NEURAL INFORMATION PROCESSING SYSTEMS

FlashBias: Fast Computation of Attention with Bias

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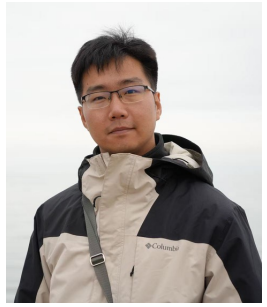
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Mingsheng Long

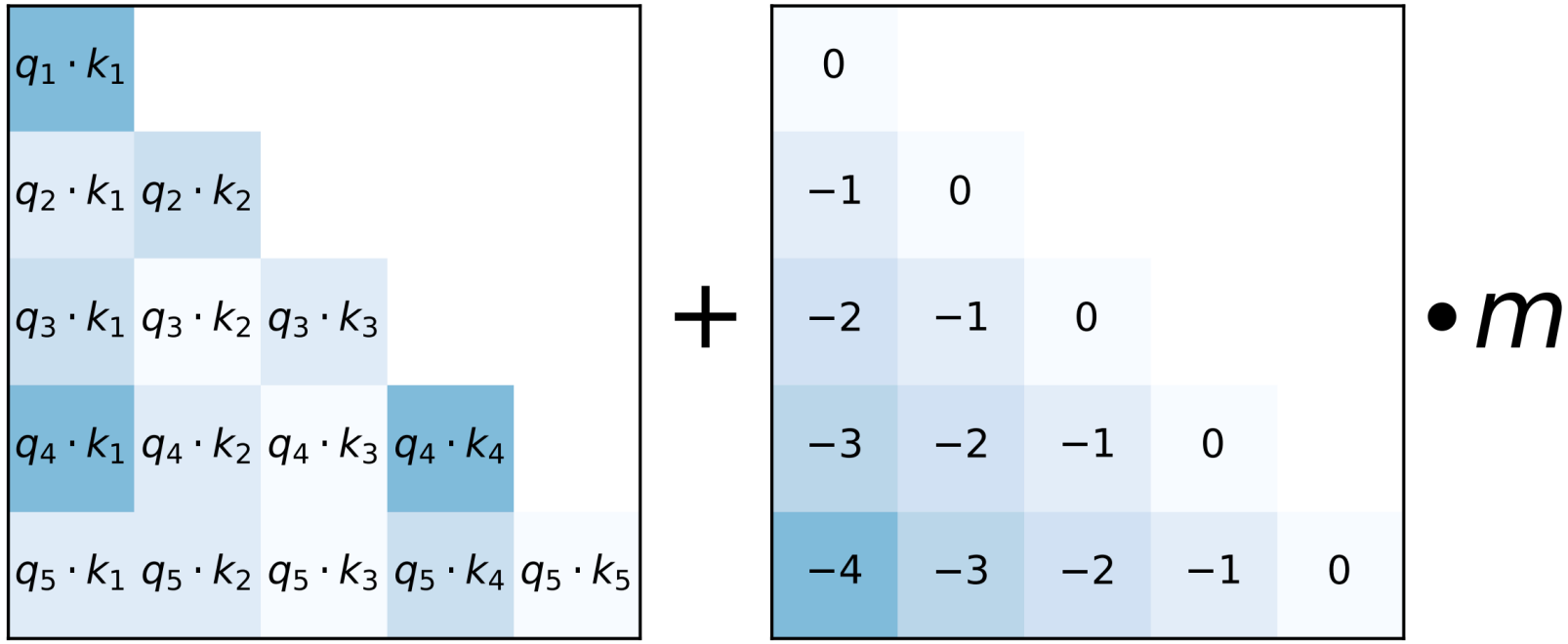
Code Link: https://github.com/thuml/FlashBias

1.5x Speedup for Pairformer in AlphaFold 3; **2x** Speedup for Swin Transformer v2. **Try FlashBias!**

Attention in Advanced Language Models

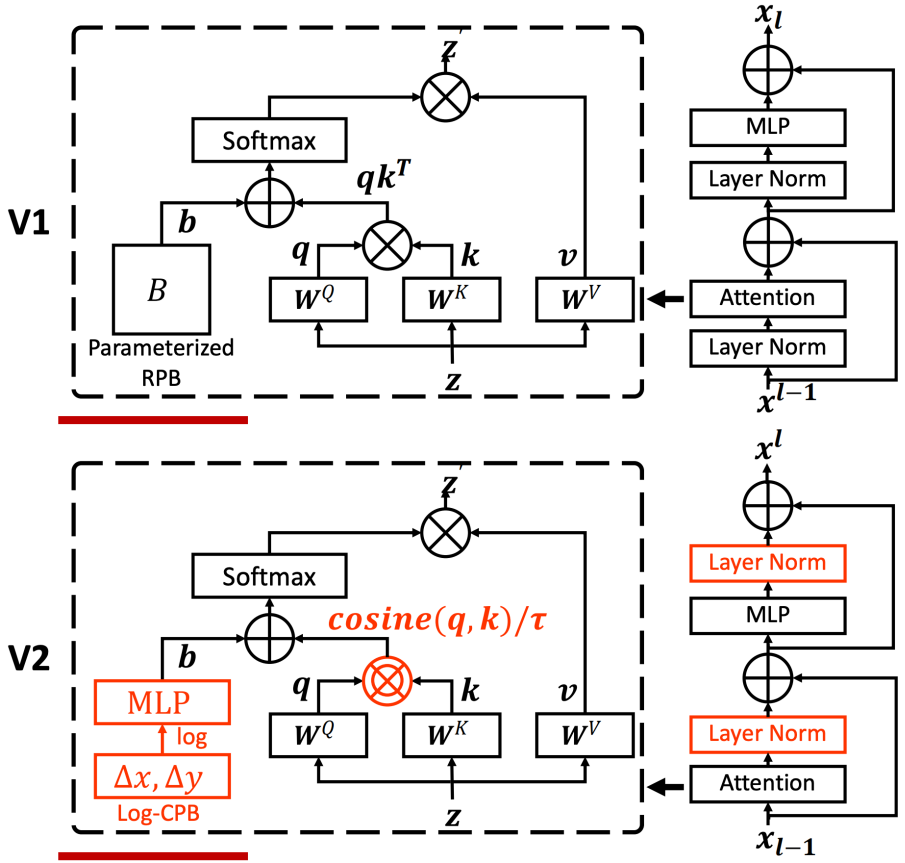
ALiBi Bias

$$\text{softmax}(\mathbf{q}_i \mathbf{K}^\top + m \cdot [-(i-1), ..., -2, -1, 0])$$



Press et al., Train Short, Test Long: Attention with Linear Biases Enables Input Length Extrapolation, ICLR 2022

