

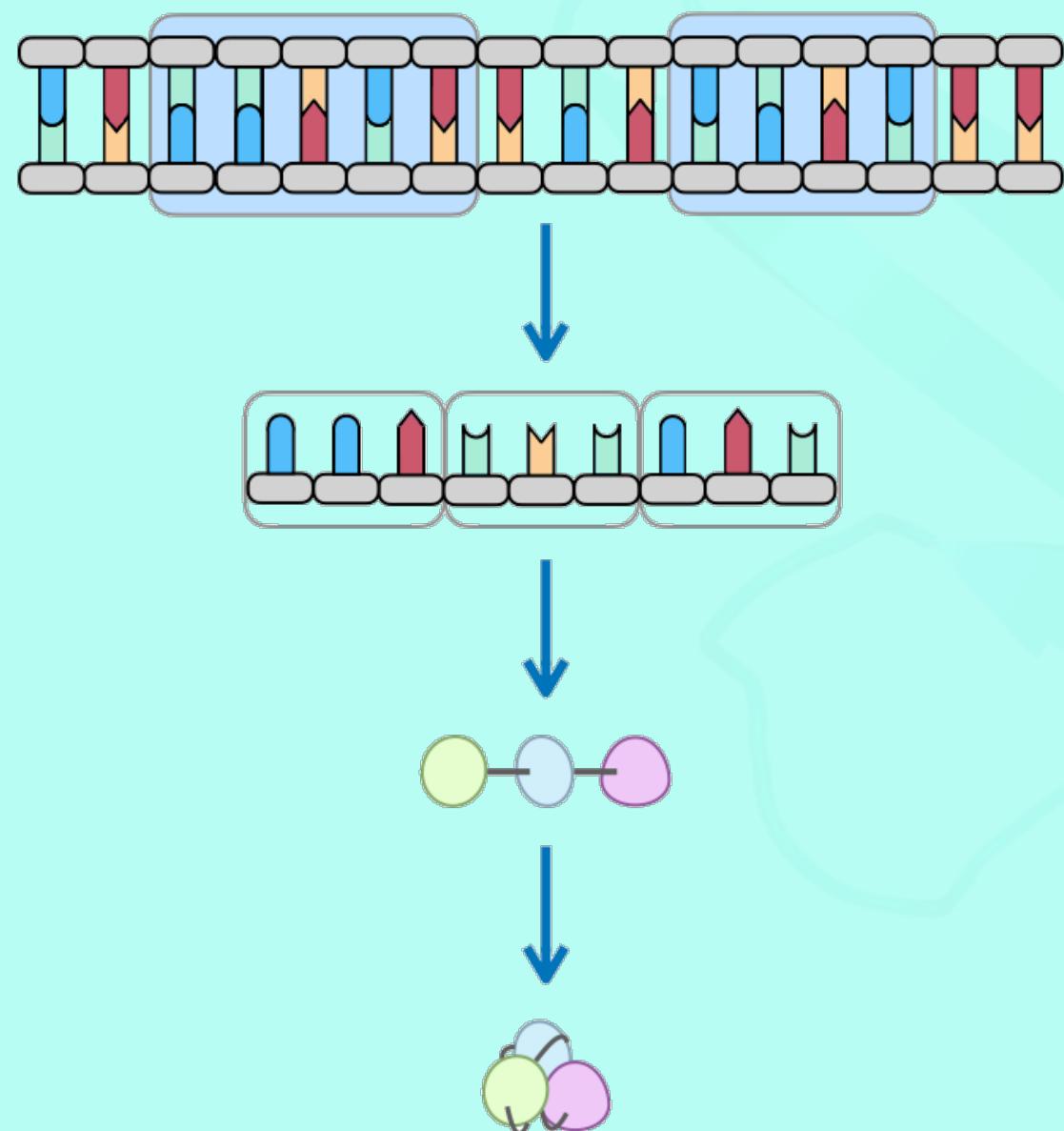
AlphaFold and Protein Structure Prediction

Janik Euskirchen

Table of Contents

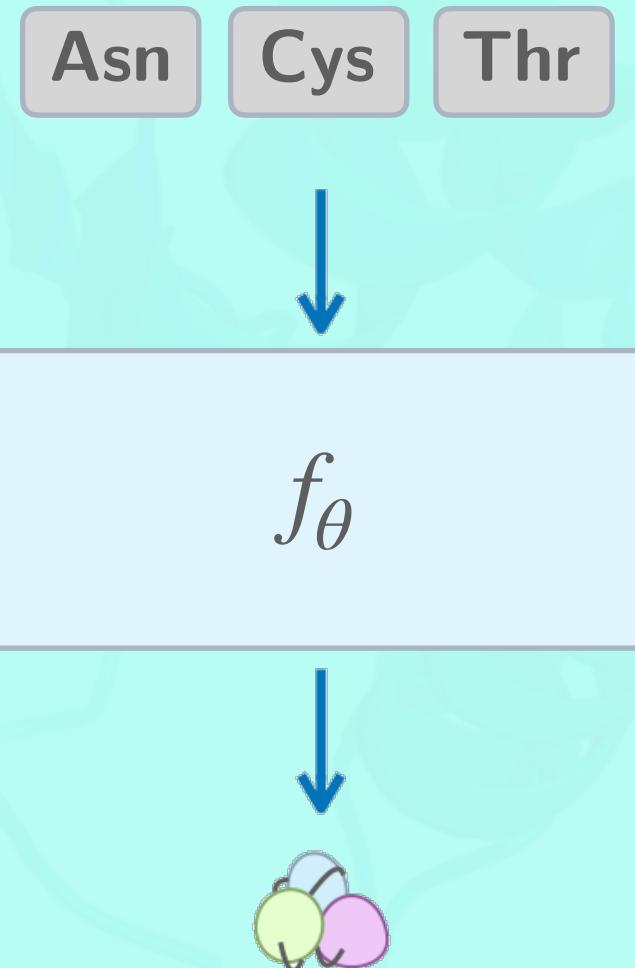
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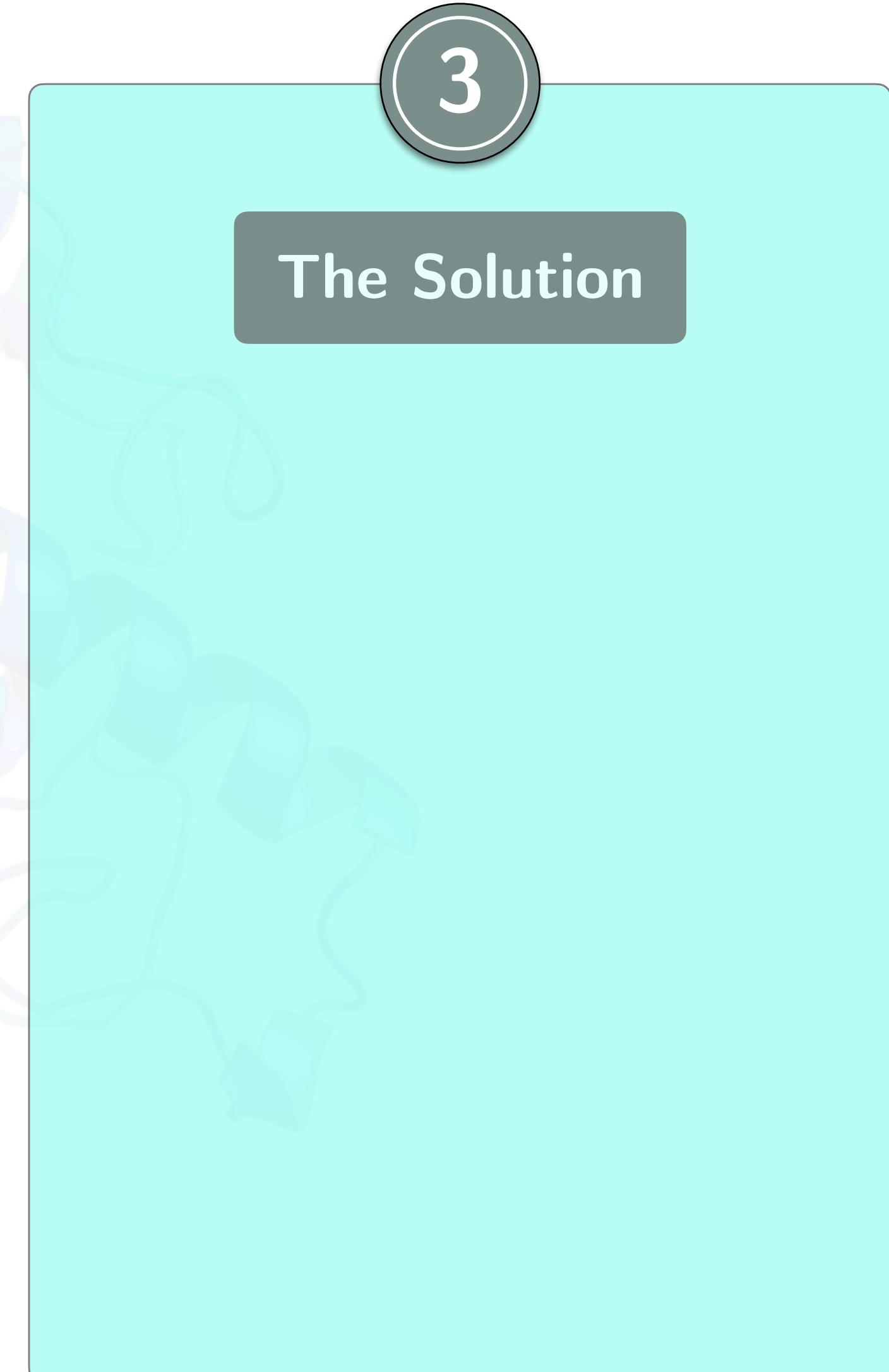
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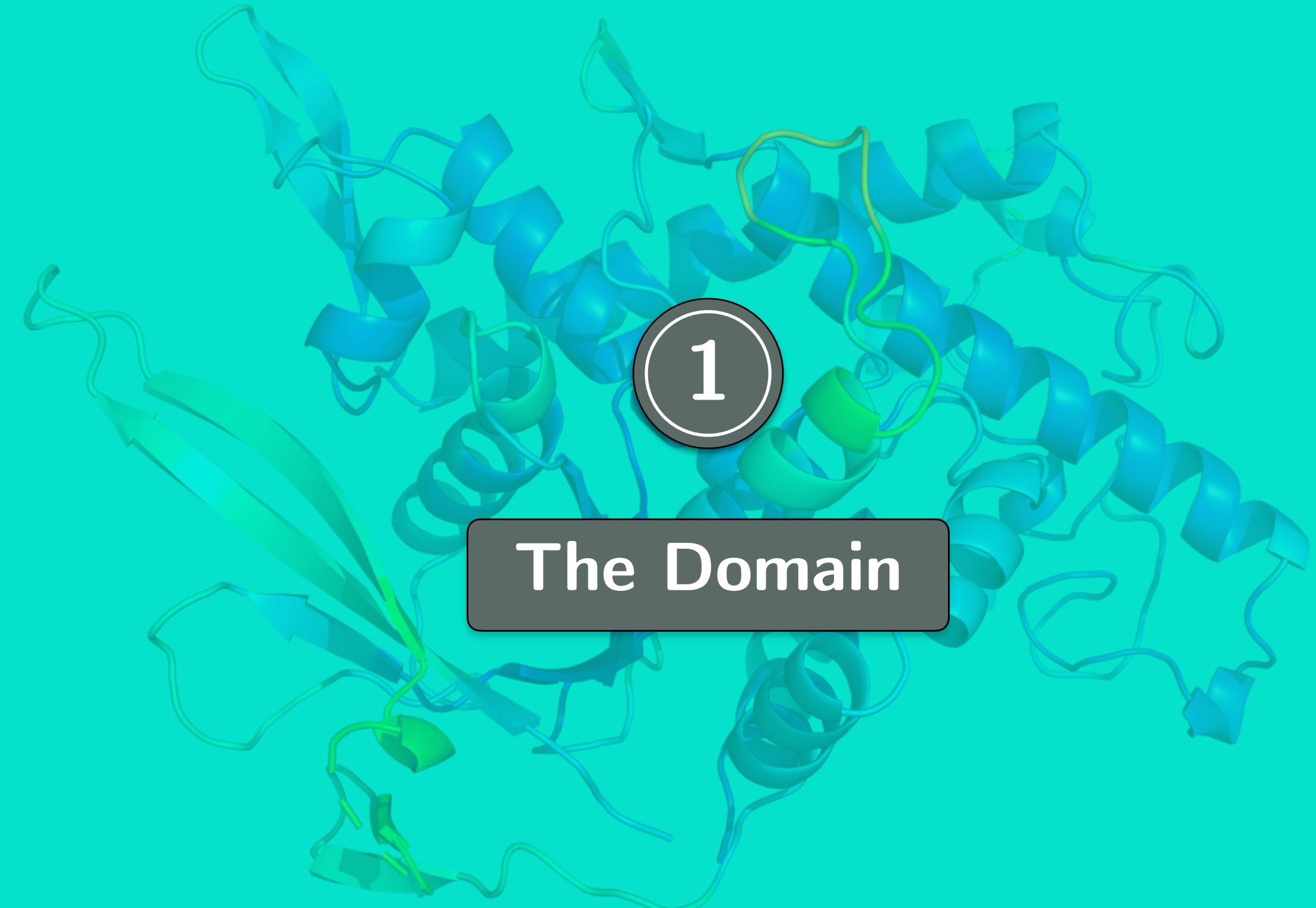
The Problem



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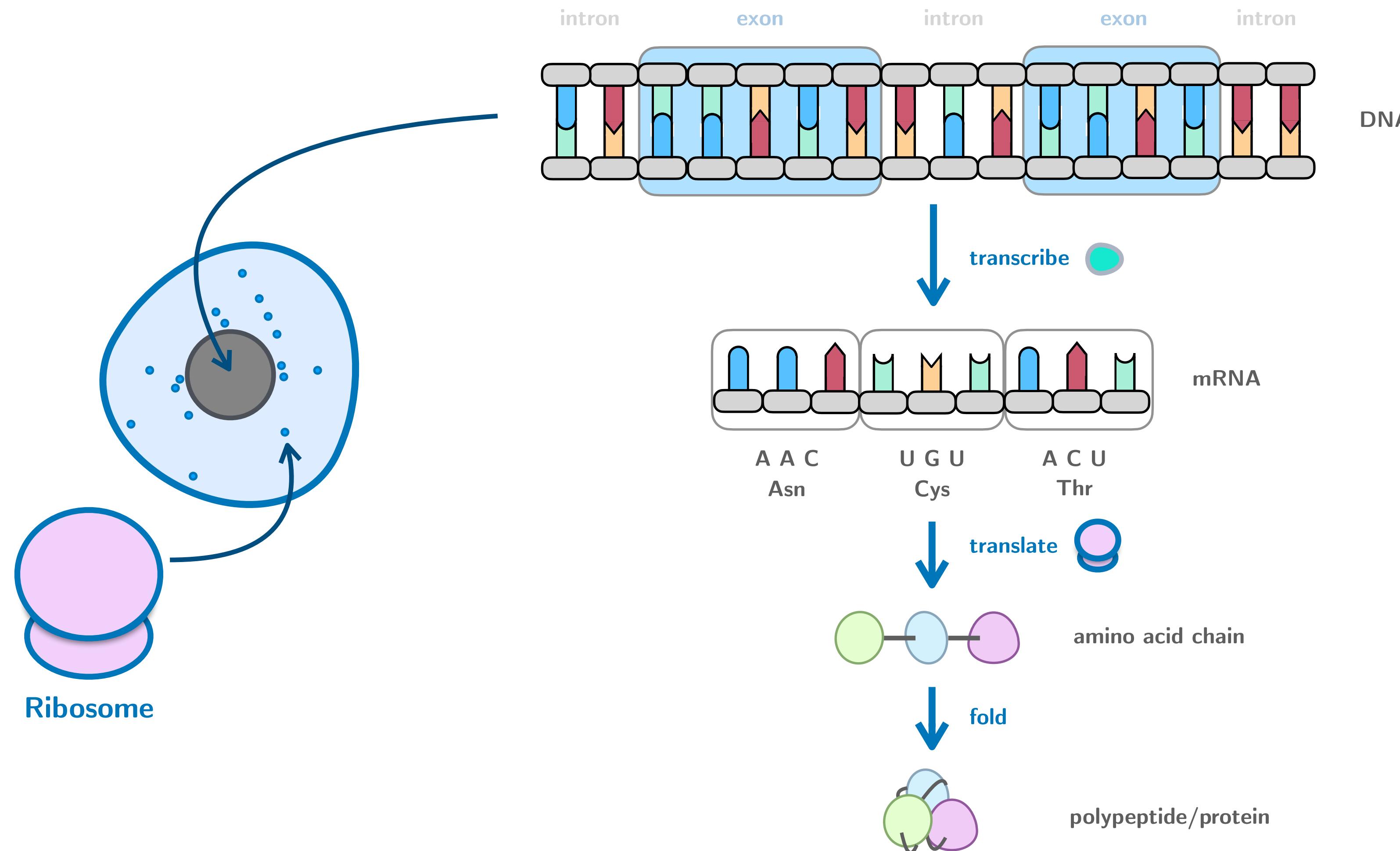
The Solution





