# Scientific Computing & Flow-based Generative Models

专题 2: AI for PDE

## 主要内容

**FNO** 核心算子定义为 $(\mathcal{K}v)(x) = \mathcal{F}^{-1}(R \cdot \mathcal{F}(v))(x)$，其中 $R$ 为可学习的低频复数权重矩阵。迭代更新规则为：

$$v_{t+1}(x) = \sigma(Wv_t(x) + (\mathcal{K}v_t)(x))$$

注：非线性激活函数 $\sigma$ 可以产生高频信息。

**Geo-FNO** 通过非均匀傅里叶变换处理不规则网格：

$$(\mathcal{F}_a v)(k) \approx \frac{1}{|\mathcal{T}_a|} \sum_{x \in \mathcal{T}_a} m(x) v(x) e^{-2i\pi \langle \phi_a^{-1}(x), k \rangle}$$

逆变换为：

$$(\mathcal{F}_a^{-1} \hat{v})(x) = \sum_k \hat{v}(k) e^{2i\pi \langle \phi_a^{-1}(x), k \rangle}$$

**GCN** 图卷积层的特征更新公式：

$$H^{(l+1)} = \sigma\left(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)}\right)$$

**GAT** 引入注意力机制计算节点间权重：

$$e_{ij} = \mathrm{LeakyReLU}\left(\vec{a}^T [\mathbf{W}\vec{h}_i \parallel \mathbf{W}\vec{h}_j]\right), \quad \alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k \in \mathcal{N}_i} \exp(e_{ik})}$$

$$\vec{h}_i' = \sigma\left(\sum_{j \in \mathcal{N}_i} \alpha_{ij} \mathbf{W} \vec{h}_j\right)$$

**MeshGraphNets** 基于消息传递机制的物理仿真：

$$\mathbf{e}_{ij}' = f^M(\mathbf{e}_{ij}, \mathbf{v}_i, \mathbf{v}_j) \qquad \text{(边更新)}$$

$$\mathbf{v}_i' = f^V\left(\mathbf{v}_i, \sum_{j \in \mathcal{N}_i} \mathbf{e}_{ij}'\right) \qquad \text{(节点更新)}$$

**RL for h-refine** 利用强化学习进行网格细化：

$$\text{目标函数:} \quad Q_t(s,a) = \mathbb{E}_\pi\left[\sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \mid S_t = s, A_t = a\right]$$

$$\text{奖励函数:} \quad R(S_t, a_t) = \pm[\log(\Delta u_h + \epsilon) - \log \epsilon] - \gamma_c [B(p^{t+1}) - B(p^t)]$$

$$\Delta u_h = \sum \int_K |u_h^{t+1} - u_h^t| dK, \quad B(p) = \frac{\sqrt{p}}{1-p}$$

**r-refine** 基于最优传输理论的网格移动（Moving Mesh）：

**等分布约束**：

$$M(x)\det(\nabla_\xi x) = C$$

$L^2$ **距离最小化**：

$$I[x] = \int_{\Omega_c} \|x(\xi) - \xi\|^2 d\xi$$

**Brenier 定理**：最优传输映射 $x(\xi)$ 必定是某凸函数 $P(\xi)$ 的梯度，即 $x(\xi) = \nabla P(\xi)$

**Monge-Ampère 方程**：

$$\det(H(P)) \cdot M = C$$

求解 Monge-Ampère 方程的过程也可以使用 GAT 来进行，注意损失函数：

$$L_{vol}(\theta) = \mathbb{E}_{(\xi, m_\xi; V_r, T_r)\in\mathcal{D}} \left[ \frac{1}{|T_a|} \sum_{i=1}^{n_2} |Vol(t_i) - Vol(q_i)| \right]$$

$$L_{cd}(\theta) = \mathbb{E}_{(\xi, m_\xi; V_r, T_r)\in\mathcal{D}} \left[ \frac{1}{|V_a|} \sum_{x_i\in V_a} \min_{y_j\in V_r} \|x_i - y_j\|_2 + \frac{1}{|V_r|} \sum_{y_j\in V_r} \min_{x_i\in V_a} \|x_i - y_j\|_2 \right]$$

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## 参考文献


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[5] Mingrui Zhang et al. “Towards Universal Mesh Movement Networks”. In: *The Thirty-eighth Annual Conference on Neural Information Processing Systems*. 2024. https://openreview.net/forum?id=lcALCNF2qe.