Attention in Advanced Vision Models



$$\mathrm{SoftMax}(QK^T/\sqrt{d}+B)V,$$

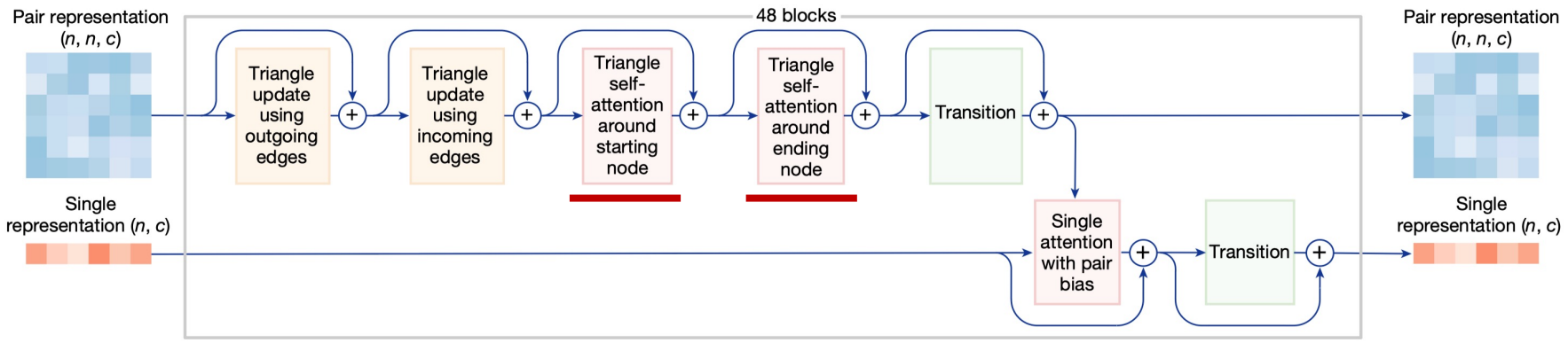
Relative Position Bias

$$\cos(\mathbf{q}_i,\mathbf{k}_j)/\tau + B_{ij}$$

Relative Position Bias

Liu et al., Swin Transformer V2: Scaling Up Capacity and Resolution, CVPR 2022

Attention in Advanced Scientific Models



 # Attention

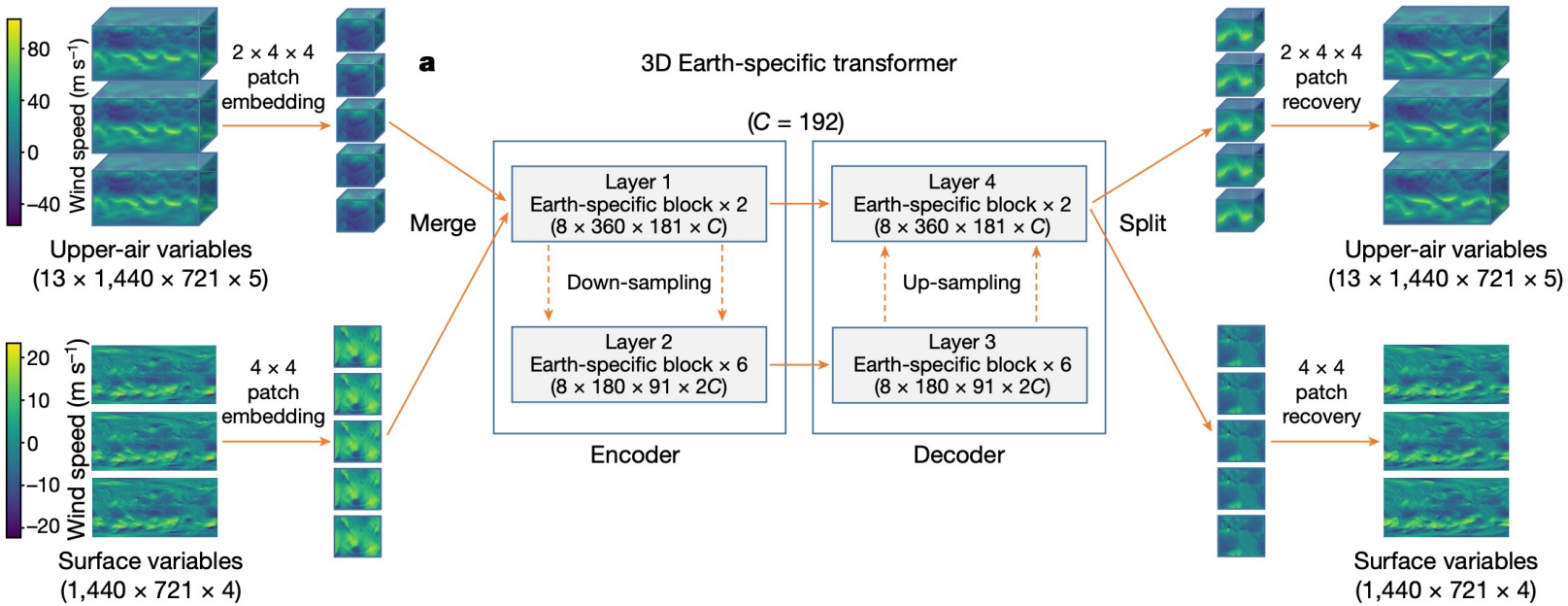
$$5:\ a_{ijk}^h = \mathrm{softmax}_k\left(\frac{1}{\sqrt{c}}\,\mathbf{q}_{ij}^{h\top}\mathbf{k}_{ik}^h + b_{jk}^h\right)$$

$$6:\ \mathbf{o}_{ij}^h = \mathbf{g}_{ij}^h \odot \textstyle\sum_k a_{ijk}^h \mathbf{v}_{ik}^h$$

Pair Representation Bias

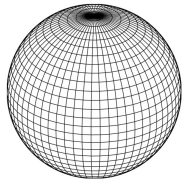
Abramson et al., Accurate structure prediction of biomolecular interactions with AlphaFold 3, Nature 2024

Attention in Advanced Scientific Models



$$\mathrm{Attention}(\mathbf{Q},\mathbf{K},\mathbf{V}) = \mathrm{SoftMax}(\mathbf{Q}\mathbf{K}^{\top}/\sqrt{D} + \mathbf{B})\mathbf{V}$$

Earth-specific Positional Bias



Bi et al., Accurate medium-range global weather forecasting with 3D neural networks, Nature 2023

Attention with Bias

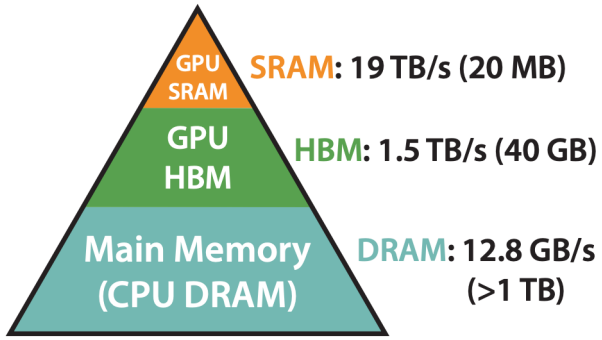
$$\mathbf{o} = \mathrm{softmax}(\frac{\mathbf{q}\mathbf{k}^\top}{\sqrt{C}} + \mathbf{b})\mathbf{v}.$$

queries $\mathbf{q} \in \mathbb{R}^{N\times C}$, keys $\mathbf{k} \in \mathbb{R}^{M\times C}$ and values $\mathbf{v} \in \mathbb{R}^{M\times C}$, bias $\mathbf{b} \in \mathbb{R}^{N\times M}$

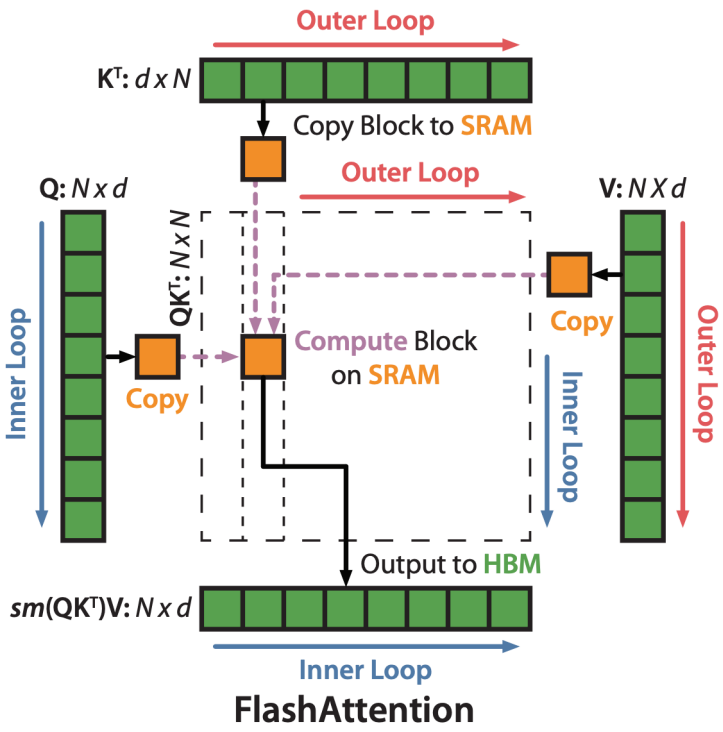
Introduce prior knowledge to guide attention learning

Vanilla FlashAttention

$$\mathbf{o} = \text{softmax}(\frac{\mathbf{q}\mathbf{k}^\top}{\sqrt{C}} + \mathbf{b})\mathbf{v}.$$

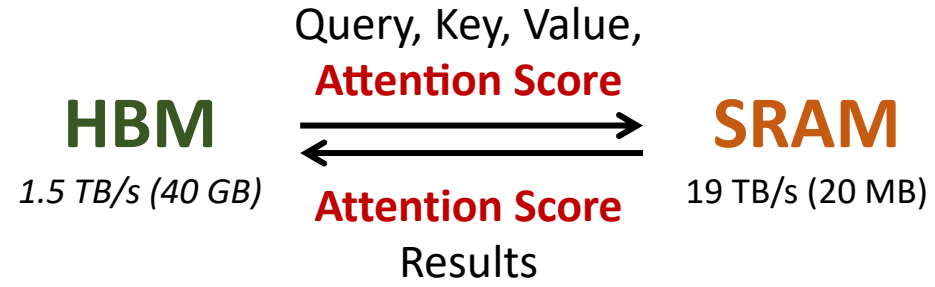


Memory Hierarchy with Bandwidth & Memory Size

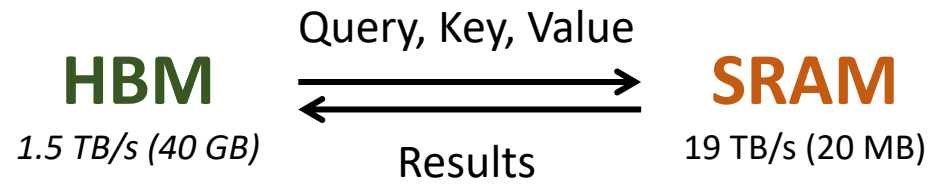


FlashAttention

- Standard Implementation: **Quadratic IO Complexity**



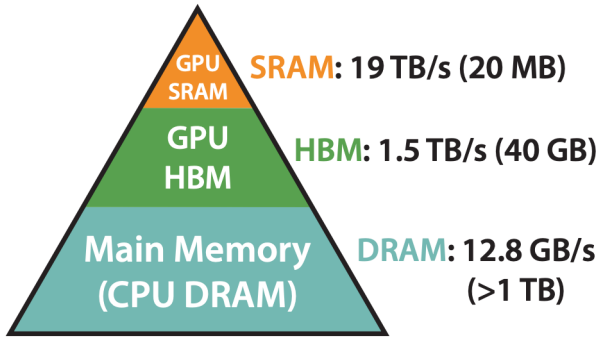
- FlashAttention: **Reduced IO Complexity**



