Diffusion-Based Particle Configuration Generator

Detailed Technical Documentation

Overview

This project implements a conditional diffusion model to generate particle configurations in accelerators while preserving collective effects. The approach treats particle generation as a denoising process, where the model learns to transform random noise into physically plausible particle arrangements.

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1. Mathematical Foundation

1.1 Diffusion Process Theory

Forward Process (Adding Noise):

```
q(x_t | x_{t-1}) = N(x_t; √(1-β_t)x_{t-1}, β_t I)
```

Where:

- `x_t` is the noisy data at timestep t
- `β_t` is the noise schedule (increases from 0.0001 to 0.02)
- `N(μ, σ²)` represents a Gaussian distribution

Reverse Process (Denoising):

```
p_θ(x_{t-1} | x_t) = N(x_{t-1}; μ_θ(x_t, t), Σ_θ(x_t, t))
```

The neural network learns to predict the noise `ε_θ(x_t, t, c)` where `c` is the conditioning information (beam energy).

1.2 Physics Integration

Coulomb Force Calculation:

```
F_i = Σ_j (q_i × q_j × r_ij) / |r_ij|³
```

Where:

- `q_i, q_j` are particle charges

- `r_ij` is the distance vector between particles i and j
- This captures the collective effects between particles

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2. Code Architecture Analysis

2.1 ParticleDataGenerator Class

Purpose: Generate synthetic particle accelerator data with realistic collective effects.

Key Methods:

`coulomb_force(positions, charges)`

python

```python
def coulomb_force(self, positions, charges):
    forces = np.zeros_like(positions)
    for i in range(len(positions)):
        for j in range(len(positions)):
            if i != j:
                r_vec = positions[i] - positions[j]
                r_dist = np.linalg.norm(r_vec)
                if r_dist > 0.1:  # Avoid singularity
                    force = charges[i] * charges[j] * r_vec / (r_dist**3)
                    forces[i] += force
    return forces
```

Technical Details:

- Implements $O(N^2)$ force calculation between all particle pairs
- Uses regularization (`r_dist > 0.1`) to avoid numerical instability
- Returns force vectors for each particle
- **Physics Significance:** This is the core collective effect - particles influence each other's positions

`generate_configuration(beam_energy, charge_ratio)`

python

```python
def generate_configuration(self, beam_energy=1.0, charge_ratio=0.5):
    # Initial beam-like distribution
    positions = np.random.normal(0, 0.5, (self.n_particles, 2))
    positions[:, 0] += np.random.normal(0, 0.1, self.n_particles)

    # Assign charges
    charges = np.ones(self.n_particles)
    n_negative = int(self.n_particles * charge_ratio)
    charges[:n_negative] = -1

    # Apply collective effects
    forces = self.coulomb_force(positions, charges)
    positions += forces * 0.01

    return positions, charges, beam_energy
```

Technical Details:

- Creates realistic beam distribution (Gaussian in transverse, focused in longitudinal)
- Mixes positive and negative charges based on `charge_ratio`
- Applies force-based displacement to simulate collective effects
- **Beam Energy Effect:** Higher energy → more spread in longitudinal direction

2.2 SimpleDiffusionModel Class

Purpose: Neural network that predicts noise in particle configurations.

Architecture:

python

```python
self.network = nn.Sequential(
    nn.Linear(input_dim + condition_dim + 1, hidden_dim),  # +1 for timestep
    nn.ReLU(),
    nn.Linear(hidden_dim, hidden_dim),
    nn.ReLU(),
    nn.Linear(hidden_dim, hidden_dim),
    nn.ReLU(),
    nn.Linear(hidden_dim, input_dim)
)
```

Technical Details:

- **Input:** Flattened particle positions + timestep + beam energy condition
- **Output:** Predicted noise with same shape as input positions
- **Hidden Layers:** 3 layers with ReLU activation for non-linearity
- **Conditioning:** Beam energy is concatenated to input, enabling energy-dependent generation

forward(x, t, condition)

python

```python
def forward(self, x, t, condition):
    x_flat = x.view(x.size(0), -1)  # Flatten positions
    t_embed = t.unsqueeze(1) if t.dim() == 1 else t
    condition = condition.unsqueeze(1) if condition.dim() == 1 else condition

    input_tensor = torch.cat([x_flat, t_embed, condition], dim=1)
    noise_pred = self.network(input_tensor)

    return noise_pred.view(x.shape)  # Reshape back
```

Technical Details:

- Flattens 2D particle positions to 1D vector for neural network
- Concatenates timestep and condition information
- Returns noise prediction in original shape
- **Key Innovation:** Conditional generation based on beam energy

2.3 DiffusionTrainer Class

Purpose: Handles the training and sampling process for the diffusion model.