The Domain

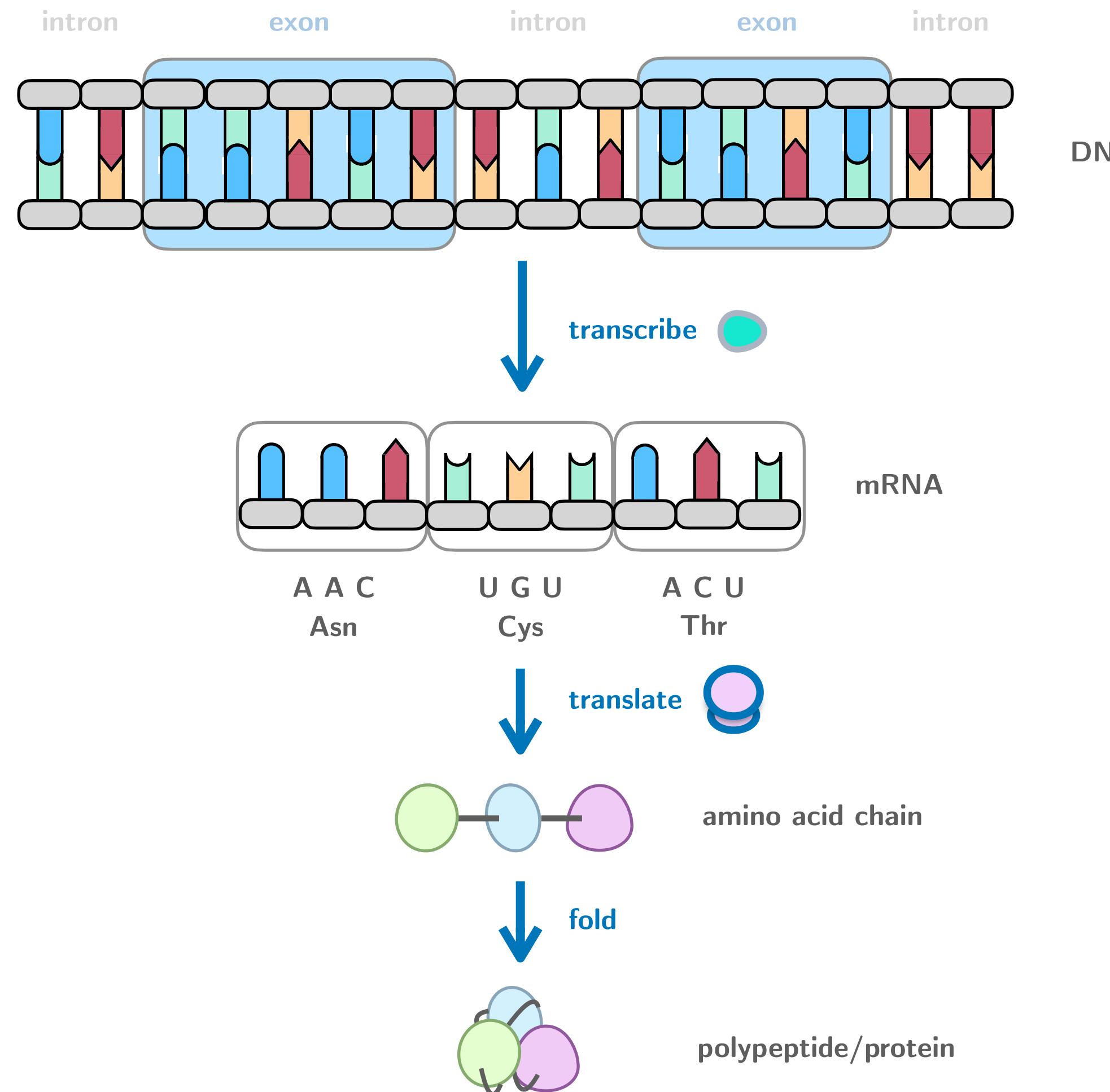
Central Dogma of Molecular Biology



AlphaFold and Protein Structure Prediction

The Domain

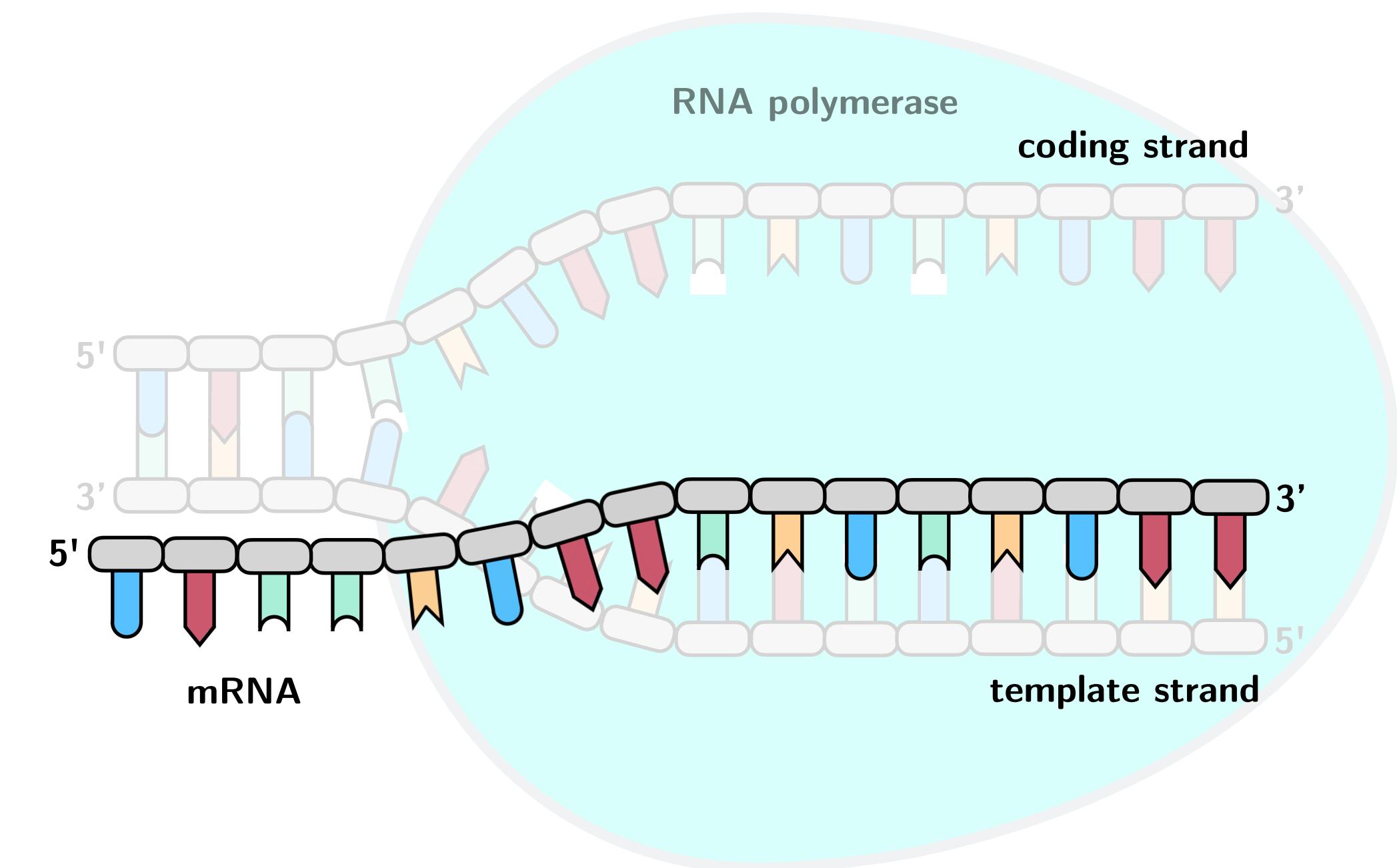
Central Dogma of Molecular Biology



Source (tRNA graphic): National Human Genome Research Institute

Source (template for most graphics): ...

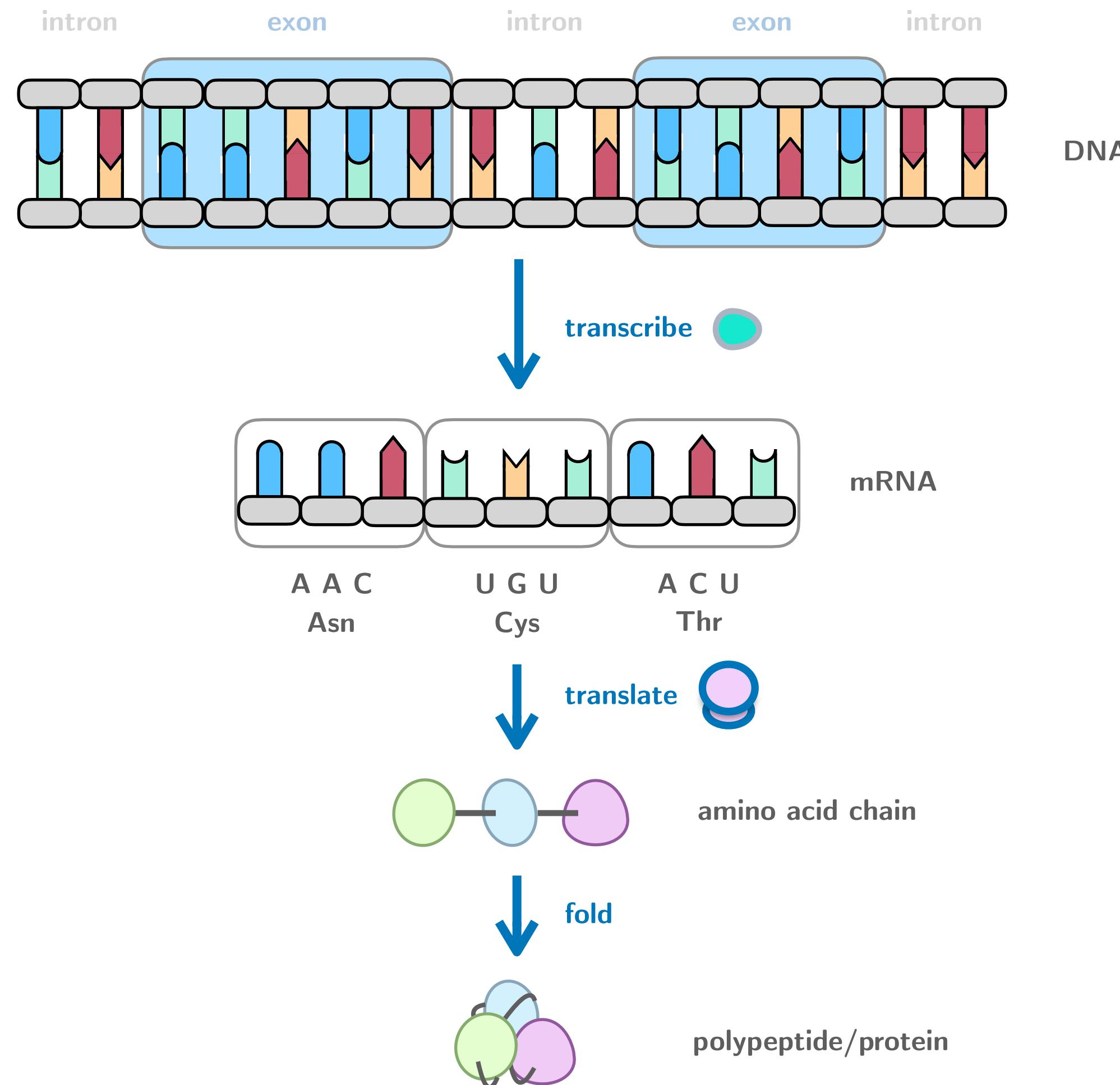
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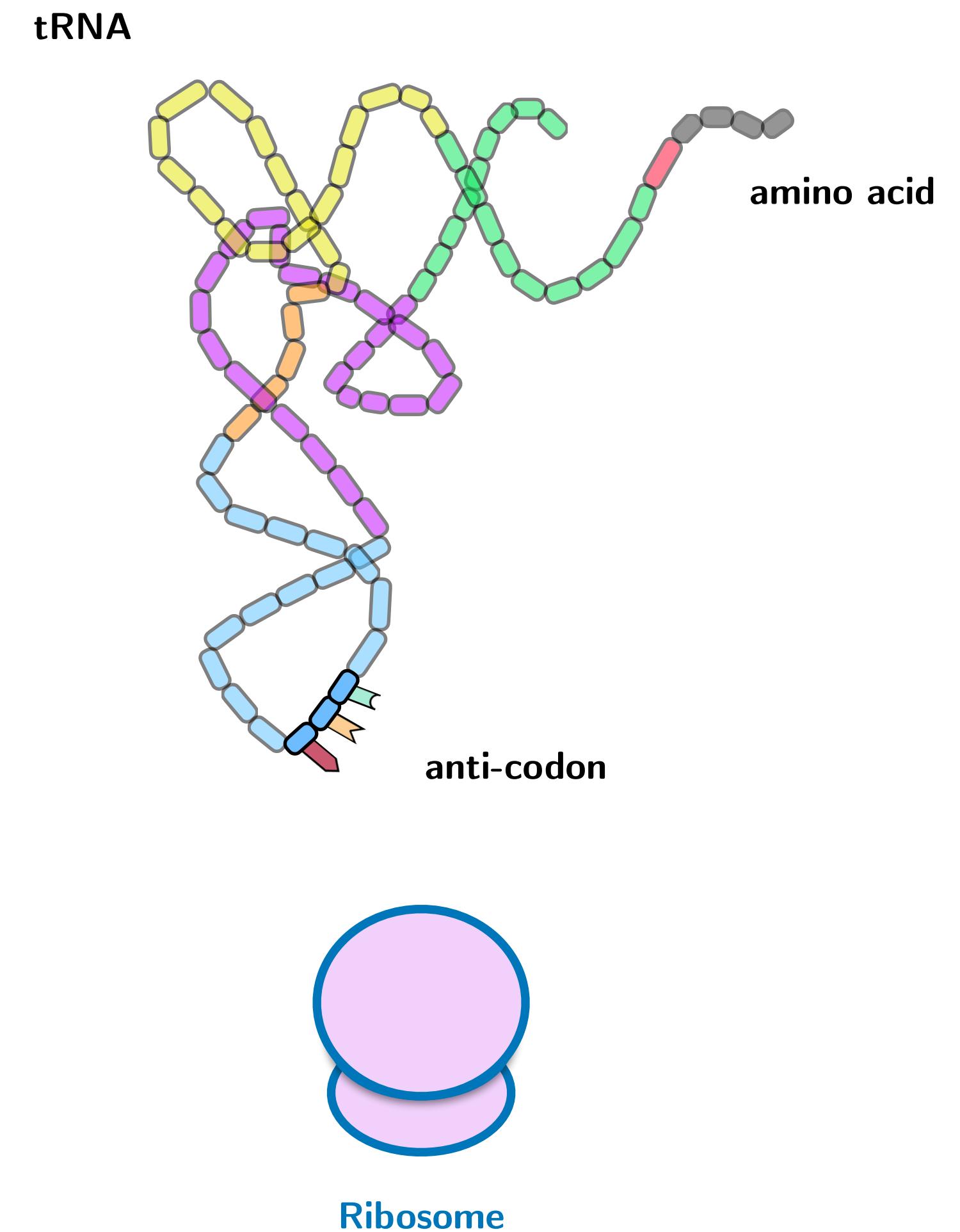
AlphaFold and Protein Structure Prediction