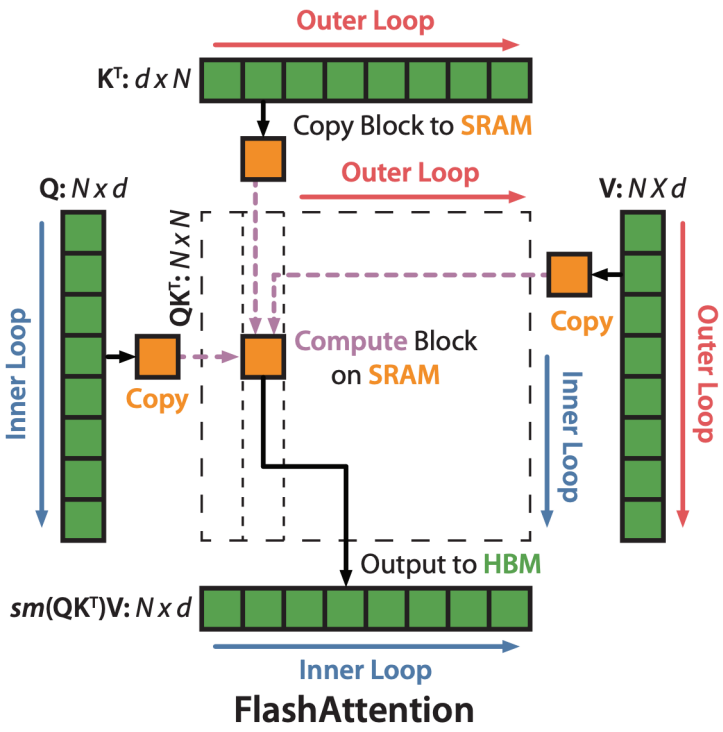
Dao et al., FlashAttention: Fast and Memory-Efficient Exact Attention with IO-Awareness, NeurIPS 2022
Dao et al., FlashAttention-2: Faster Attention with Better Parallelism and Work Partitioning, ICLR 2024

Vanilla FlashAttention Fails

$$\mathbf{o} = \text{softmax}(\frac{\mathbf{q}\mathbf{k}^\top}{\sqrt{C}} + \mathbf{b})\mathbf{v}.$$

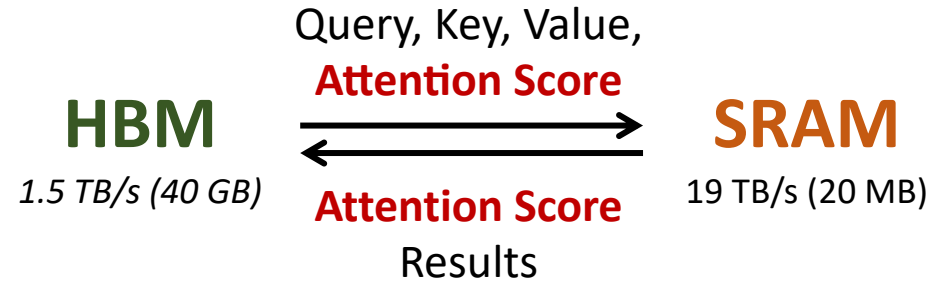


Memory Hierarchy with Bandwidth & Memory Size

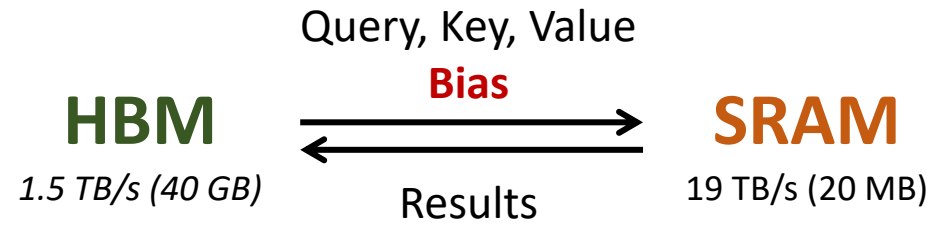


FlashAttention

- Standard Implementation: **Quadratic IO Complexity**



- FlashAttention: **Quadratic IO Complexity**



Dao et al., FlashAttention: Fast and Memory-Efficient Exact Attention with IO-Awareness, NeurIPS 2022

Dao et al., FlashAttention-2: Faster Attention with Better Parallelism and Work Partitioning, ICLR 2024

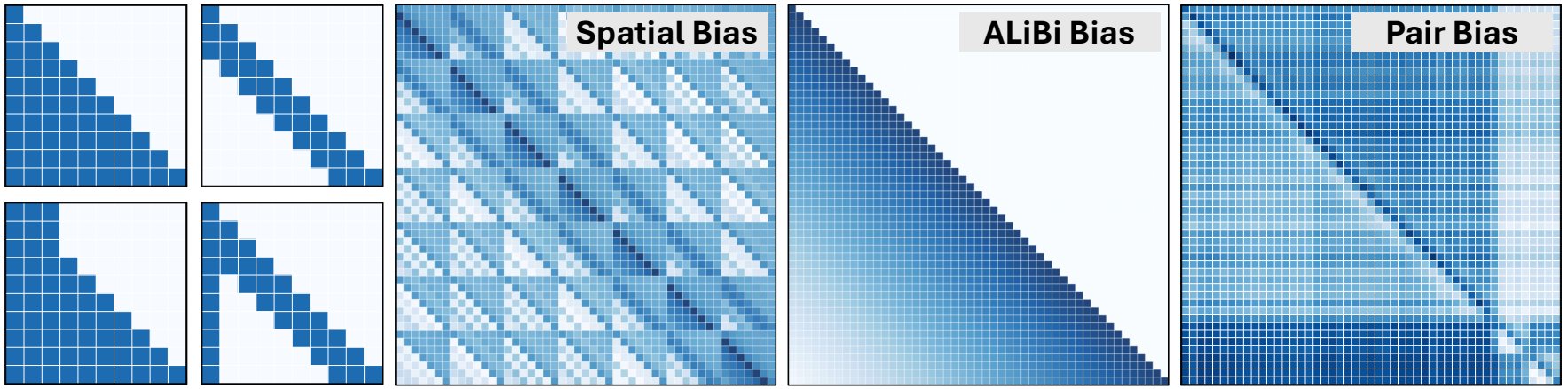
Challenge in Optimizing Attention with Bias

$$\mathbf{o} = \text{softmax}(\frac{\mathbf{q}\mathbf{k}^\top}{\sqrt{C}} + \mathbf{b})\mathbf{v}.$$

queries $\mathbf{q} \in \mathbb{R}^{N\times C}$, keys $\mathbf{k} \in \mathbb{R}^{M\times C}$ and values $\mathbf{v} \in \mathbb{R}^{M\times C}$, bias $\mathbf{b} \in \mathbb{R}^{N\times M}$