Noise Schedule

python

```python
self.betas = torch.linspace(self.beta_start, self.beta_end, self.timesteps)
self.alphas = 1 - self.betas
self.alpha_cumprod = torch.cumprod(self.alphas, dim=0)
```

Technical Details:

- **Beta Schedule:** Linear from 0.0001 to 0.02 over 100 timesteps
- **Alpha Values:** $\alpha_t = 1 - \beta_t$ (amount of signal preserved)

- **Cumulative Alpha:** `ᾱ_t = ∏(α_i)` (total signal after t steps)
- **Purpose:** Controls how much noise is added at each timestep

`add_noise(x, noise, t)`

```python
def add_noise(self, x, noise, t):
    alpha_cumprod_t = self.alpha_cumprod[t].view(-1, 1, 1)
    return torch.sqrt(alpha_cumprod_t) * x + torch.sqrt(1 - alpha_cumprod_t) * noise
```

Mathematical Implementation:

```
x_t = √(ᾱ_t) × x_0 + √(1 - ᾱ_t) × ε
```

Where:

- `x_0` is the original clean data
- `ε` is random noise
- `ᾱ_t` controls the noise level at timestep t

`train_step(batch_positions, batch_conditions, optimizer)`

```python
def train_step(self, batch_positions, batch_conditions, optimizer):
    # Sample random timesteps
    t = torch.randint(0, self.timesteps, (batch_size,), device=self.device)

    # Sample noise
    noise = torch.randn_like(batch_positions)

    # Add noise to positions
    noisy_positions = self.add_noise(batch_positions, noise, t)

    # Predict noise
    predicted_noise = self.model(noisy_positions, t.float(), batch_conditions)

    # Calculate loss
    loss = nn.MSELoss()(predicted_noise, noise)

    return loss.item()
```

Training Process:

1. **Random Timestep:** Sample t uniformly from [0, T]
2. **Noise Addition:** Add noise according to schedule
3. **Noise Prediction:** Model predicts the added noise
4. **Loss Calculation:** MSE between predicted and actual noise
5. **Backpropagation:** Update model parameters

sample(n_samples, condition, shape)

python

```python
def sample(self, n_samples, condition, shape):
    # Start with random noise
    x = torch.randn(n_samples, *shape, device=self.device)

    # Reverse diffusion process
    for t in reversed(range(self.timesteps)):
        t_tensor = torch.tensor([t] * n_samples, dtype=torch.float32, device=self.device)

        # Predict noise
        predicted_noise = self.model(x, t_tensor, condition_tensor)

        # Remove noise (DDPM sampling)
        alpha_t = self.alphas[t]
        alpha_cumprod_t = self.alpha_cumprod[t]
        beta_t = self.betas[t]

        x = (1 / torch.sqrt(alpha_t)) * (x - (beta_t / torch.sqrt(1 - alpha_cumprod_t)) * predicted_noise)

        # Add noise for non-final steps
        if t > 0:
            noise = torch.randn_like(x)
            x = x + torch.sqrt(beta_t) * noise

    return x
```

Sampling Process:

1. **Initialize:** Start with pure noise
2. **Reverse Steps:** Iteratively remove noise for T steps
3. **Denoising Formula:**

```
x_{t-1} = (1/√α_t) × (x_t - (β_t/√(1-ᾱ_t)) × ε_θ(x_t, t, c))
```

4. **Stochastic Component:** Add small noise except at final step
5. **Conditioning:** Use beam energy to guide generation

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3. Data Flow and Processing

3.1 Training Data Pipeline

1. **Configuration Generation:**

```
Raw Parameters → Coulomb Forces → Particle Positions
```

2. **Data Preprocessing:**

python

```python
positions_flat = positions_tensor.view(-1, positions_tensor.size(-1))
positions_flat_norm = scaler.fit_transform(positions_flat)
```

- Flattens 3D tensor (samples × particles × coordinates) to 2D
- Applies StandardScaler for normalization
- Reshapes back to original structure

3. **Batch Processing:**

python

```python
dataset = TensorDataset(positions_tensor, conditions_tensor)
dataloader = DataLoader(dataset, batch_size=32, shuffle=True)
```

3.2 Model Input/Output Shapes

Training:

- Input: `(batch_size, n_particles, 2)` - particle positions
- Condition: `(batch_size, 1)` - beam energy
- Timestep: `(batch_size, 1)` - diffusion timestep
- Output: `(batch_size, n_particles, 2)` - predicted noise