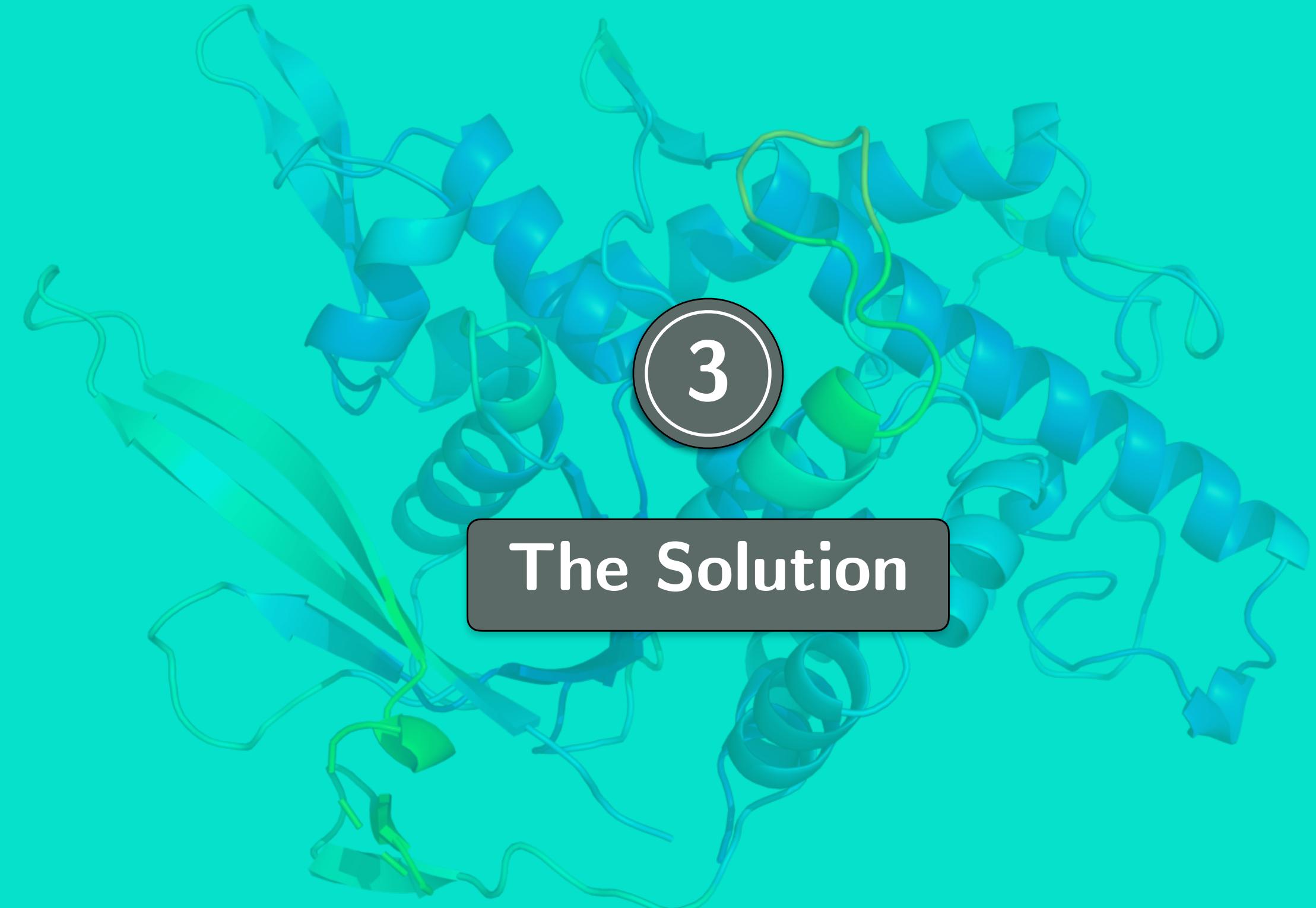
The Domain

Central Dogma of Molecular Biology



Translation

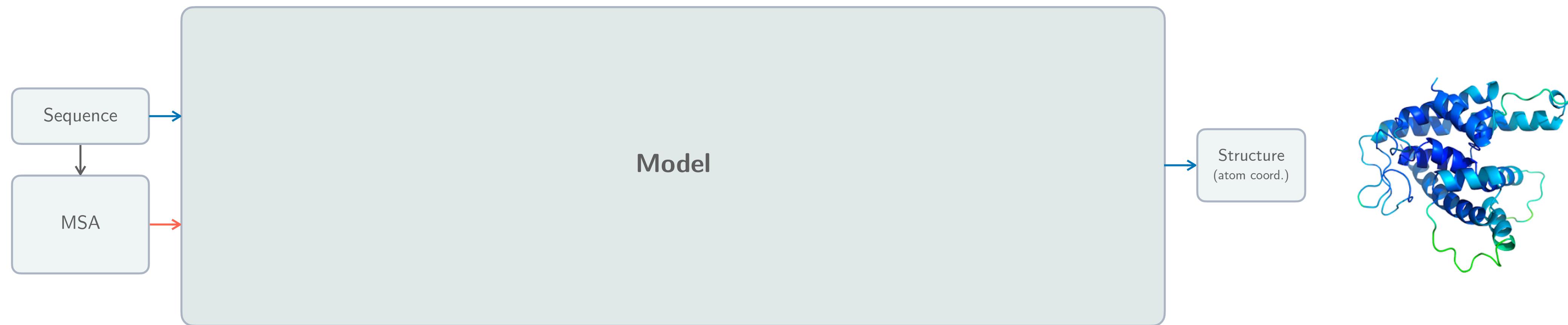






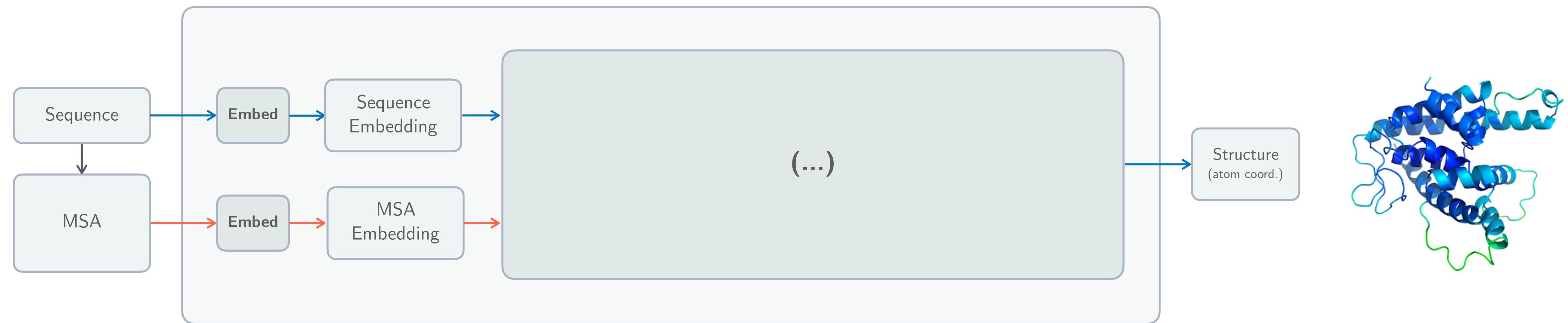
The Solution AlphaFold 2

Model



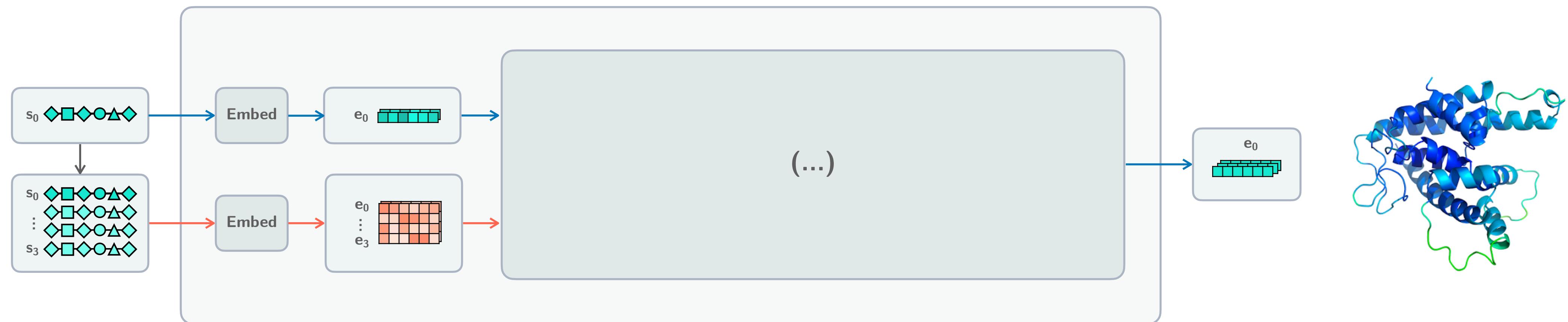
The Solution AlphaFold 2

Embedding & Structure Module



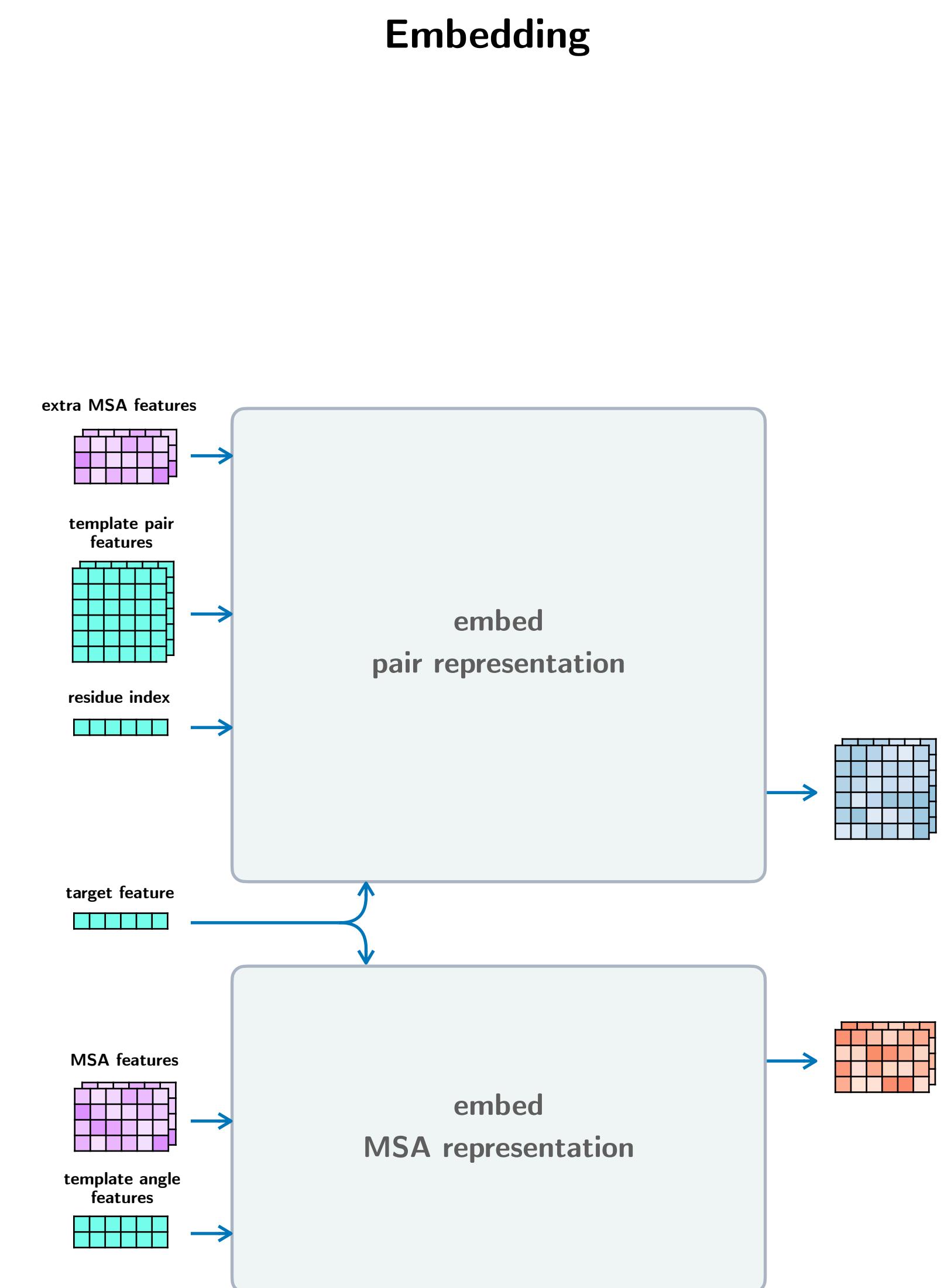
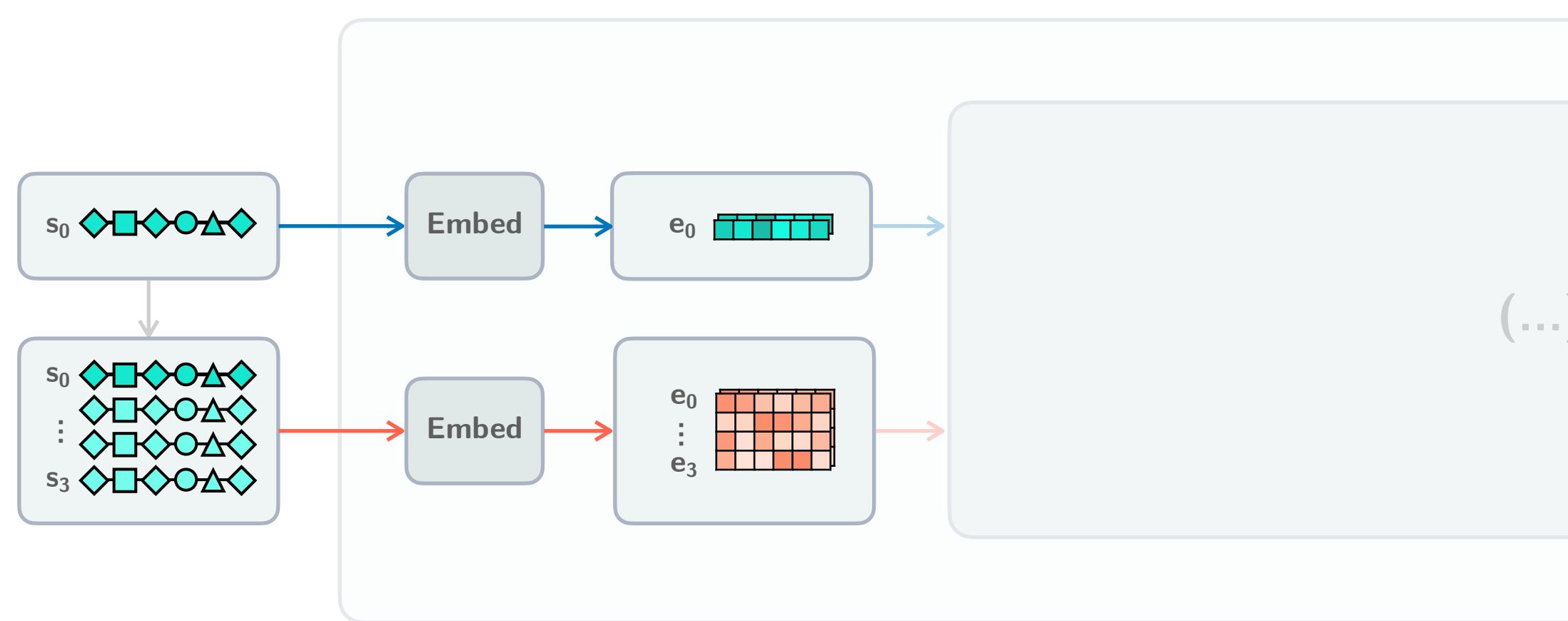
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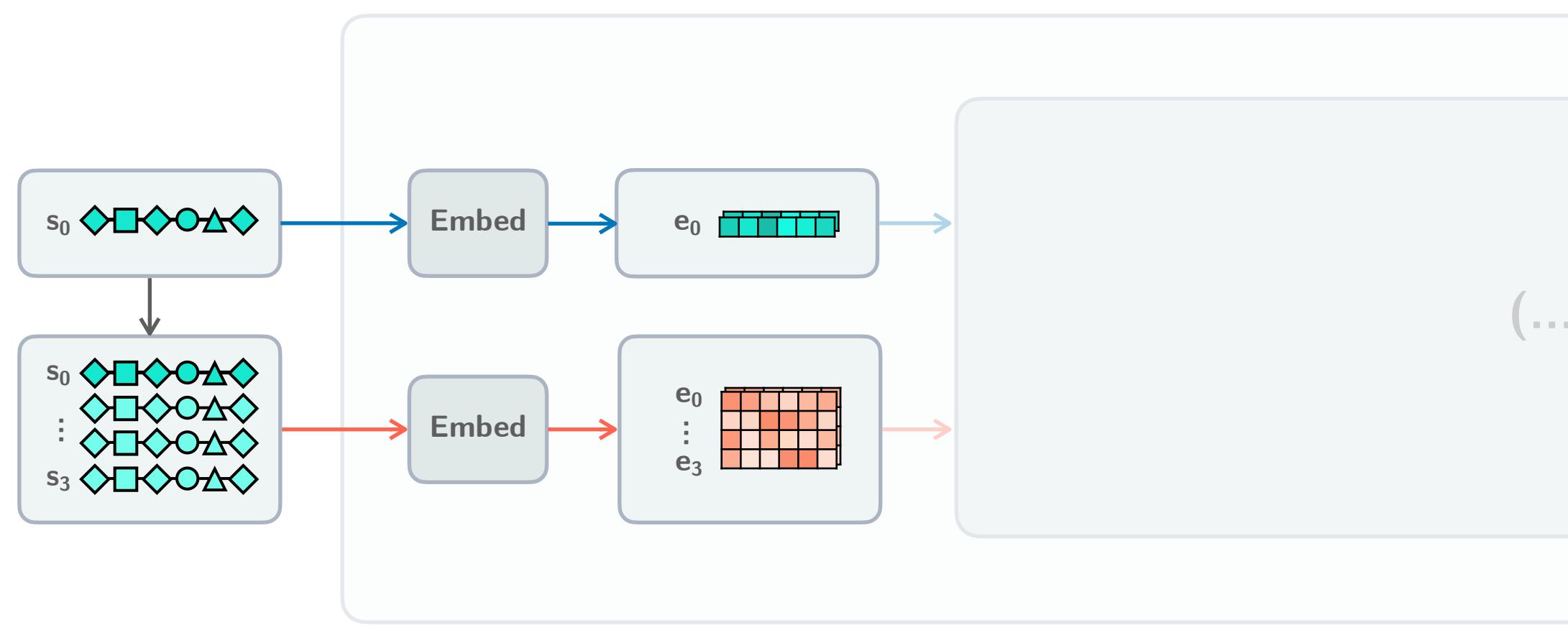
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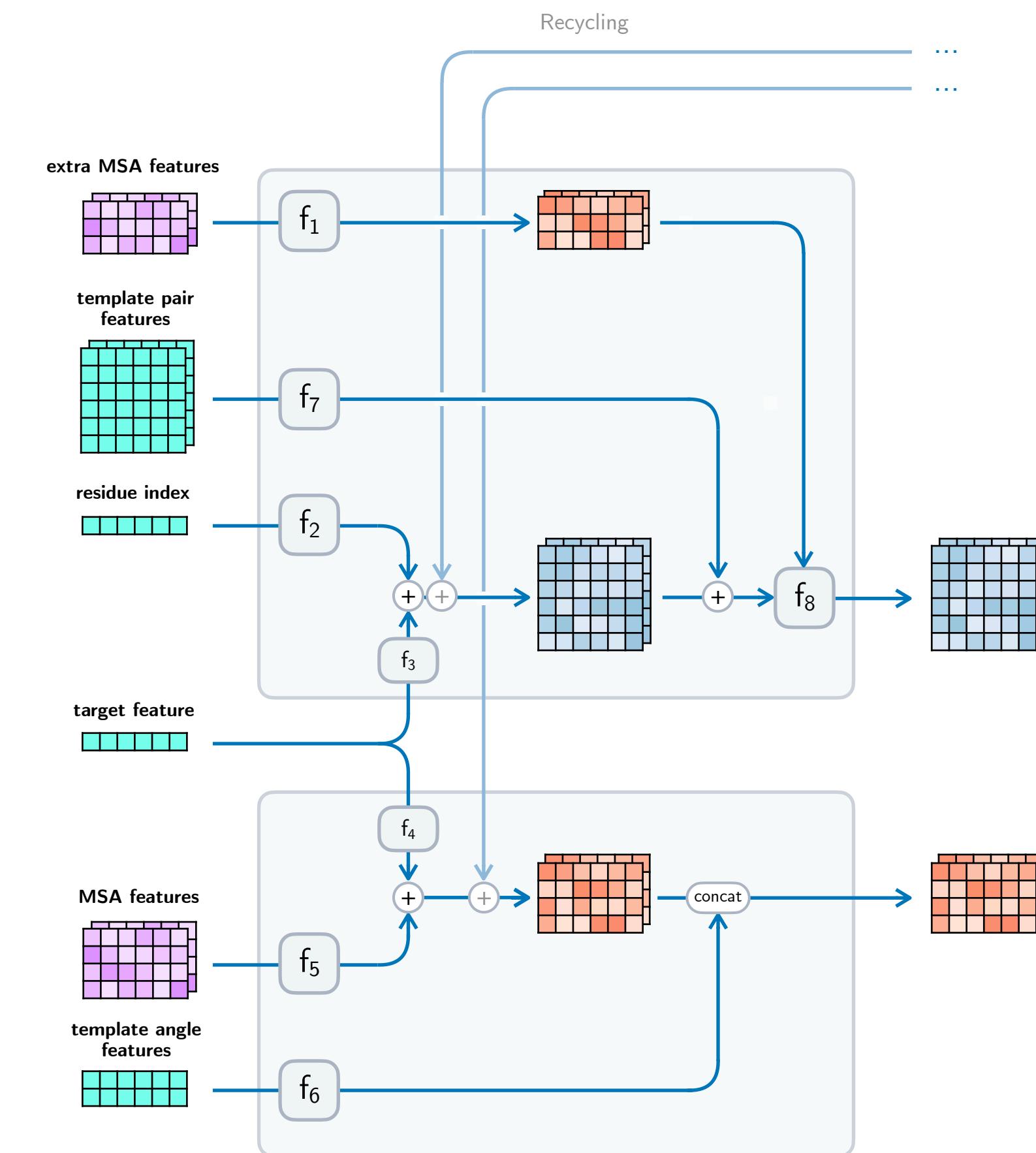