Introduce prior knowledge to guide attention learning

Sparse

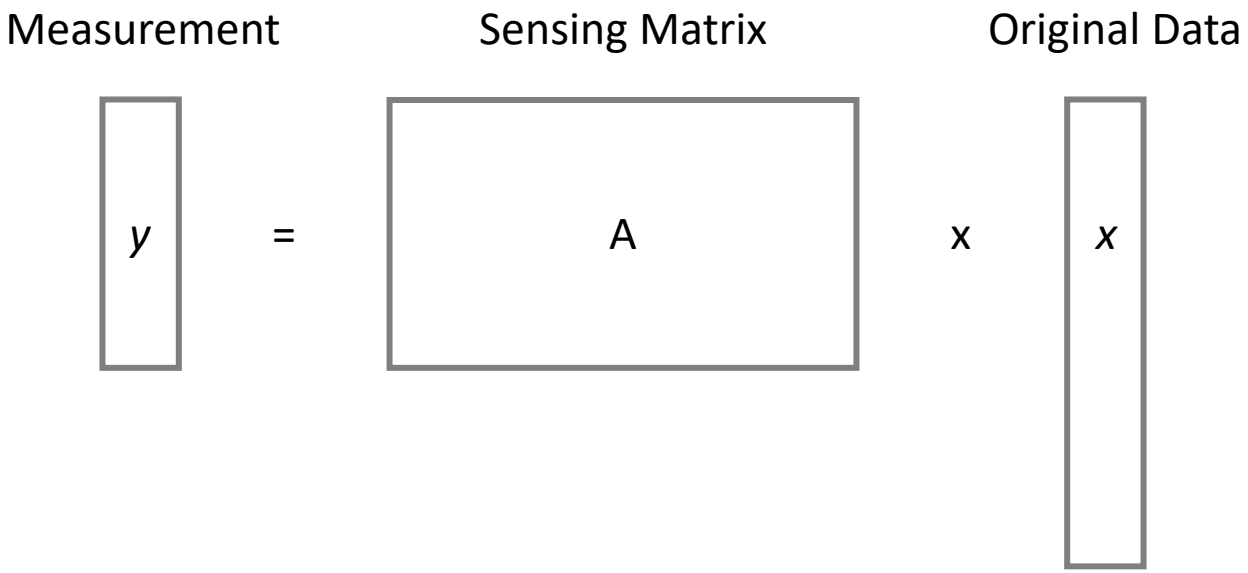


Dense
Continuous

(a) Attention Mask (b) Attention Bias in Famous Transformers

Inevitable IO complexity for loading the dense bias matrix

A Typical Compressed Sensing Problem

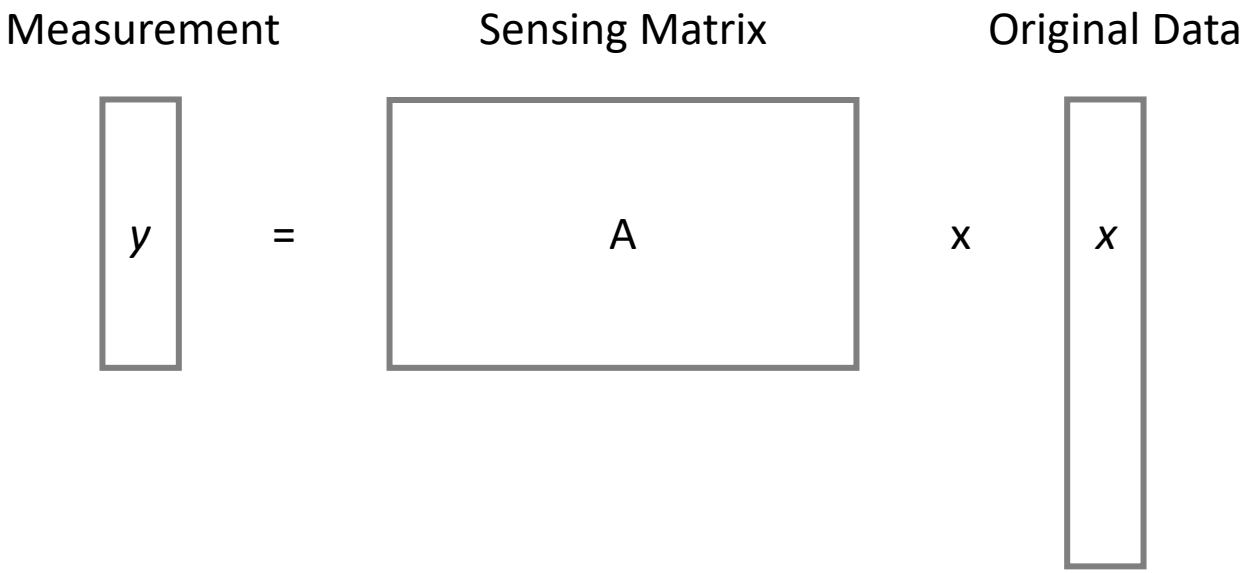


- **Compressed Sensing:** “measurement” (storage) is expensive, but the computation is cheap
- **Attention Computation:** IO is slow, but on-chip computation is fast

If we can compress the original data (Bias Matrix), we can reduce the IO complexity.

Donoho et al., Compressed sensing. IEEE Transactions on information theory 2006

A Typical Compressed Sensing Problem



Theorem (from Emmanuel J. Candès and Terence Tao)

For an *N*x*N* dense Matrix with rank-*R*, the smallest measurement is $\Theta(NR)$.

Determined by the rank of matrix

Candès et al., The power of convex relaxation: Near-optimal matrix completion. IEEE Transactions on information theory 2010

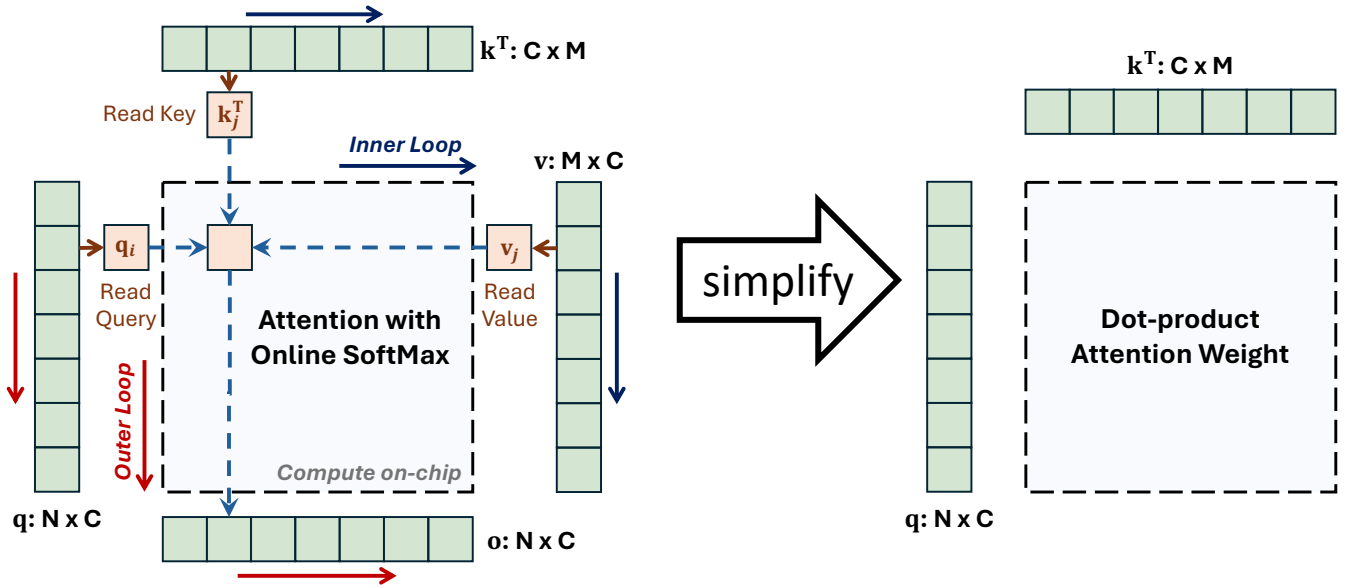
Why FlashAttention is Fast? Underlying low rank assumption

Given Sequence len *N*, Channel dim *C*, SRAM size *S* and $C=\alpha N,\ S=\beta NC$

1) FlashAttention IO Complexity is $\Theta\left(\left(1+\frac{1}{\alpha}\right)\beta\right)$ *smaller than standard attention*

2) Suppose dot-product attention weight $\mathbf{s}=\mathbf{q}\mathbf{k}^{\mathrm{T}}$ *is of rank R,* $\alpha \geq \frac{R}{N}$

The speedup ratio of FlashAttention $\propto \frac{1}{\alpha}$ and $\propto \beta$. β is usually fixed. **α determines performance.**



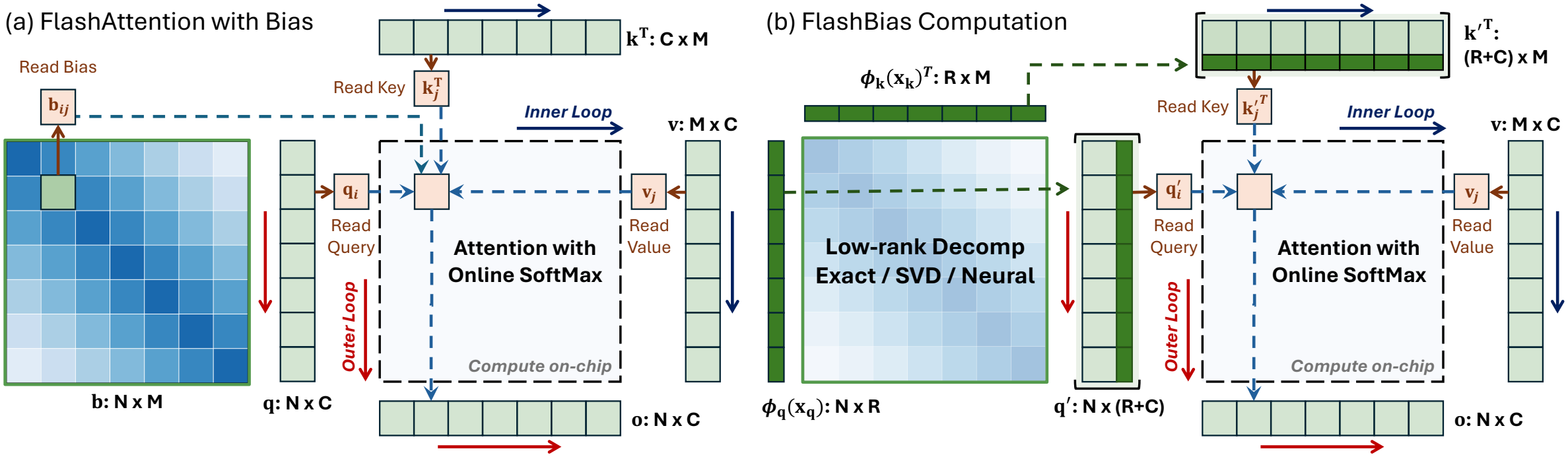
Reverse thinking 💡

Query and key are from low-rank decomposition of attention score.

