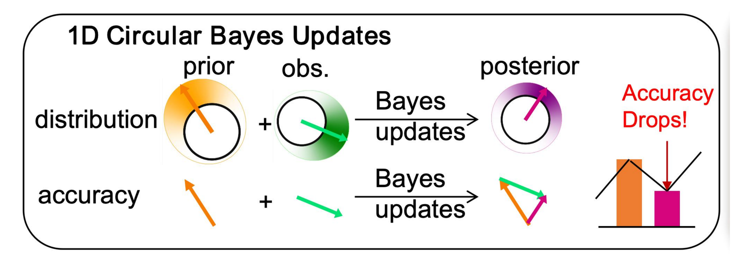
## ② Periodic Data Are Everywhere

- Crystals: Fractional coordinates lie on a torus.
- CLF: Distinct periodic phases can render identical intensities.
  - ➢ A key step toward glasses-free 3D display.



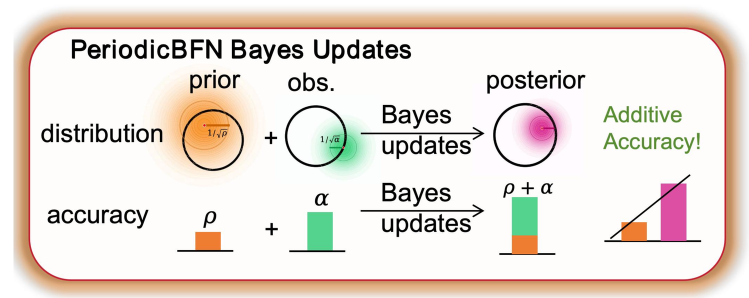

## ③ Problem: Circular BFNs Break Additivity

- 1D circular BFN: posterior accuracy depends on mean direction.
- Accuracy no longer follows the additive law ρ ← ρ + α.
- Training becomes schedule-sensitive and needs heuristic stabilization.

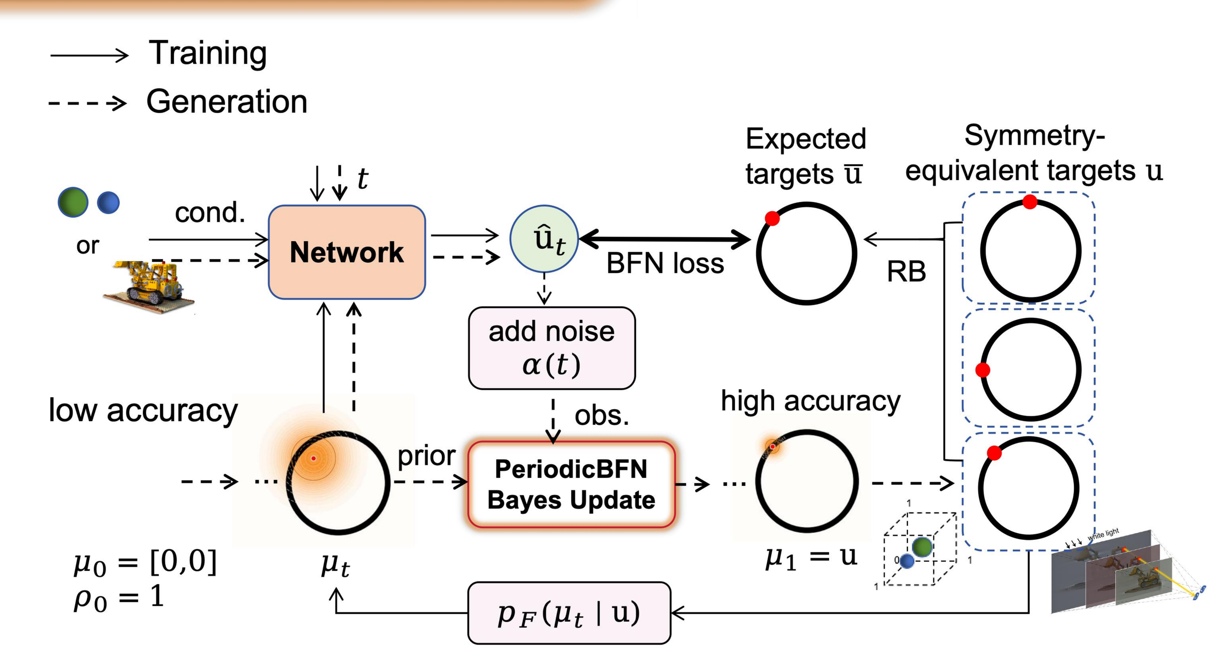



**Core issue** Circular updates mix direction and confidence; BFN loses its clean information clock.

## ④ PeriodicBFN: 2D Embedding + RB




**Feat.** Additive-accuracy structure yields a clean continuous-time and geometric loss




- Embed each periodic scalar θ as (cos θ, sin θ); run Gaussian BFN updates in 2D.
- Precision is scalar again; μ carries periodic geometry.

**RB target: posterior mean over symmetries**

$$\bar{u}_{RB} = E_g [\, u(g \cdot x) \mid \mu_t \,] \qquad L_{RB} = E_t \,\|\, \hat{u}_\theta(\mu_t, t) - \bar{u}_{RB} \,\|^2$$

**CSP: g = δ periodic translation | CLF: g = s ∈ {±1} sign / π ambiguity**

Averaging equivalent targets reduces denoising-target variance.

## ⑤ Experiments: CSP and CLF

### Crystal Structure Prediction (multi-seed mean ± std)

| Method | MP-20 MR↑ | MP-20 RMSE↓ | MPTS MR↑ | MPTS RMSE↓ |
|---|---|---|---|---|
| CDVAE | 33.93±0.15 | 0.1069±0.0018 | 5.21±0.13 | 0.2083±0.0023 |
| DiffCSP | 51.89±0.30 | 0.0611±0.0015 | 13.95±0.11 | 0.1422±0.0053 |
| EquiCSP | 57.48±0.18 | 0.0510±0.0010 | 14.48±0.19 | 0.1201±0.0029 |
| FlowMM | 61.26±0.14 | 0.0572±0.0014 | 16.11±0.17 | 0.1831±0.0021 |
| CrysBFN | 64.33±0.24 | 0.0445±0.0010 | 19.71±0.72 | 0.1112±0.0077 |
| **PeriodicBFN** | **70.05±0.04** | **0.0370±0.0009** | **27.03±0.13** | **0.1105±0.0024** |

+5.7 / +7.3 match-rate points over strongest prior BFN on MP-20 / MPTS-52.

### Ablation on MP-20

| Variant | MR↑ | RMSE↓ |
|---|---|---|
| **PeriodicBFN** | **70.05** | **0.0370** |
| w/o RB | 66.11 | 0.0507 |
| w/o 2D emb. | 60.02 | 0.0569 |

### CLF phase synthesis

| Method | PSNR↑ | FPS↑ |
|---|---|---|
| Conj. Grad. | 34.31±1.21 | 1.45 |
| EyeReal | 27.46±1.18 | 51.55 |
| **EyeReal + PeriodicBFN** | **31.40±1.05** | **28.49** |