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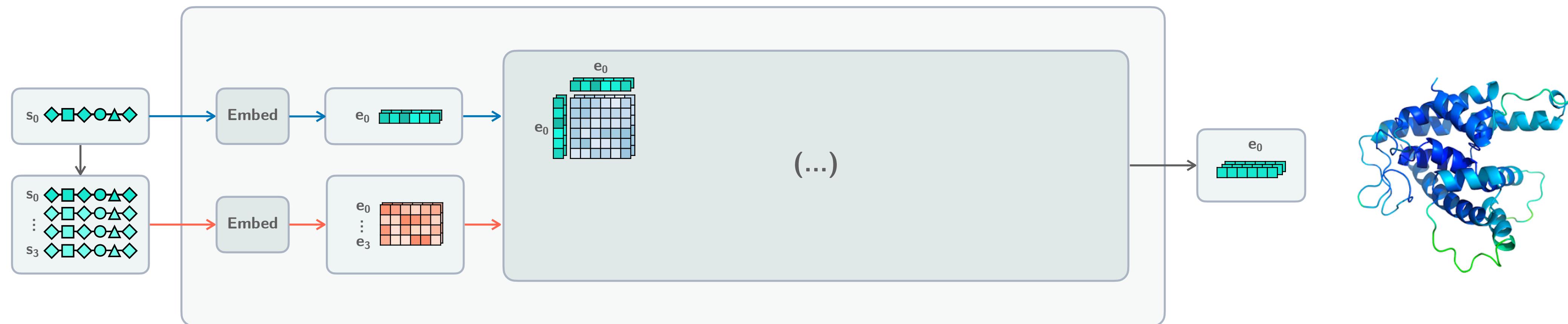


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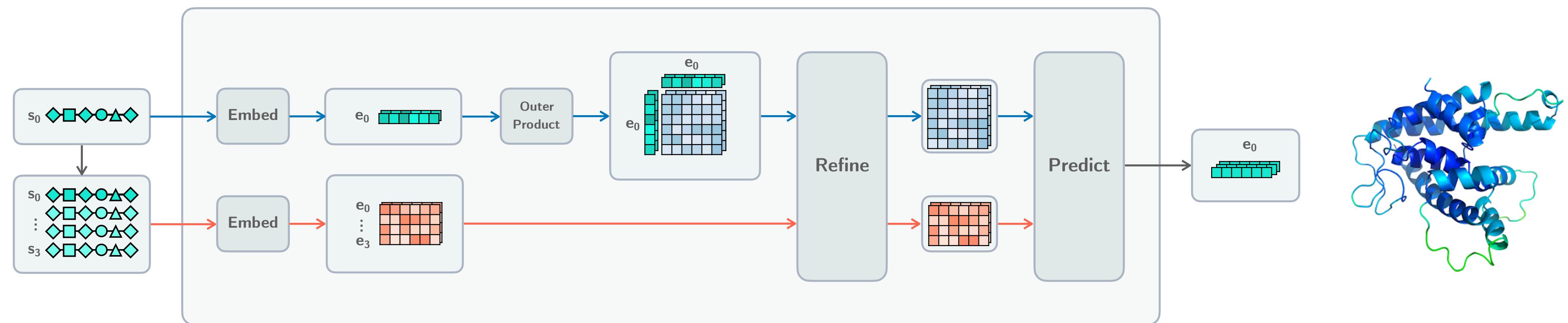
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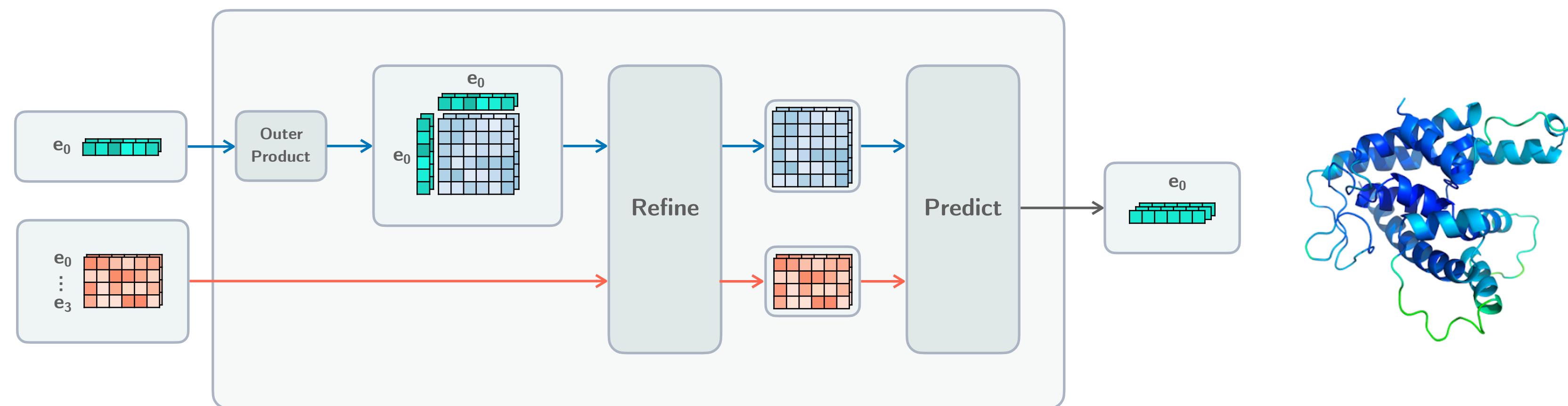


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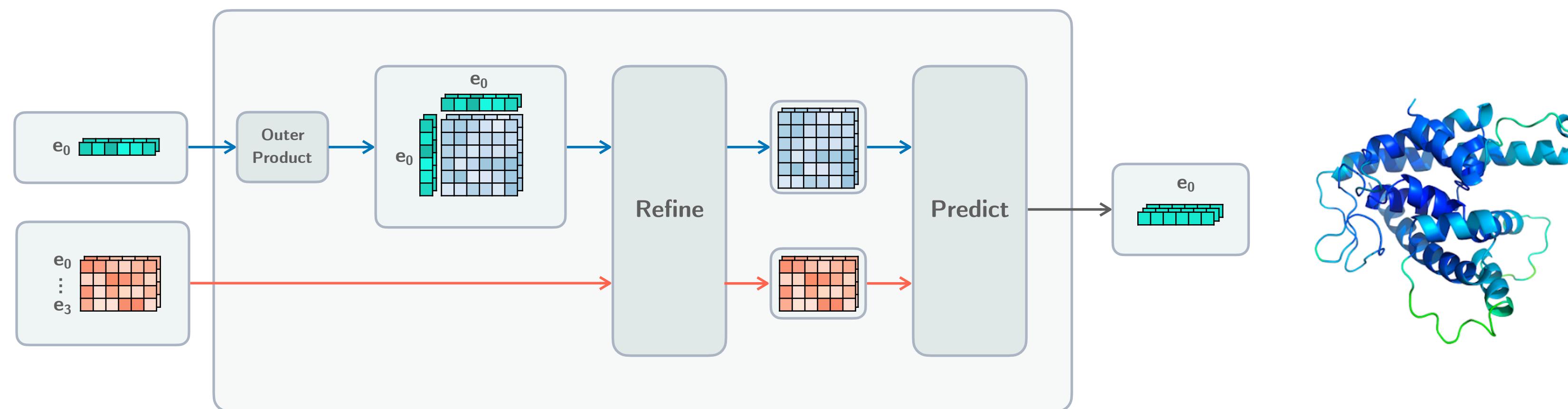


Structure Module



The Solution AlphaFold 2

Refining & Predicting

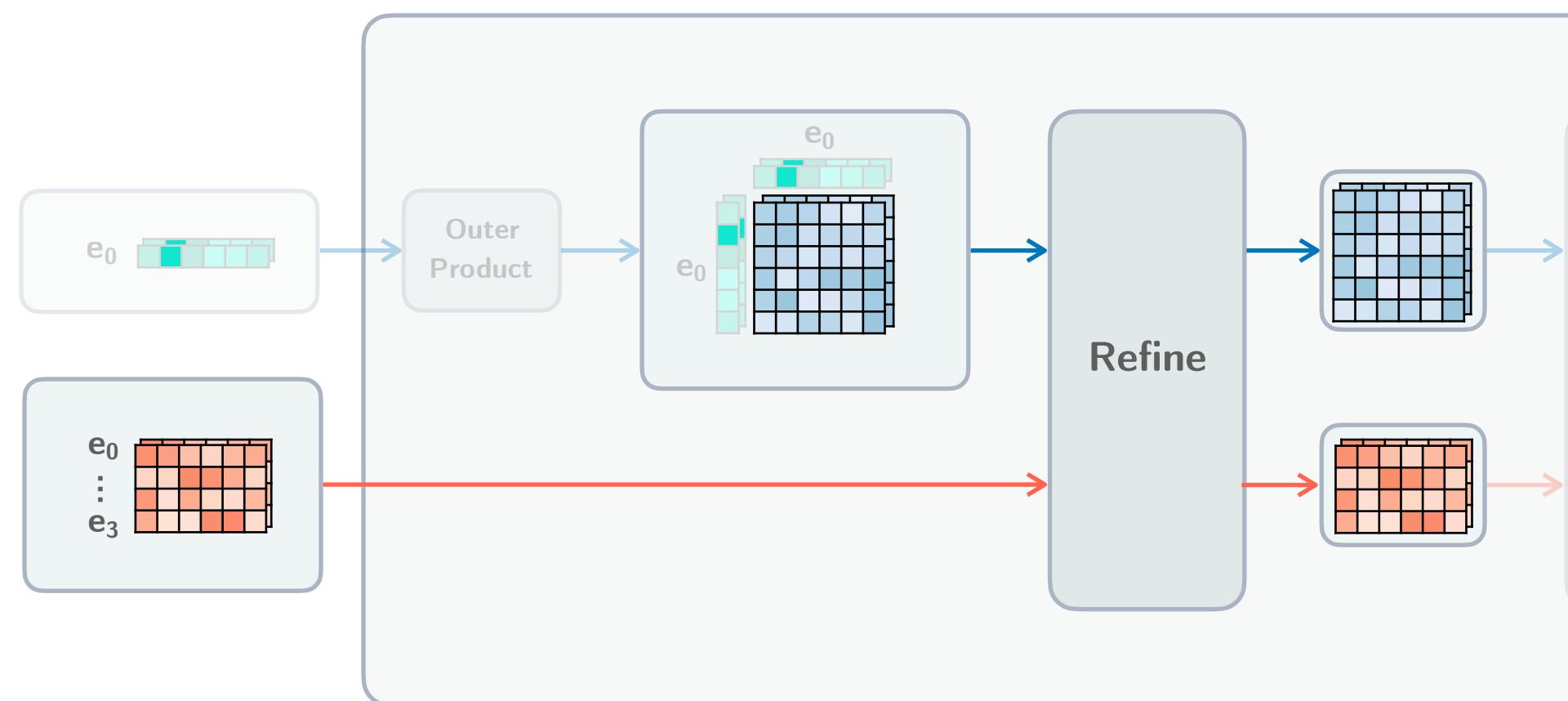


AlphaFold and Protein Structure Prediction

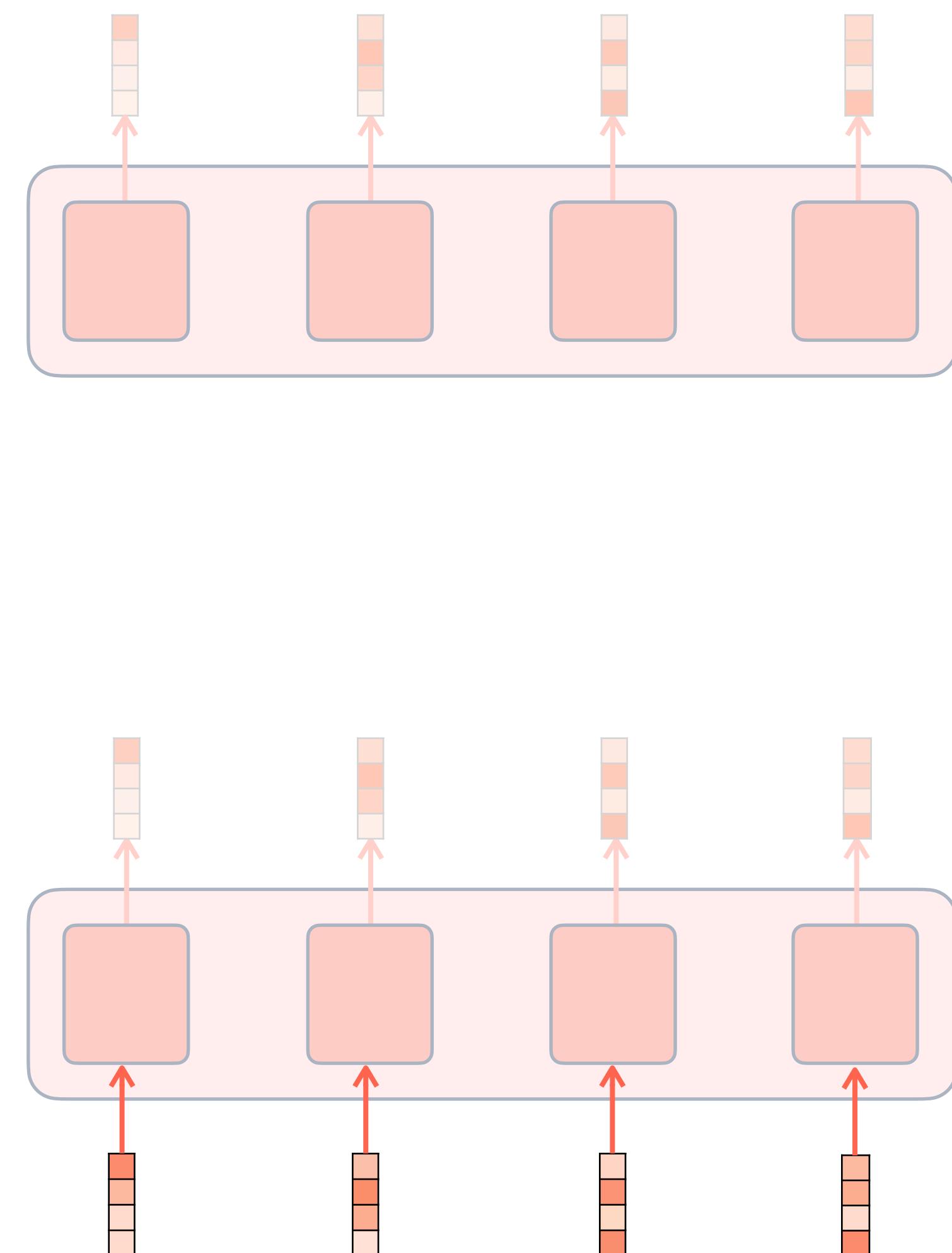
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