Sampling:

- Input: `(n_samples, n_particles, 2)` - random noise
- Output: `(n_samples, n_particles, 2)` - generated configurations

4. Physics Interpretation

4.1 Collective Effects Modeling

What the Model Learns:

- Spatial correlations between particles due to electromagnetic forces
- Energy-dependent beam spreading
- Charge distribution effects on particle arrangements
- Realistic beam envelope shapes

Physical Validation:

- Generated configurations should show repulsion between like charges
- Higher beam energy should produce more spread configurations
- Particle density should follow beam-like distributions

4.2 Conditional Generation

Beam Energy Conditioning:

- Low energy (0.8): Tight beam, less spreading
- Medium energy (1.2): Moderate spreading
- High energy (1.6): Significant spreading

Physical Meaning:

- Higher energy particles have more momentum
- Collective effects become more pronounced
- Beam envelope expands with energy

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5. Technical Advantages

5.1 Compared to Traditional Methods

Traditional Particle Simulation:

- Requires expensive N-body calculations
- Computationally intensive for large particle numbers
- Difficult to explore parameter space efficiently

Diffusion Model Approach:

- Fast generation once trained
- Inherently probabilistic (captures uncertainty)
- Conditional generation for parameter exploration
- Learns complex collective effects implicitly

5.2 Compared to Other Generative Models

vs. GANs:

- More stable training (no adversarial dynamics)
- Better mode coverage (less mode collapse)
- Easier to condition on physical parameters

vs. VAEs:

- Higher generation quality
- Better handling of multi-modal distributions
- More flexible conditioning mechanisms

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6. Potential Extensions

6.1 Physics Enhancements

- **Relativistic Effects:** Modify force calculations for high-energy particles
- **Magnetic Fields:** Add Lorentz force terms
- **3D Geometry:** Extend to full 3D particle tracking
- **Time Evolution:** Model temporal dynamics

6.2 Model Improvements

- **Transformer Architecture:** Better handling of particle interactions
- **Graph Neural Networks:** Explicit modeling of particle relationships
- **Multi-Scale Modeling:** Different resolution levels
- **Uncertainty Quantification:** Bayesian neural networks

6.3 Applications

- **Accelerator Design:** Optimize beam configurations

- **Digital Twins:** Real-time simulation of accelerator states
- **Anomaly Detection:** Identify unusual particle behaviors
- **Control Systems:** Predictive control based on generated scenarios

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7. Limitations and Considerations

7.1 Current Limitations

- **Simplified Physics:** Only Coulomb forces, no magnetic effects
- **2D Geometry:** Real accelerators are 3D
- **Static Generation:** No temporal evolution
- **Limited Particle Numbers:** Scalability to thousands of particles

7.2 Numerical Considerations

- **Normalization:** Critical for stable training
- **Noise Schedule:** Affects generation quality
- **Architecture Size:** Balance between capacity and overfitting
- **Training Time:** Requires sufficient epochs for convergence

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8. Validation and Testing

8.1 Physics Validation

- **Force Conservation:** Check if generated configurations respect physical laws
- **Energy Scaling:** Verify beam energy effects on particle distribution
- **Charge Separation:** Ensure like charges repel, unlike charges attract

8.2 Statistical Validation

- **Distribution Matching:** Compare generated vs. real particle distributions
- **Correlation Analysis:** Check spatial correlations in generated data
- **Conditional Consistency:** Verify energy conditioning works correctly

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9. References and Further Reading

9.1 Core Papers

- **Diffusion Models:** Ho et al., "Denoising Diffusion Probabilistic Models" (2020)

- **Conditional Generation:** Dhariwal & Nichol, "Diffusion Models Beat GANs on Image Synthesis" (2021)
- **Physics-Informed ML:** Raissi et al., "Physics-informed neural networks" (2019)

9.2 Accelerator Physics

- **Beam Dynamics:** Wiedemann, "Particle Accelerator Physics" (2007)
- **Collective Effects:** Chao & Tigner, "Handbook of Accelerator Physics" (2013)
- **Simulation Methods:** Qiang et al., "An object-oriented parallel particle-in-cell code" (2006)

9.3 Related ML Work

- **Point Cloud Networks:** Qi et al., "PointNet: Deep Learning on Point Sets" (2017)
- **Graph Neural Networks:** Battaglia et al., "Relational inductive biases" (2018)
- **Scientific ML:** Karniadakis et al., "Physics-informed machine learning" (2021)

This documentation provides a comprehensive technical understanding of the diffusion-based particle configuration generator, covering both the machine learning methodology and the underlying physics principles.