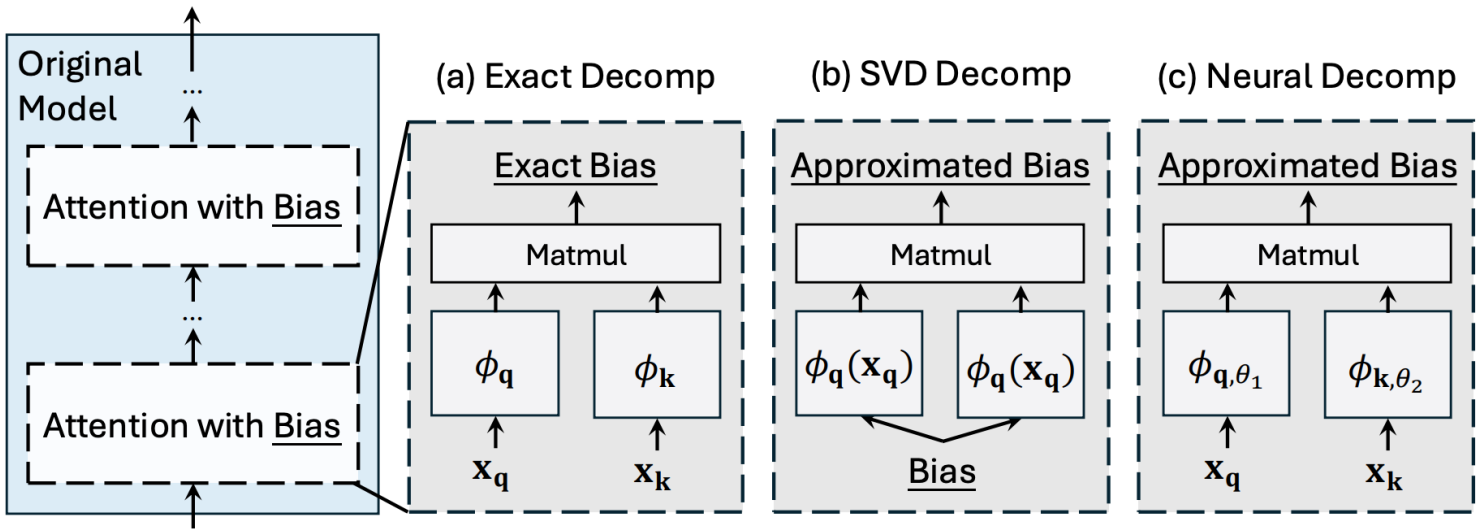
FlashBias: Achieving theoretically optimal complexity

1) Low-rank Decomp $\mathbf{b} = f(\mathbf{x_q}, \mathbf{x_k}) = \phi_\mathbf{q}(\mathbf{x_q})\phi_\mathbf{k}(\mathbf{x_k})^\top, \ \ \phi_\mathbf{q}, \phi_\mathbf{k} : \mathbb{R}^{C'} \to \mathbb{R}^R.$

2) Fast computation $\mathbf{o} = \mathrm{softmax}(\frac{\mathbf{q}\mathbf{k}^\top}{\sqrt{C}} + \mathbf{b})\mathbf{v} = \mathrm{softmax}\left(\frac{[\mathbf{q}|\sqrt{C}\phi_\mathbf{q}(\mathbf{x_q})]\ [\mathbf{k}|\phi_\mathbf{k}(\mathbf{x_k})]^\top}{\sqrt{C}}\right)\mathbf{v}.$



FlashBias: Three concrete instantiations for decomposition



Domain	Bias / Model	Type
Language	ALiBi [29]	(a)
Vision	Swin Trans. [24]	(b)
Science	Spatial Distance	(a)
	Pangu-Weather [4]	(b)
	AlphaFold [1]	(c)

1) Exact Decomp: for some representative bias, such as ALiBi or spatial distance bias.

$$f(\mathbf{x_q},_i, \mathbf{x_k},_j) = i - j \ , \ \phi_{\mathbf{q}}(\mathbf{x_q},_i) = [1, i] \ and \ \phi_{\mathbf{k}}(\mathbf{x_k},_j) = [-j, 1]$$

2) SVD Decomp: when the bias term is learnable model parameters

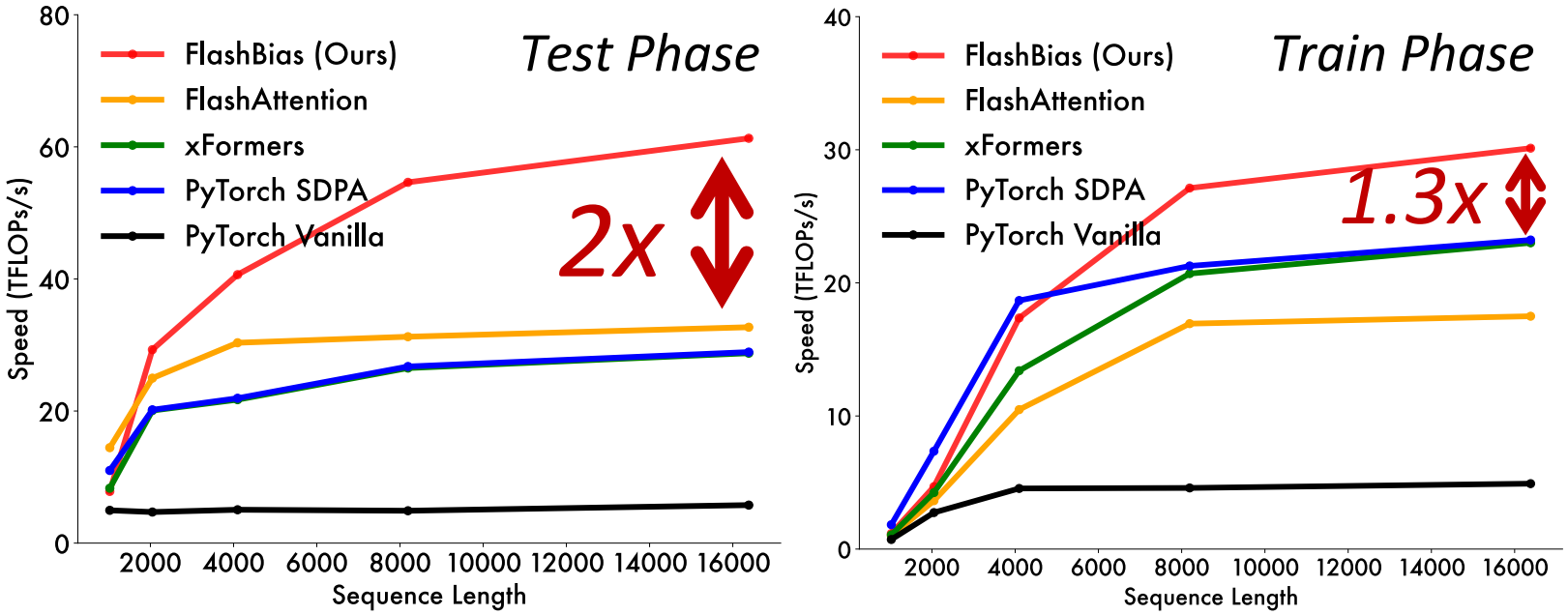
3) Neural Decomp: when the bias term is data dependent

$$\min_{\theta_1,\theta_2} \mathcal{L}(\mathbf{x_q}, \mathbf{x_k}) = \|\widehat{\phi}_{\mathbf{q},\theta_1}(\mathbf{x_q})\widehat{\phi}_{\mathbf{k},\theta_2}(\mathbf{x_k})^\top - f(\mathbf{x_q}, \mathbf{x_k})\|_2^2.$$

Relative information

Usage and Comparison

```
>> from flash_bias_triton import flash_bias_func
>> output = flash_bias_func(q, k, v, q_bias, k_bias, mask=None, causal=False, softmax_scale=1/math.sqrt(headdim))
```