Self-Attention

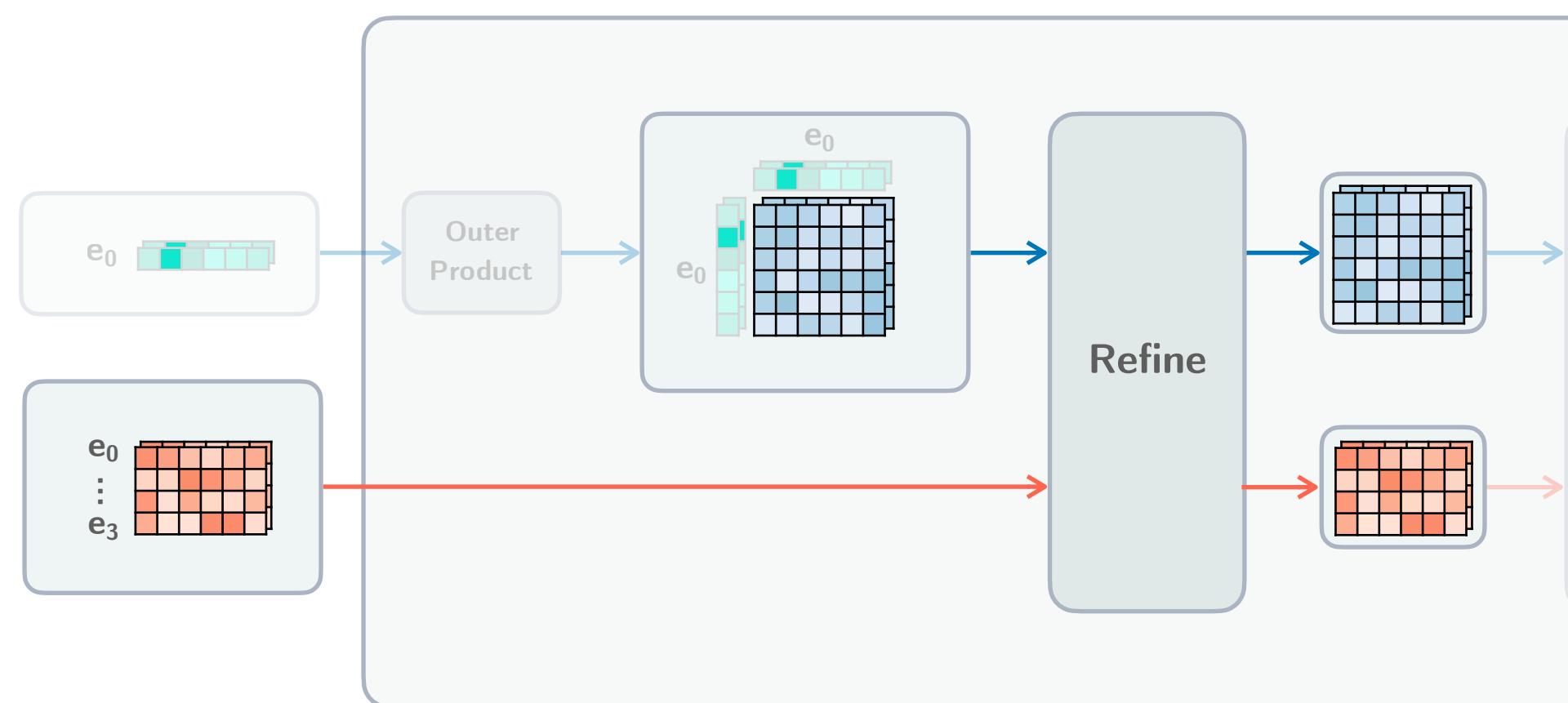


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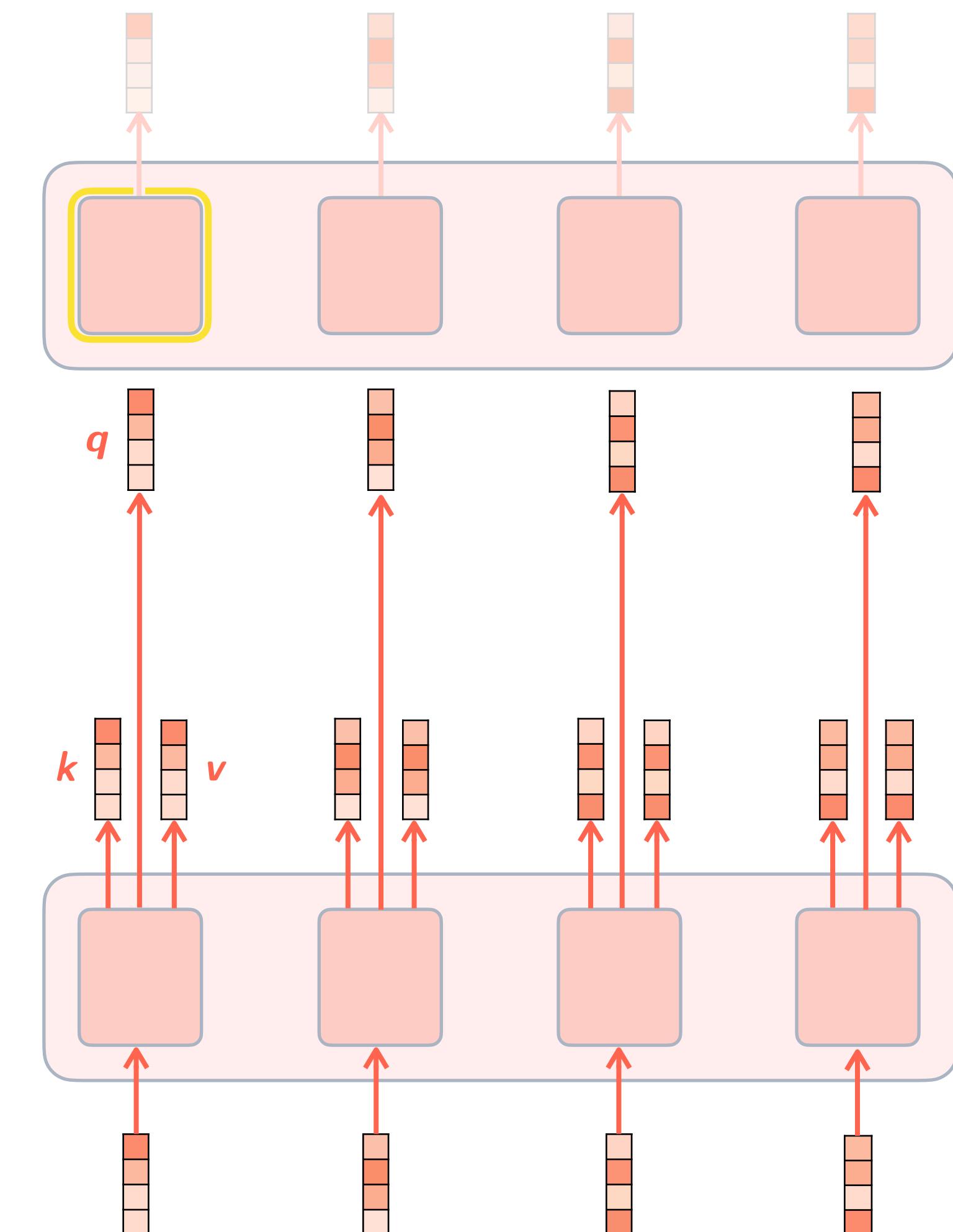
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Refining & Predicting

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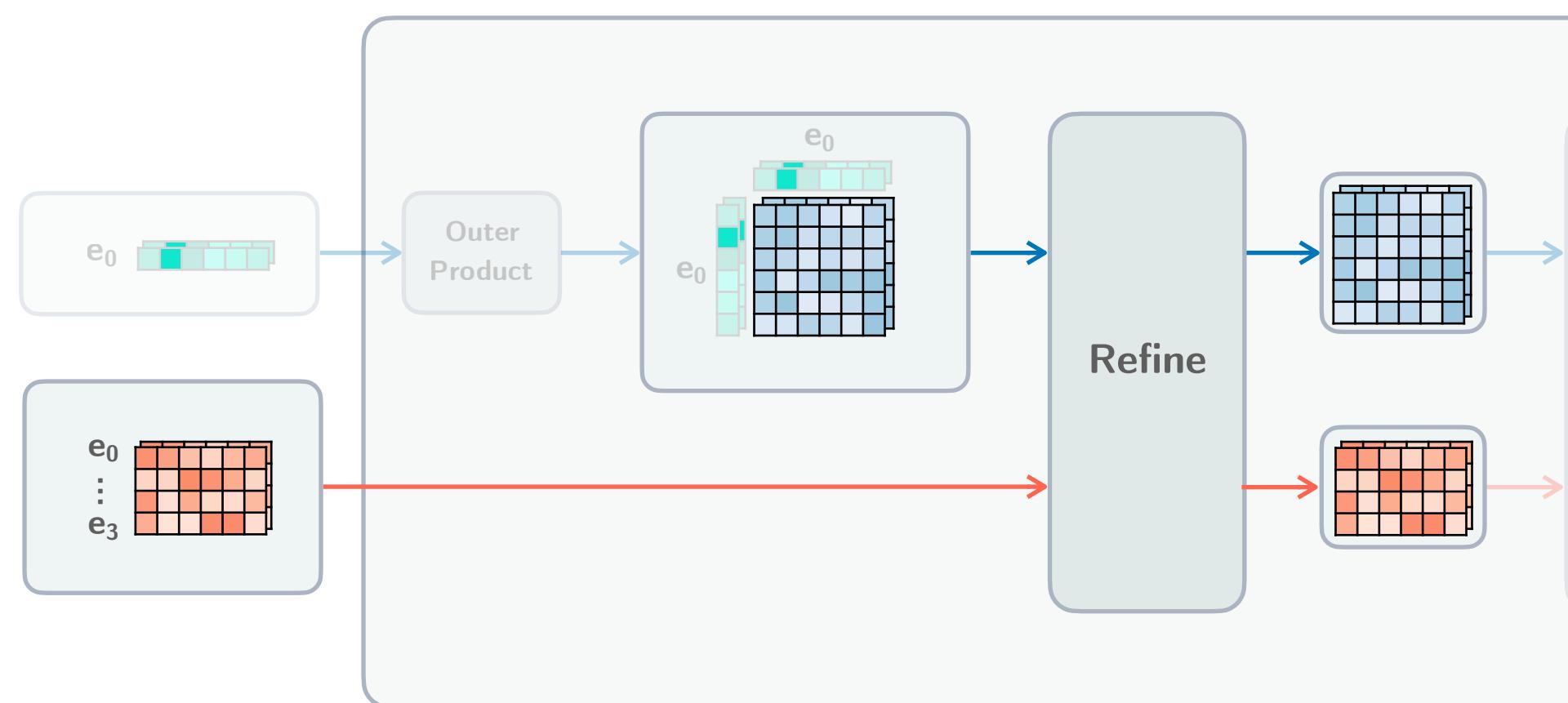


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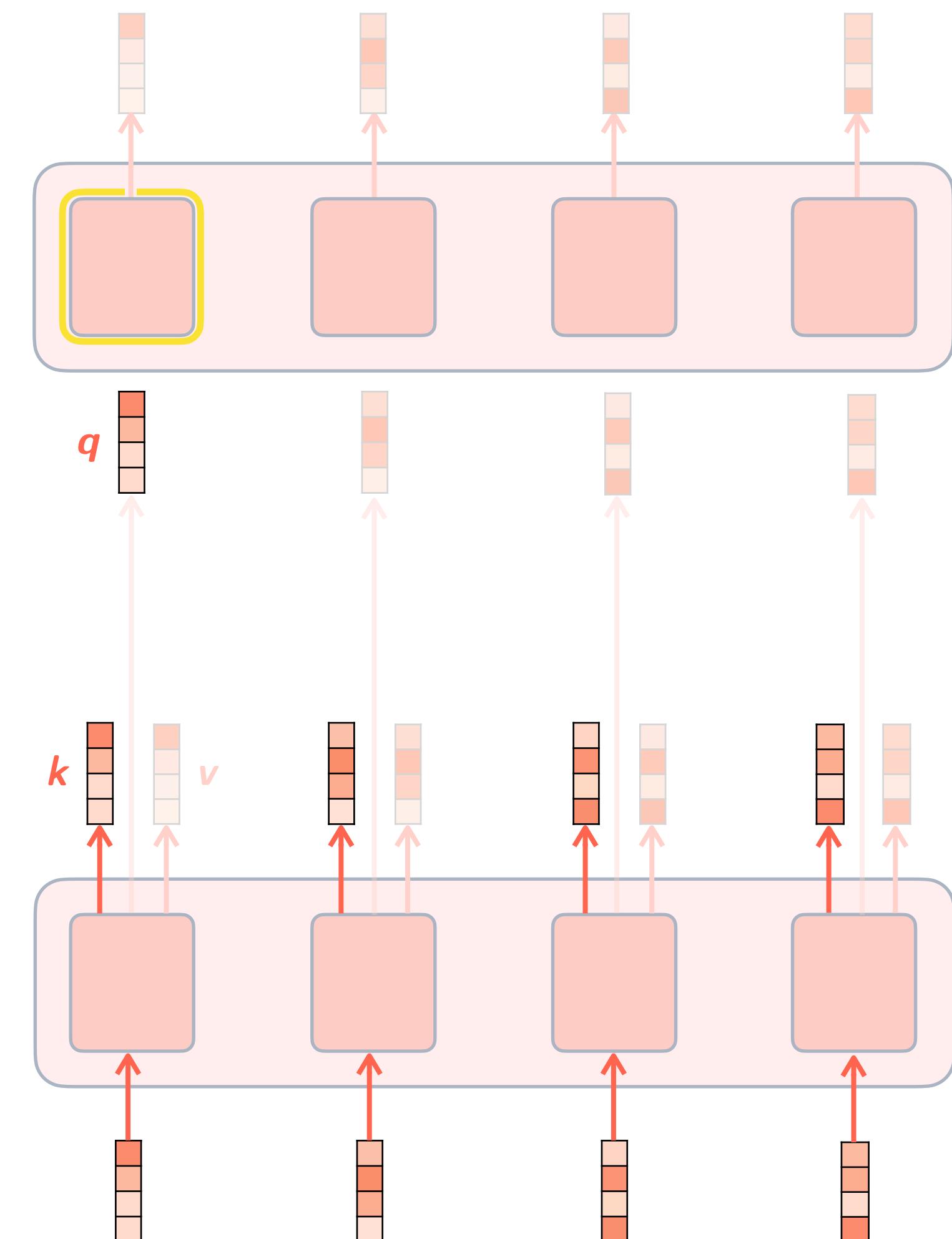
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Refining & Predicting

and contextualizing



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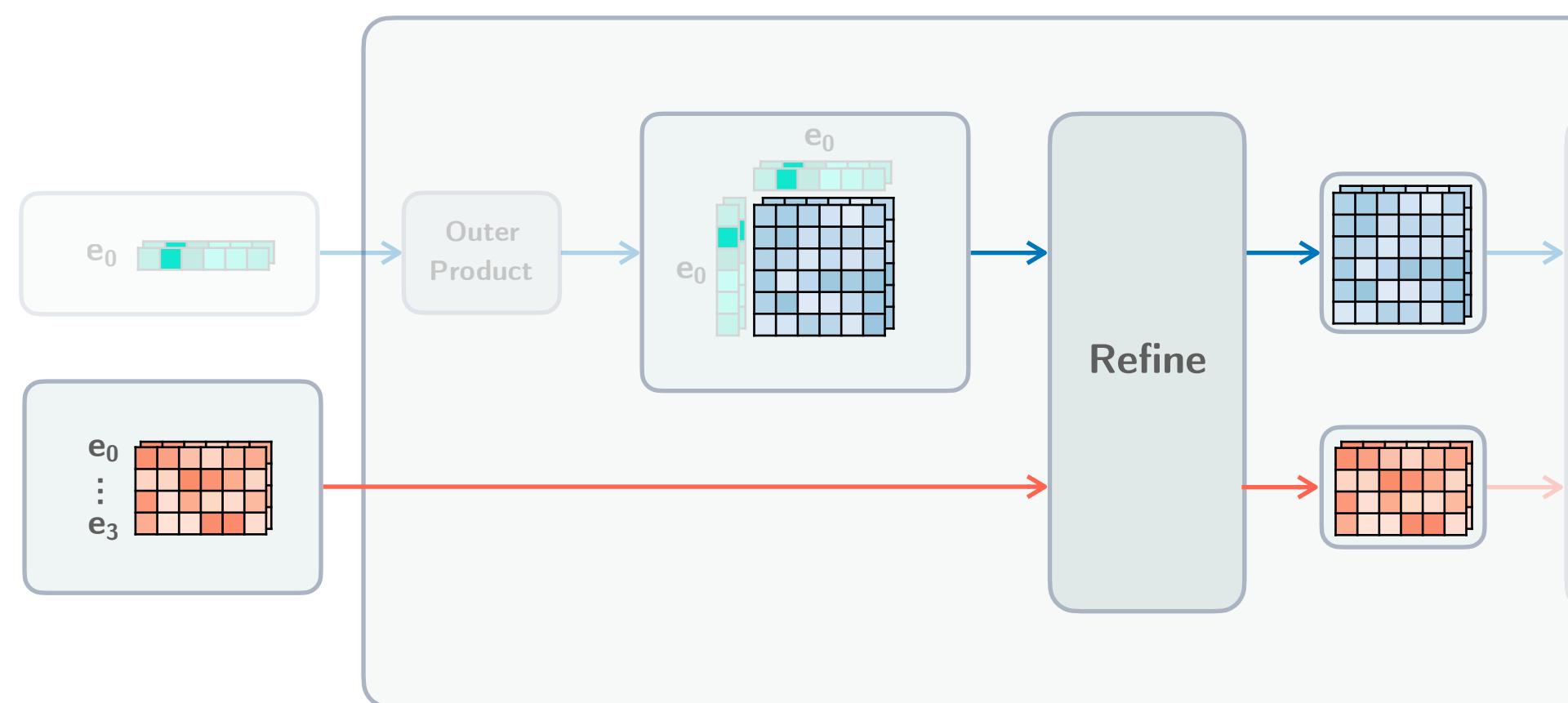


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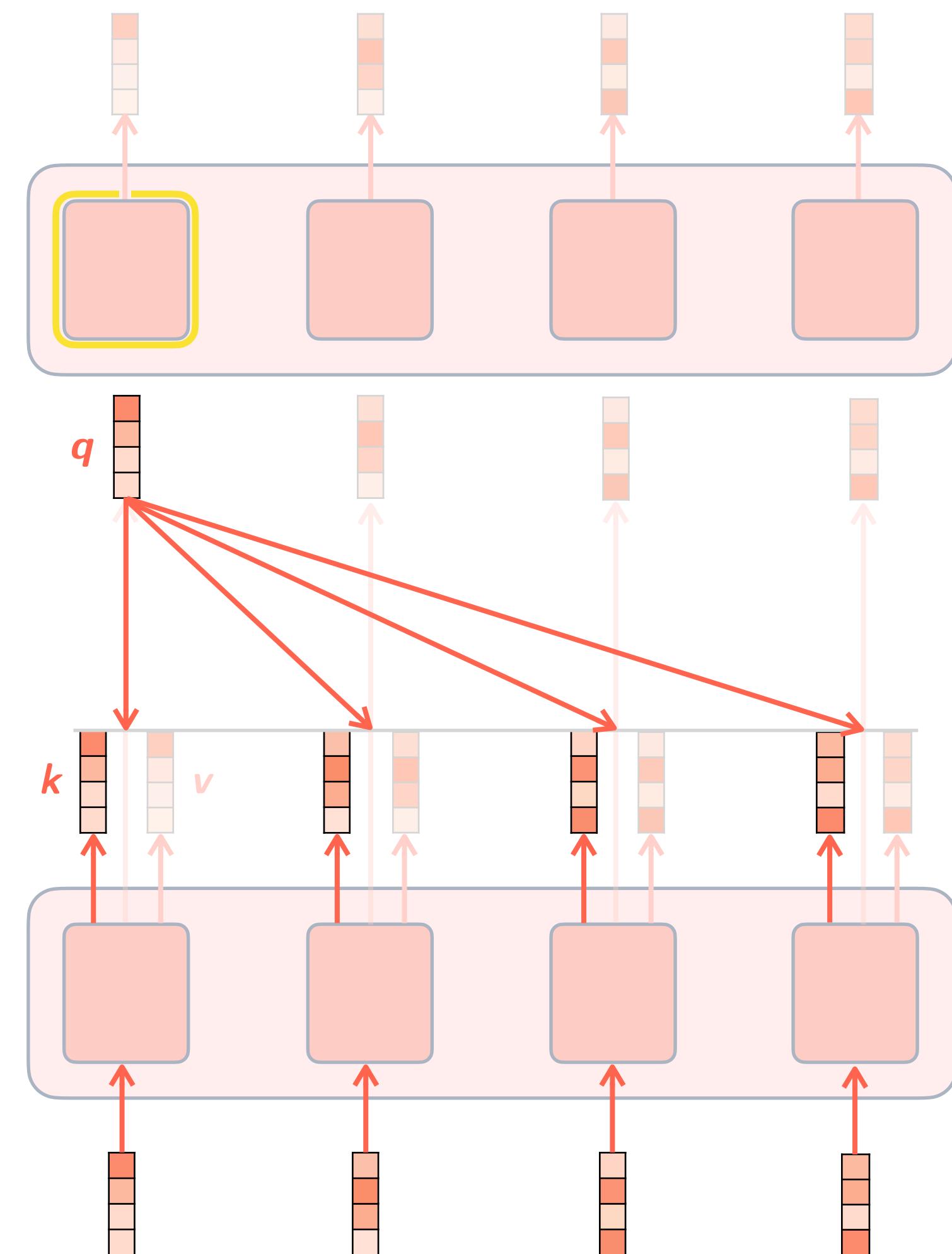
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Refining & Predicting

and contextualizing



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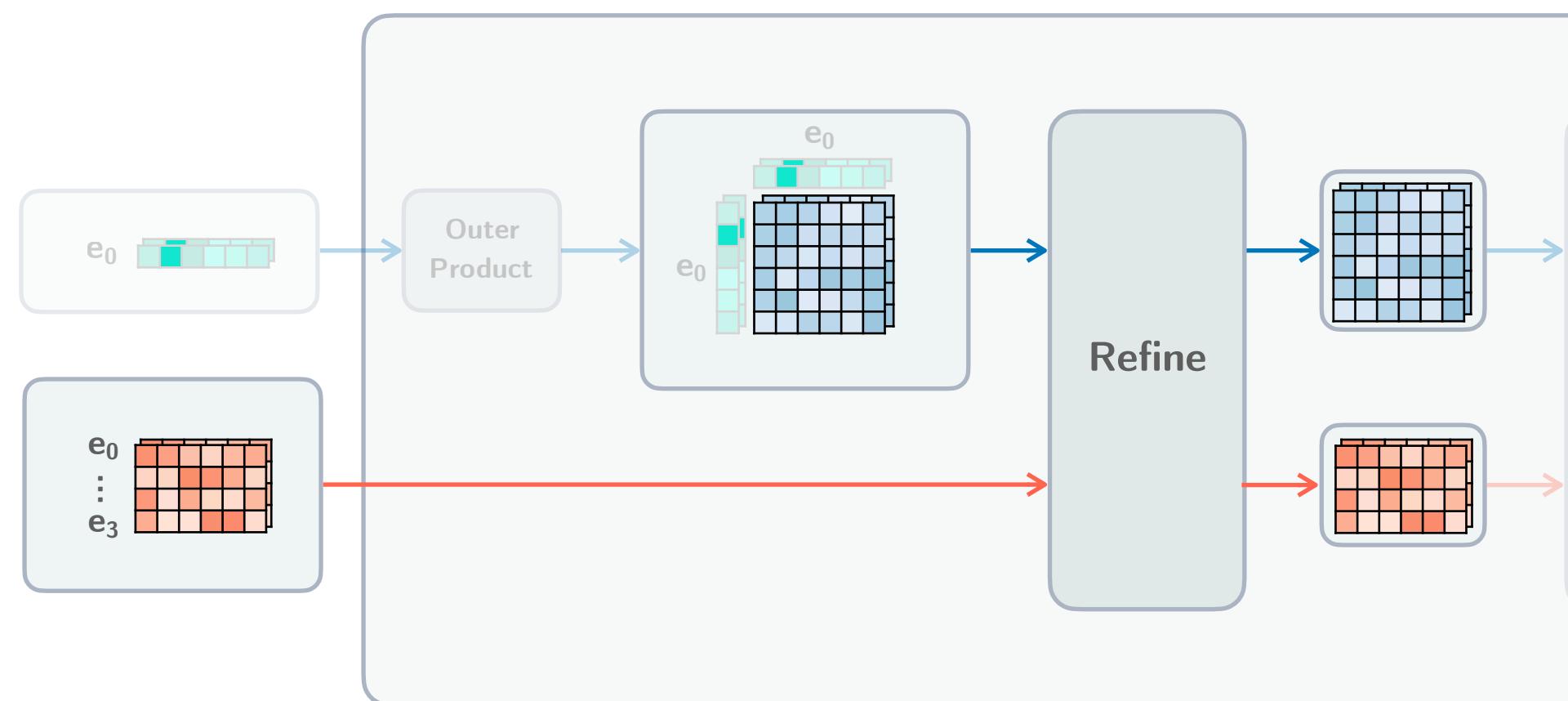


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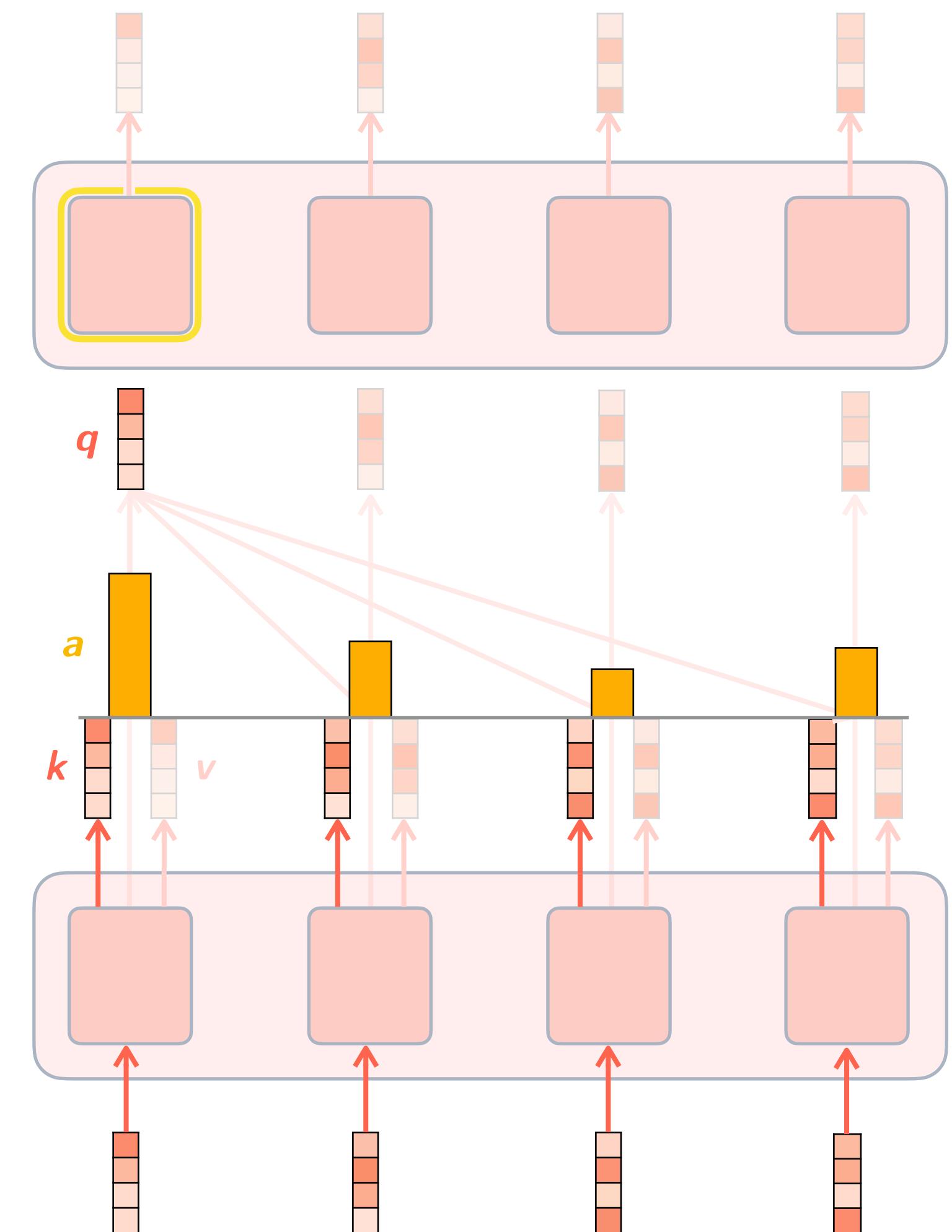
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



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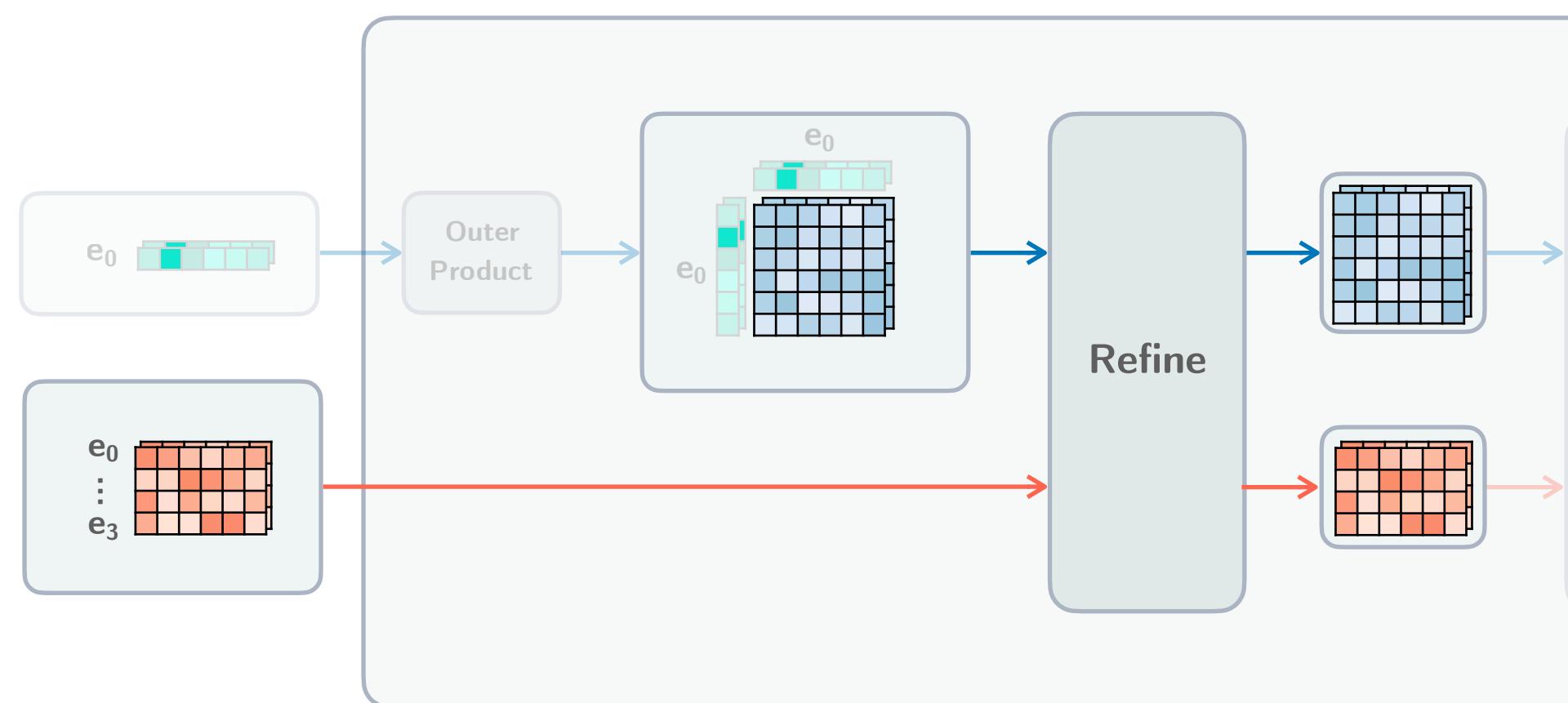