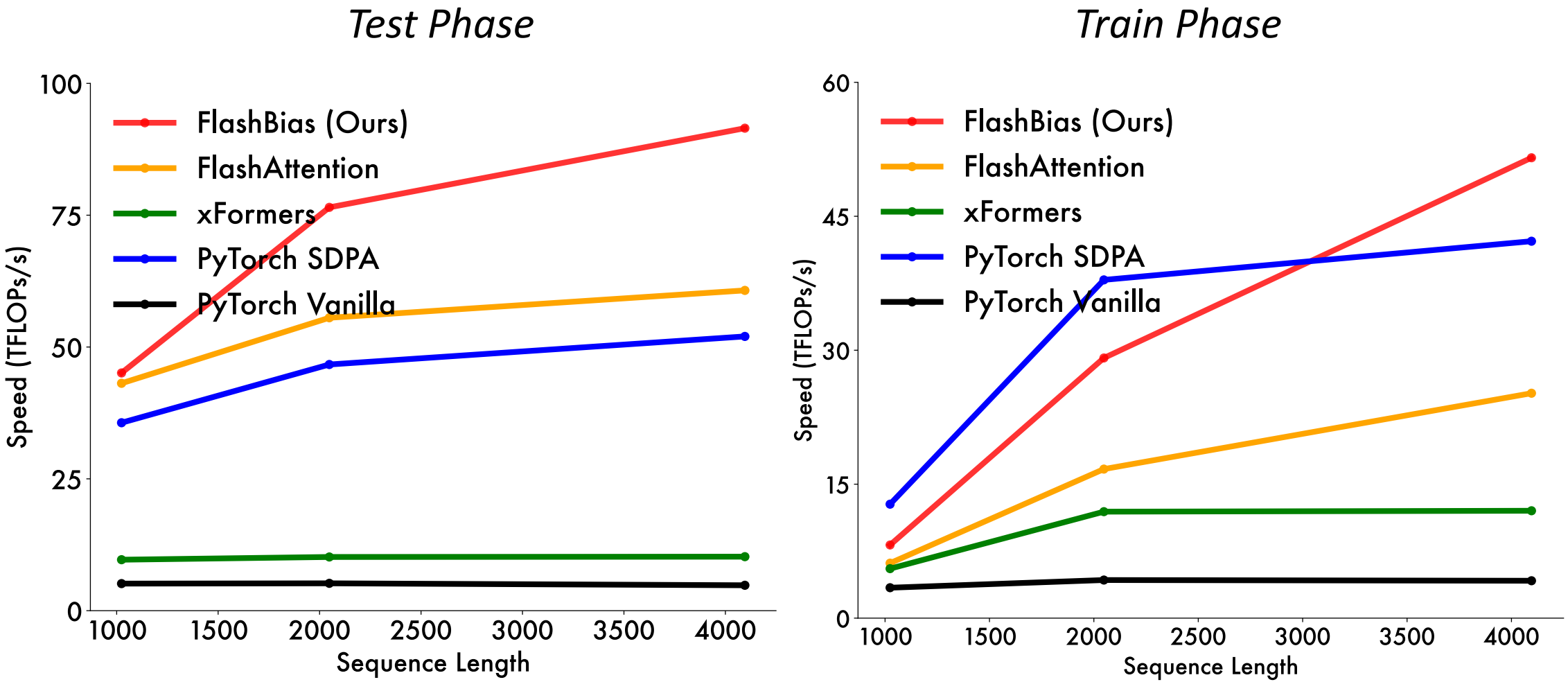
Surpass FlashAttention, PyTorch SDPA, xFormers (bs2-head4-headdim32-noncausal-rank8)

https://github.com/Dao-AILab/flash-attention

https://github.com/facebookresearch/xformers

https://docs.pytorch.org/docs/stable/generated/torch.nn.functional.scaled_dot_product_attention.html

Case 1: GPT-2 with ALiBi Bias (Exact Decomp, Causal Mask, R=2)



batchsize1-head50-headdim32-causal-rank2

Case 2: Swin Transformer V2 (SVD Decomp, R=16)

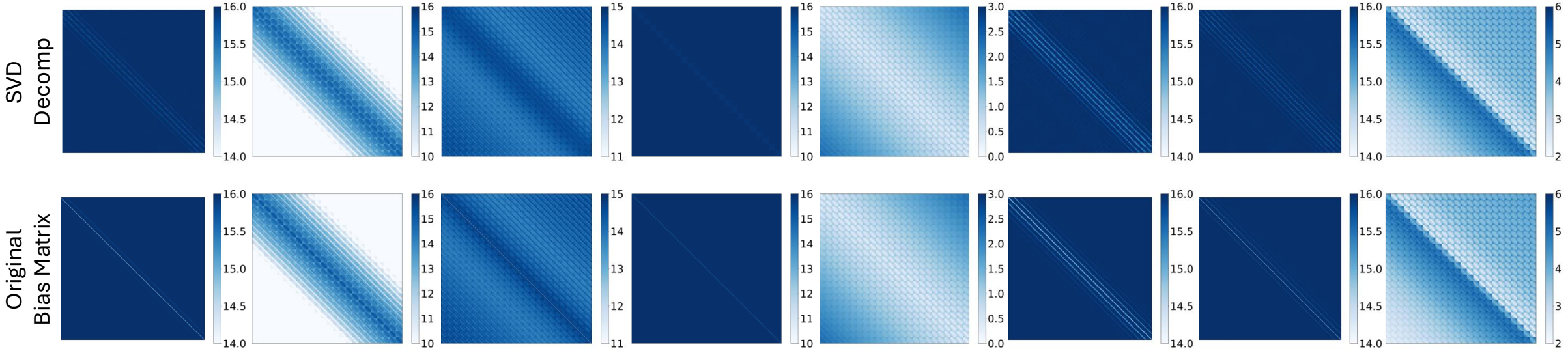
Table 4: Experiment of SwinV2-B on ImageNet-1K. #Time and #Mem correspond to inference efficiency on A100 per batch. Offline calculation of SVD for all biases takes 4.79s.

Method	Acc@1	Acc@5	Time(s)	Mem(MB)
Official Code	87.144%	98.232%	0.473	12829
Pure FlashAttention	9.376%	19.234%	0.180	3957
FlashAttention with Bias	87.142%	98.232%	0.230	11448
FlexAttention [11]	87.142%	98.232%	2.885	25986
INT8 PTQ	86.46%	*Around 22% speed up*		
FlashBias (Ours)	87.186%	98.220%	0.190	9429

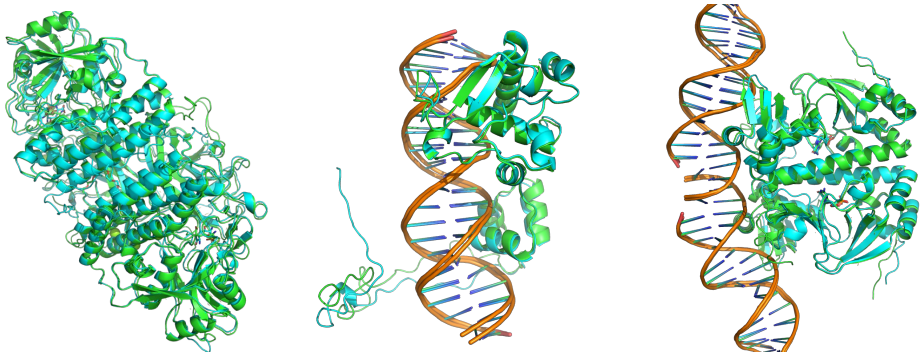
Inference time: 0.473s → 0.190s (60% reduction)

GPU memory: 12829MB → 9429MB (27% reduction)

2x speedup without any loss of accuracy



Case 3: AlphaFold 3 (Neural Decomp, R=96)



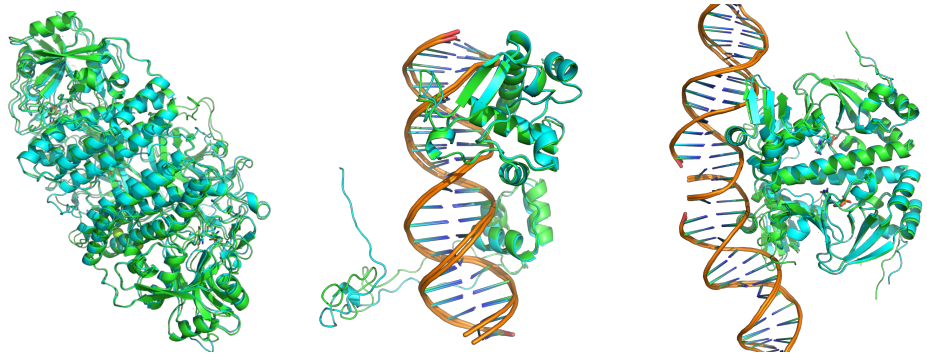
Method	Test Set	PDB ID 7wux		
	pLLDDT Loss ↓	pTM ↑	Time(s)	Mem(GB)
Open-sourced Code	3.3724	0.9500	26.85	13.62
FlashAttention w/o Bias	4.3669	0.1713	8.27	12.89
FlashAttention w/ Bias	3.3724	0.9500	20.39	13.62
FlashBias (Ours)	3.3758	0.9498	18.19	13.62