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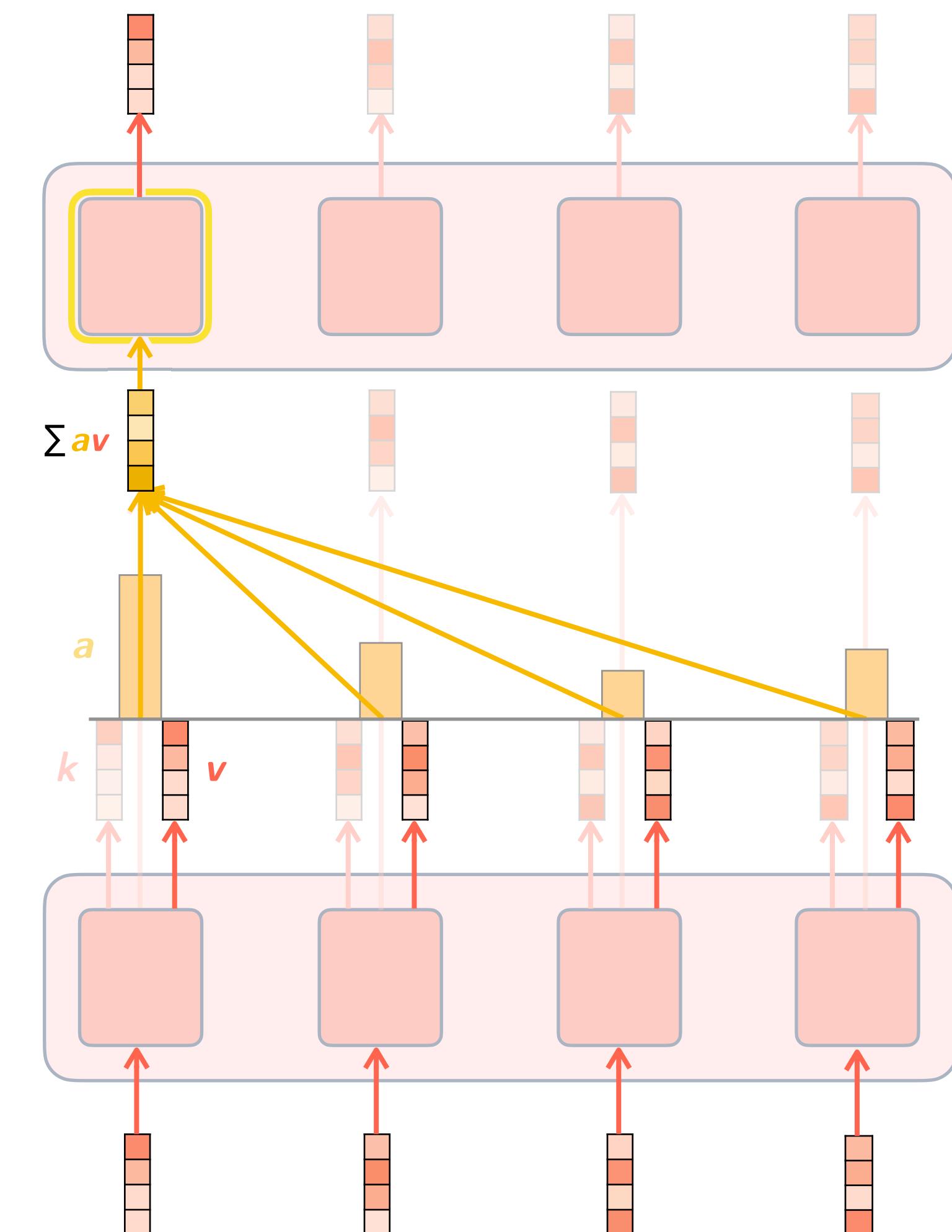
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Refining & Predicting

and contextualizing



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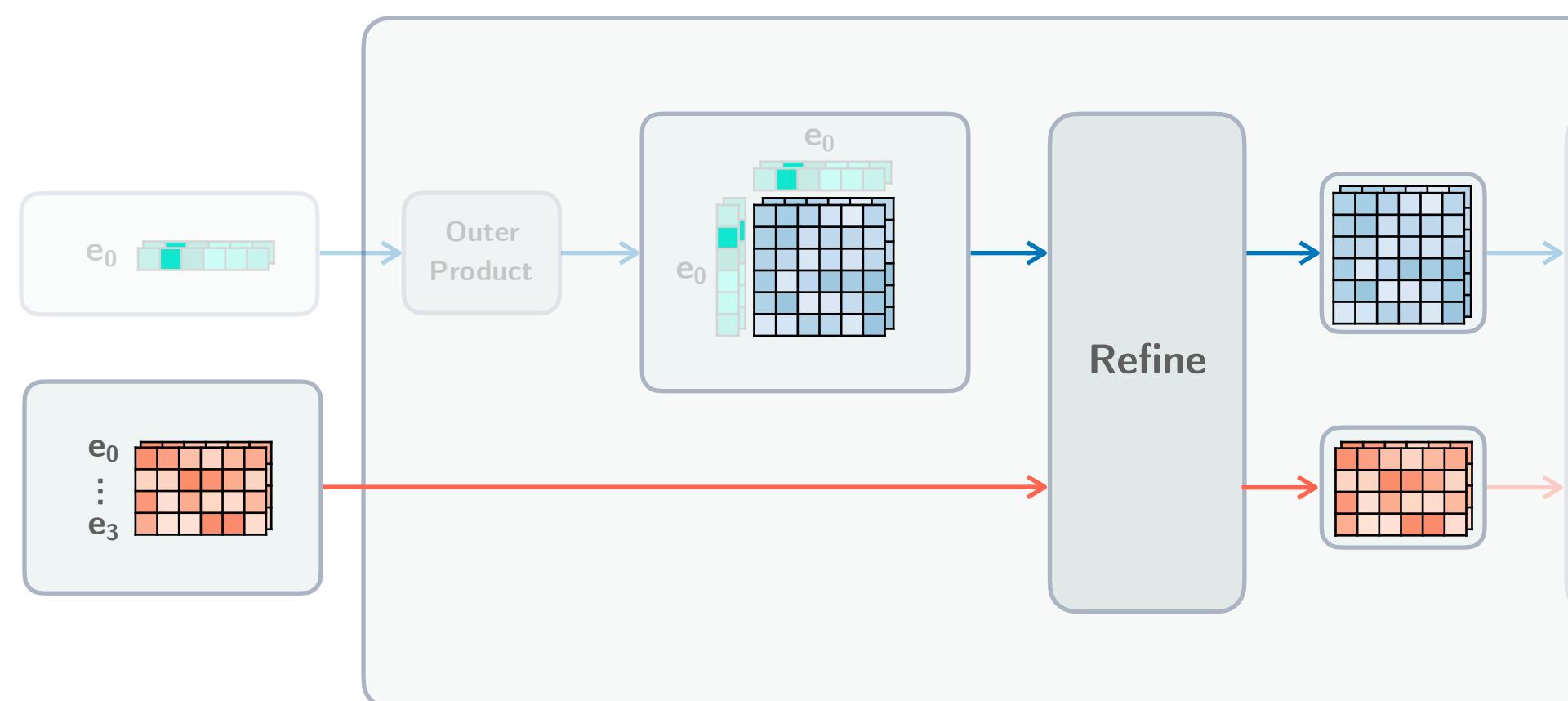


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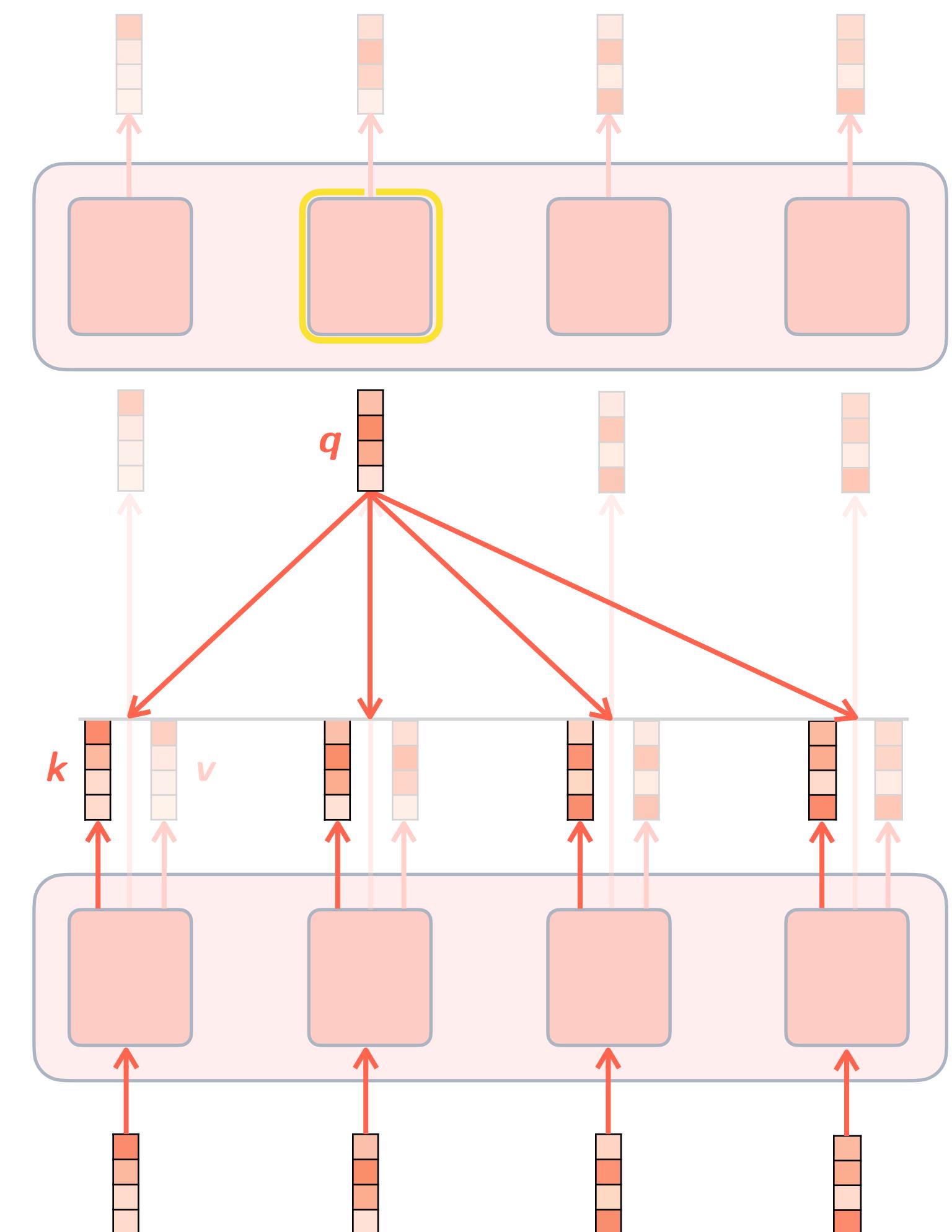
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Refining & Predicting

and contextualizing



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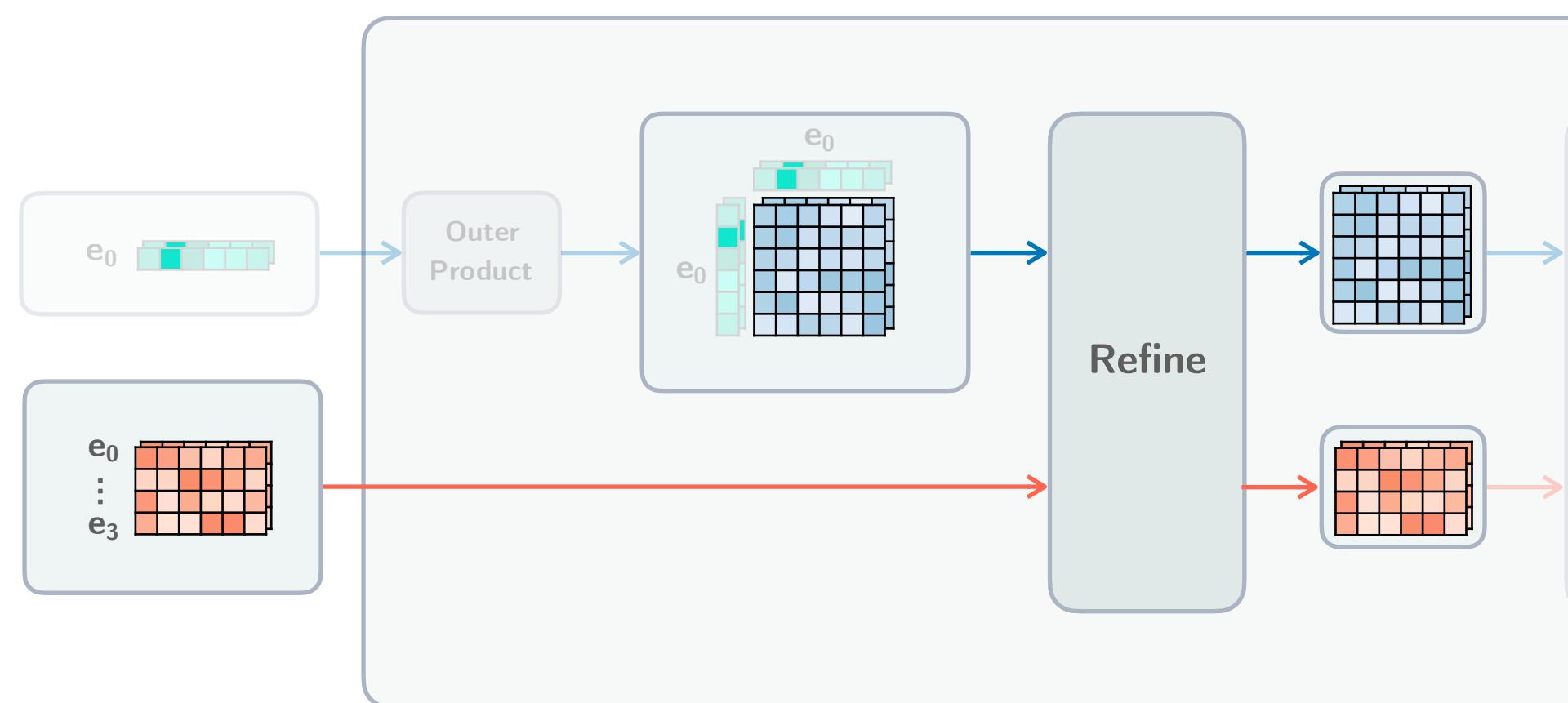