Inference time: 26.85s → 18.19s (32% reduction)

1.5x speedup without any loss of accuracy

https://github.com/bytedance/Protenix

Case 3: AlphaFold 3 (Neural Decomp, R=96)



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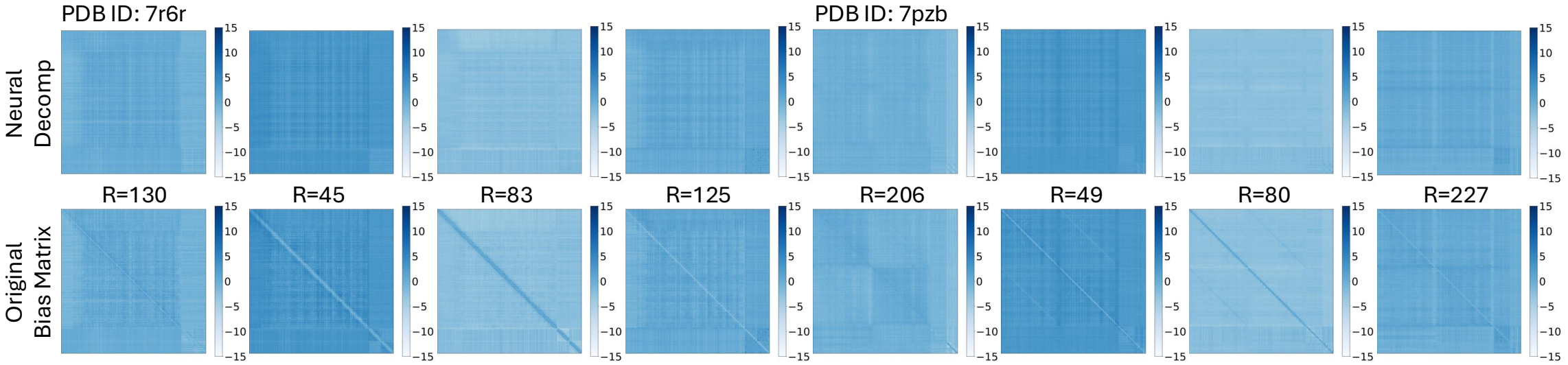
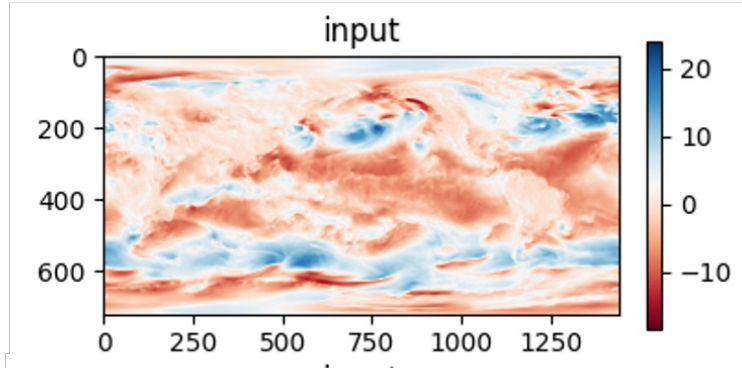


https://github.com/bytedance/Protenix

Case 4: Pangu-Weather (SVD Decomp, R=56)



Method	Output Difference	Time(s/100iters)	Mem(MB)
Open-sourced Code	-	98.022	26552
FlashAttention w/o bias	0.0128	74.089	12141
FlashAttention w/ bias	-	79.649	13186
FlashBias (Ours)	0.0003	**76.779**	**12222**

Inference time: 98s → 77s (21% reduction)

GPU memory: 26552MB → 12222MB (54% reduction)

speedup without any loss of accuracy

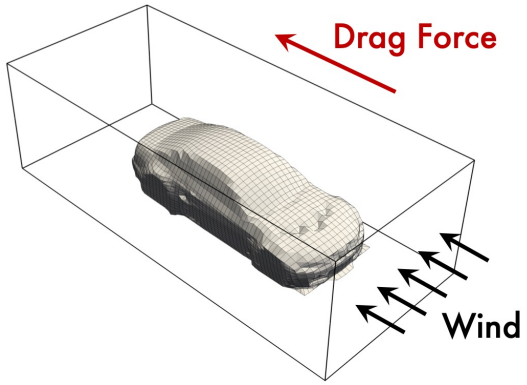
https://github.com/zhaoshan2/pangu-pytorch

Case 5: Neural Solver with Spatial Dist Bias (Exact Decomp, R=5)

For the spatial distance $f(\mathbf{x}_{\mathbf{q},i}, \mathbf{x}_{\mathbf{k},j}) = \|\mathbf{x}_{\mathbf{q},i} - \mathbf{x}_{\mathbf{k},j}\|_2^2$, *it can be exactly decomposed as:*

$$\phi_{\mathbf{q}}(\mathbf{x}_{\mathbf{q},i}) = [\mathbf{x}_{\mathbf{q},i,0}^2, 1, -2\mathbf{x}_{\mathbf{q},i,0}, \mathbf{x}_{\mathbf{q},i,1}^2, 1, -2\mathbf{x}_{\mathbf{q},i,1}, \mathbf{x}_{\mathbf{q},i,2}^2, 1, -2\mathbf{x}_{\mathbf{q},i,2}],$$
$$\phi_{\mathbf{k}}(\mathbf{x}_{\mathbf{k},j}) = [1, \mathbf{x}_{\mathbf{k},j,0}^2, \mathbf{x}_{\mathbf{k},j,0}, 1, \mathbf{x}_{\mathbf{k},j,1}^2, \mathbf{x}_{\mathbf{k},j,1}, 1, \mathbf{x}_{\mathbf{k},j,2}^2, \mathbf{x}_{\mathbf{k},j,2}]. \quad (4)$$

Based on spherical coordinates, we can further reduce R to 5.



Adaptive distance bias for better geometry information encoding:

$$f(\mathbf{x}_{\mathbf{q},i}, \mathbf{x}_{\mathbf{k},j}) = \alpha_i \|\mathbf{x}_{\mathbf{q},i} - \mathbf{x}_{\mathbf{k},j}\|_2^2$$

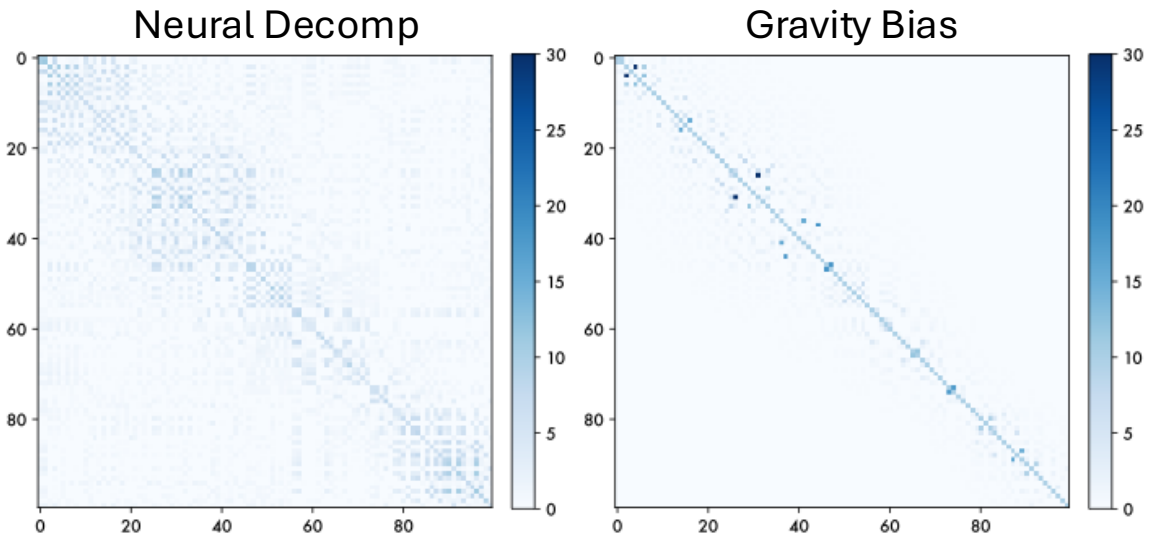
Method (Learnable Bias)	Training Phase			Inference Phase		
	8192	16384	32186	8192	16384	32186
FlashAttention	12.8 / 15.4	OOM	OOM	4.54 / 5.46	15.3 / 21.2	OOM
FlexAttention	*Not supported in current version*			21.9 / 184.0	OOM	OOM
FlashBias (Ours)	**1.46 / 4.54**	**2.02 / 14.7**	**2.97 / 51.1**	**0.98 / 1.22**	**1.03 / 3.48**	**1.13 / 12.7**

https://github.com/thuml/Neural-Solver-Library

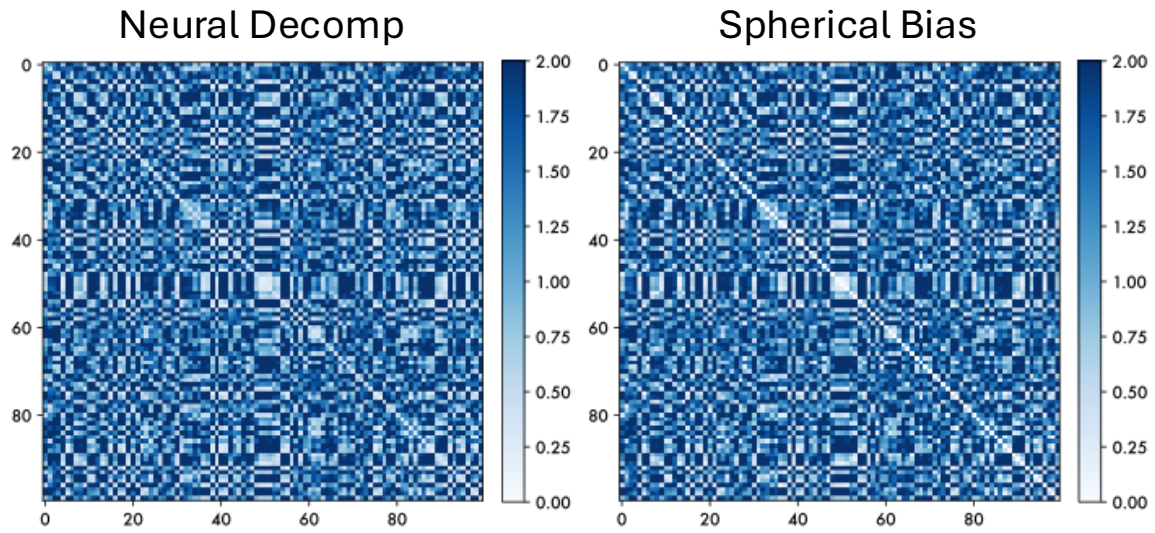
Generalization to Diverse Bias (Neural Decomp, R=32)

Gravity Bias: $$f(\mathbf{x}_{\mathbf{q},i}, \mathbf{x}_{\mathbf{k},j}) = \frac{1}{\|\mathbf{x}_{\mathbf{q},i} - \mathbf{x}_{\mathbf{k},j}\|_2^2},$$

Spherical Bias: $$f(\mathbf{x}_{\mathbf{q},i}, \mathbf{x}_{\mathbf{k},j}) = 2 \cdot \arcsin\left(\sqrt{\sin^2\left(\frac{\mathbf{x}_{\mathbf{q},i,0} - \mathbf{x}_{\mathbf{k},j,0}}{2}\right) + \cos \mathbf{x}_{\mathbf{q},i,0} \cos \mathbf{x}_{\mathbf{k},j,0} \sin^2\left(\frac{\mathbf{x}_{\mathbf{q},i,1} - \mathbf{x}_{\mathbf{k},j,1}}{2}\right)}\right)$$



(a) Gravity Bias



(b) Spherical Bias

Extension to Multiplicative Bias

$$\mathbf{o} = \text{softmax}(\frac{\mathbf{q}\mathbf{k}^\top}{\sqrt{C}} \odot \mathbf{b})\mathbf{v}$$

queries $\mathbf{q} \in \mathbb{R}^{N\times C}$, keys $\mathbf{k} \in \mathbb{R}^{M\times C}$ and values $\mathbf{v} \in \mathbb{R}^{M\times C}$, bias $\mathbf{b} \in \mathbb{R}^{N\times M}$

Introduce prior knowledge to guide attention learning

FlashBias' extension to multiplicative bias:

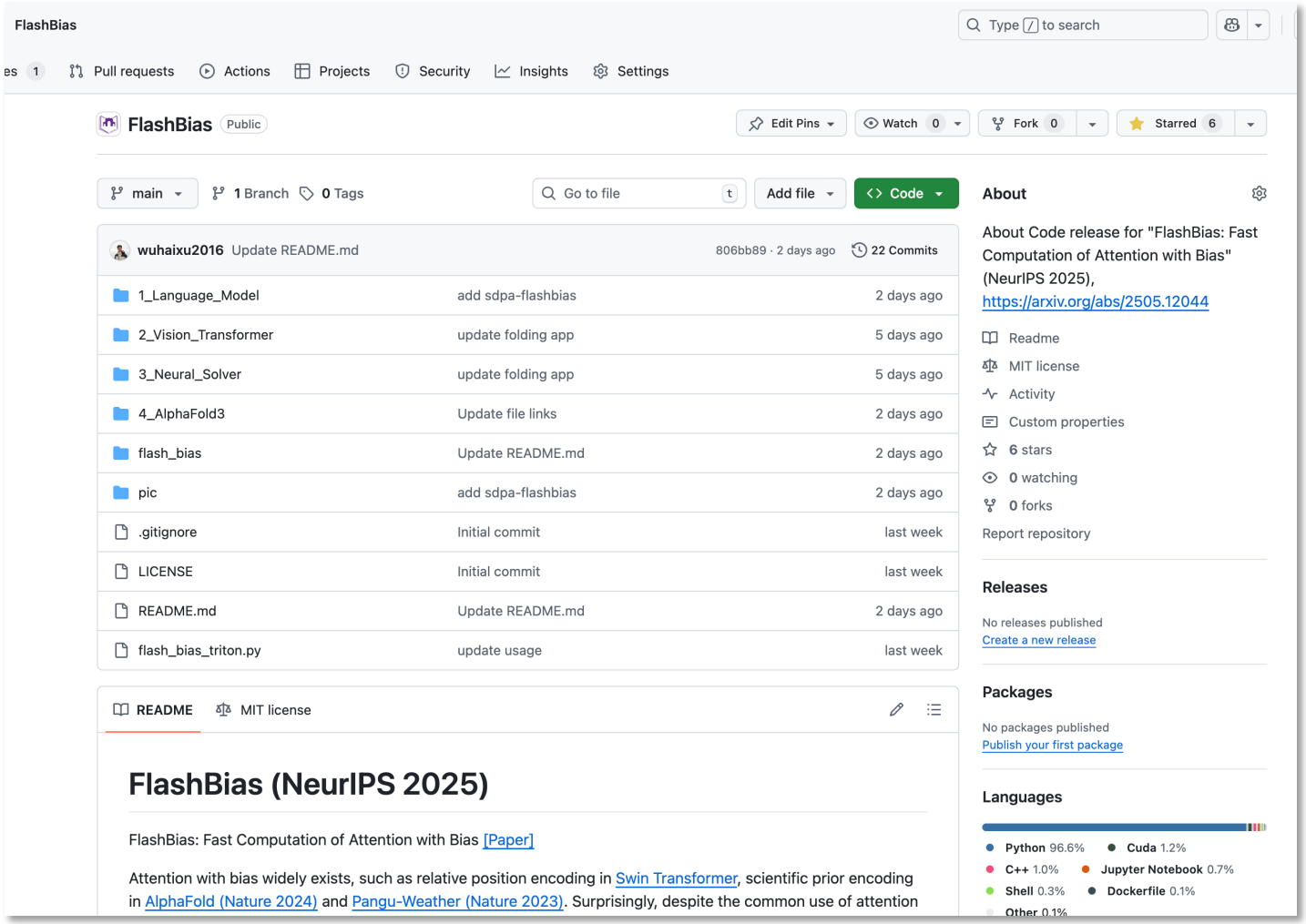
$$\mathbf{o} = \text{softmax}(\frac{\mathbf{q}\mathbf{k}^\top}{\sqrt{C}} \odot \mathbf{b})\mathbf{v} = \text{softmax}(\frac{\mathbf{q}'\mathbf{k}'^\top}{\sqrt{C}})\mathbf{v},$$

where $\mathbf{q}' = [\mathbf{q} \odot \phi_{\mathbf{q},1}, \cdots, \mathbf{q} \odot \phi_{\mathbf{q},R}] \in \mathbb{R}^{N\times CR}$, $\mathbf{k}' = [\mathbf{k} \odot \phi_{\mathbf{k},1}, \cdots, \mathbf{k} \odot \phi_{\mathbf{k},R}] \in \mathbb{R}^{N\times CR}$.

Example: $\mathbf{b}_{ij} = \cos(i-j)$

$$\phi_{\mathbf{q}}(\mathbf{x}_{\mathbf{q},i}) = [\cos(i), \sin(i)] \in \mathbb{R}^{1\times 2}, \quad \phi_{\mathbf{k}}(\mathbf{x}_{\mathbf{k},j}) = [\cos(j), \sin(j)] \in \mathbb{R}^{1\times 2}.$$

Open Source



Code is available at

https://github.com/thuml/FlashBias

NEURAL INFORMATION PROCESSING SYSTEMS

Thank You!

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Code Link: https://github.com/thuml/FlashBias

1.5x Speedup for Pairformer in AlphaFold 3; **2x** Speedup for Swin Transformer v2.

Try FlashBias!