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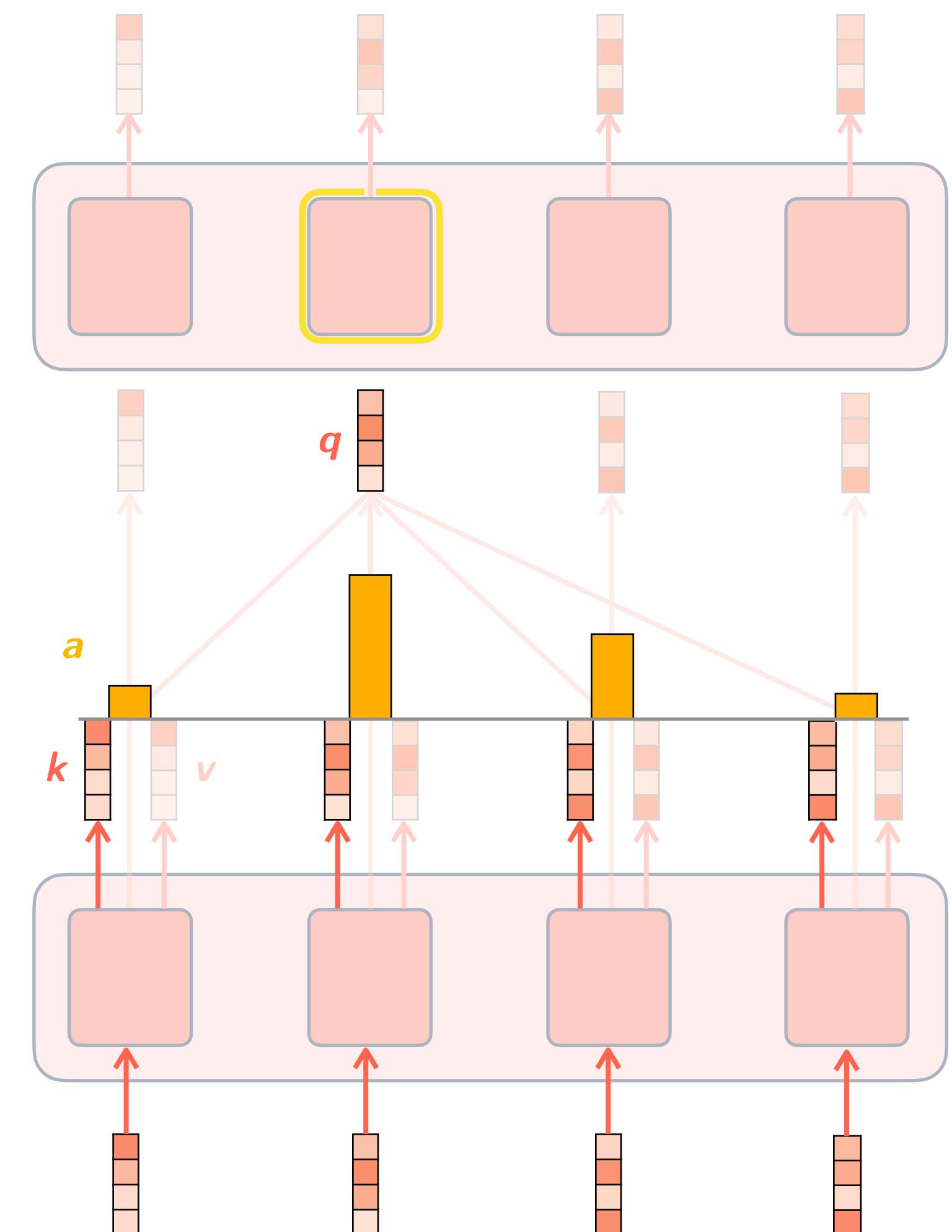
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



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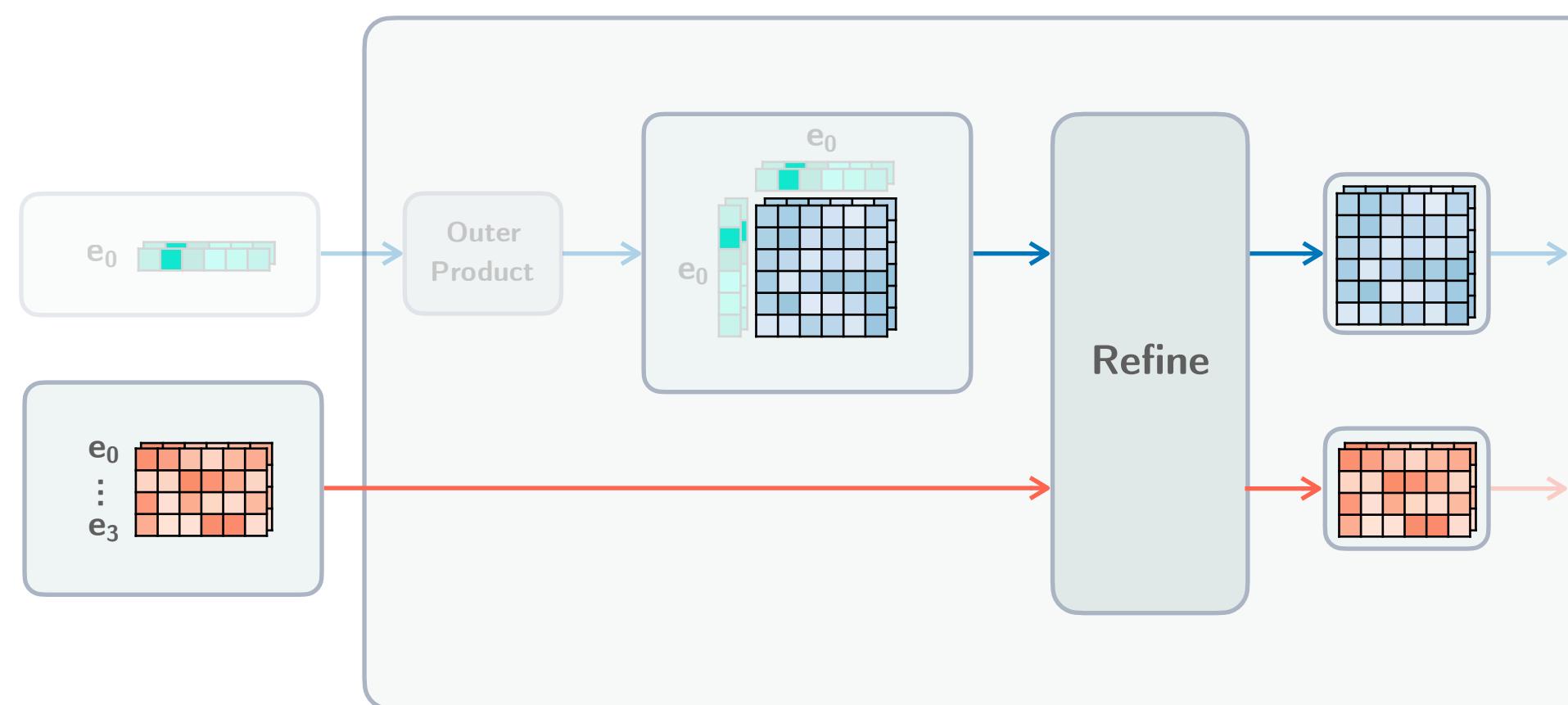


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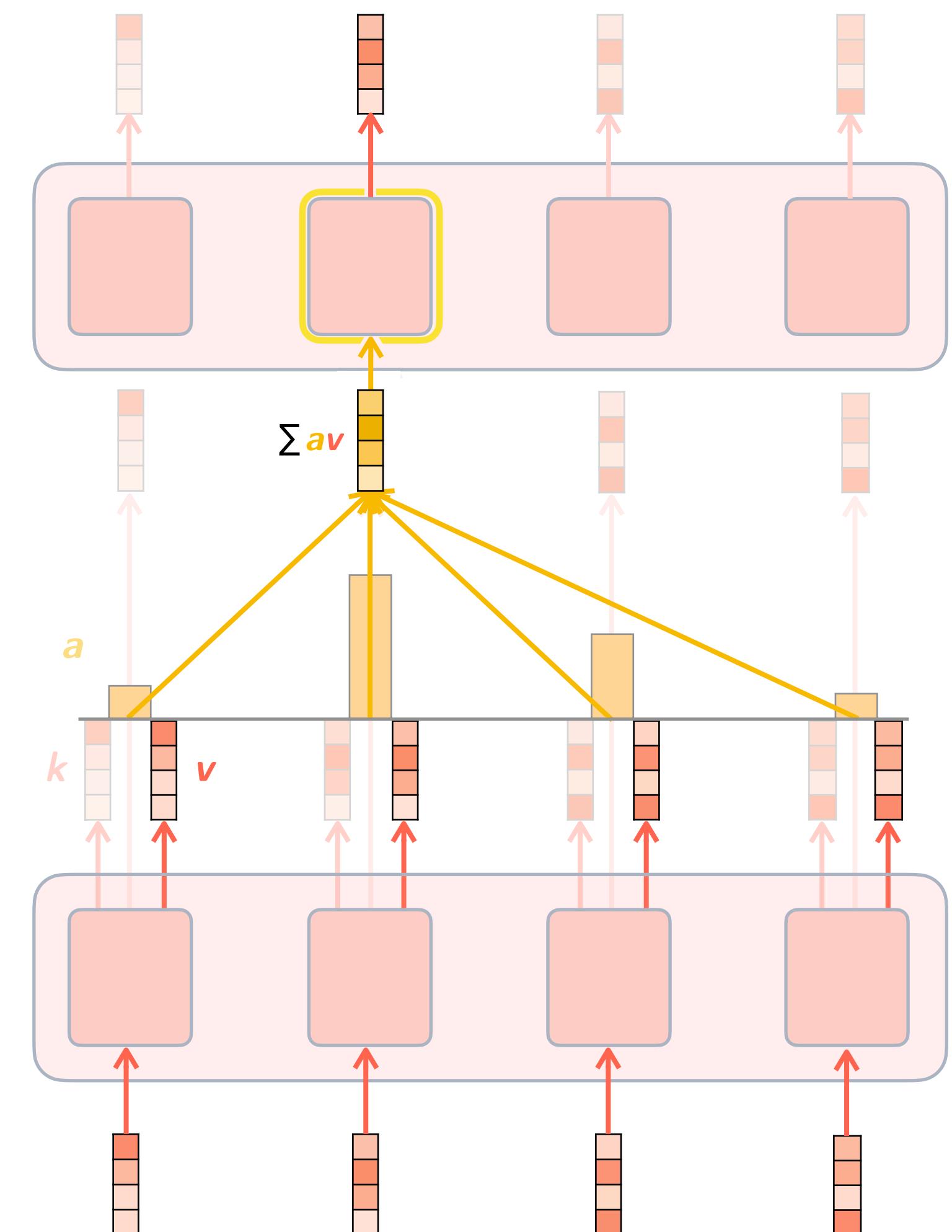
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



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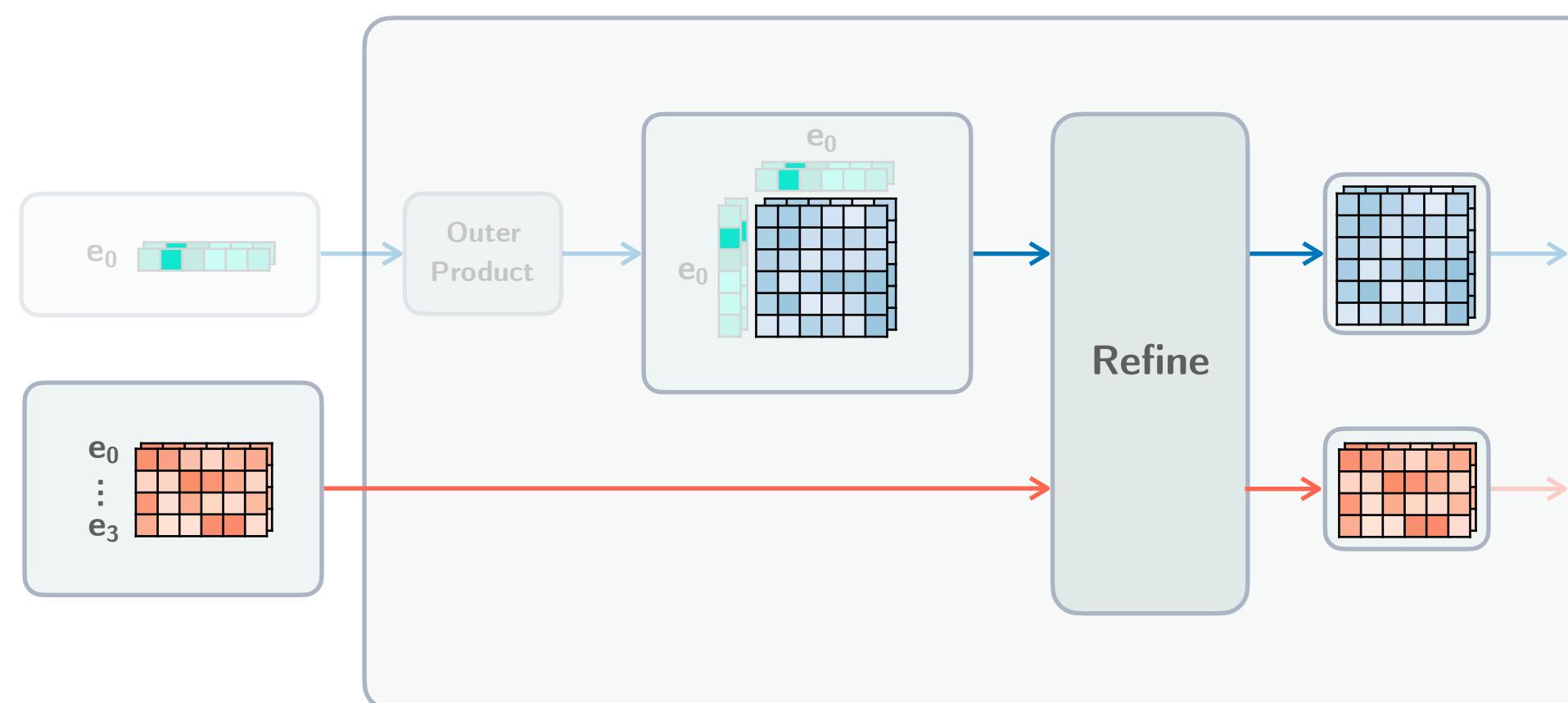


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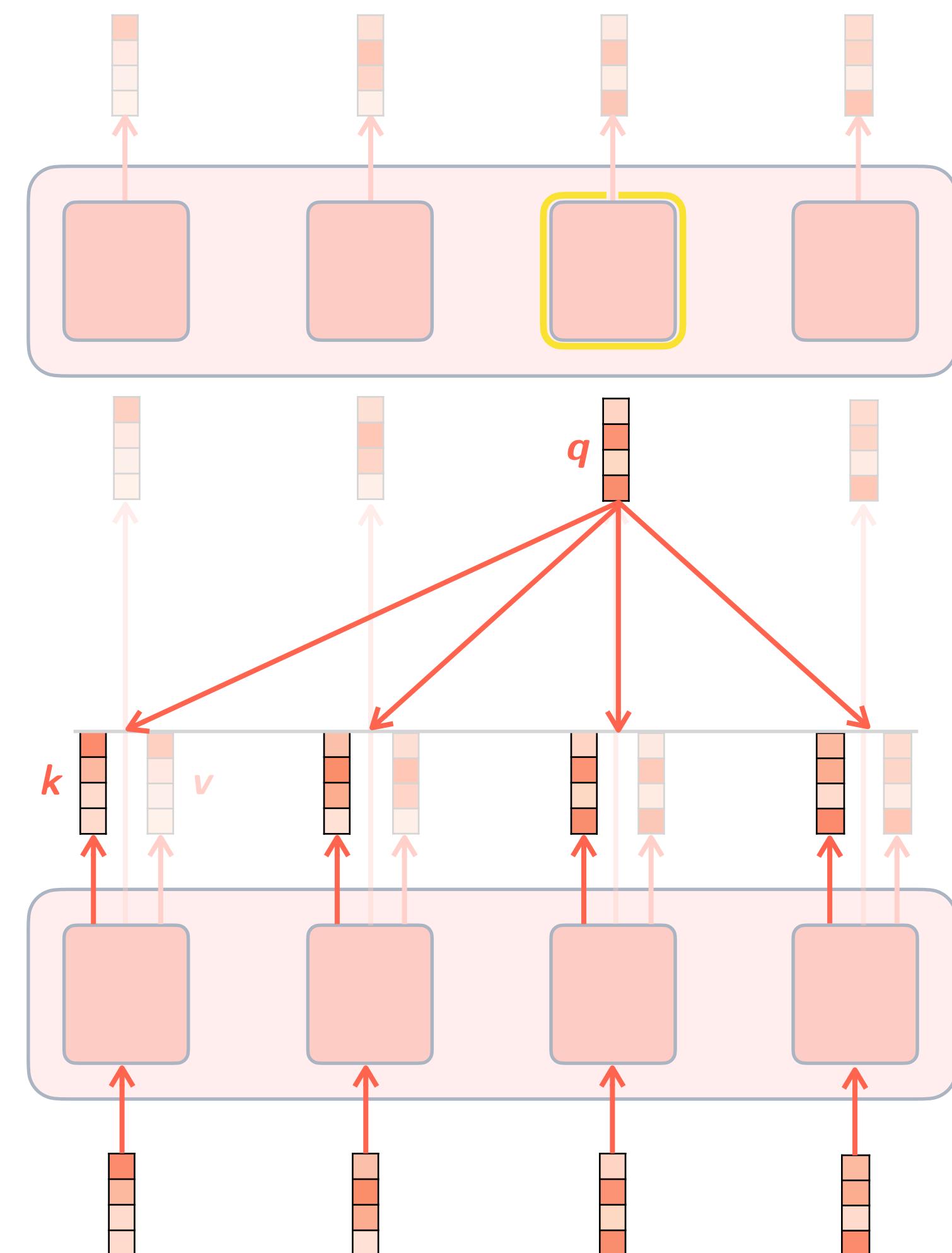
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



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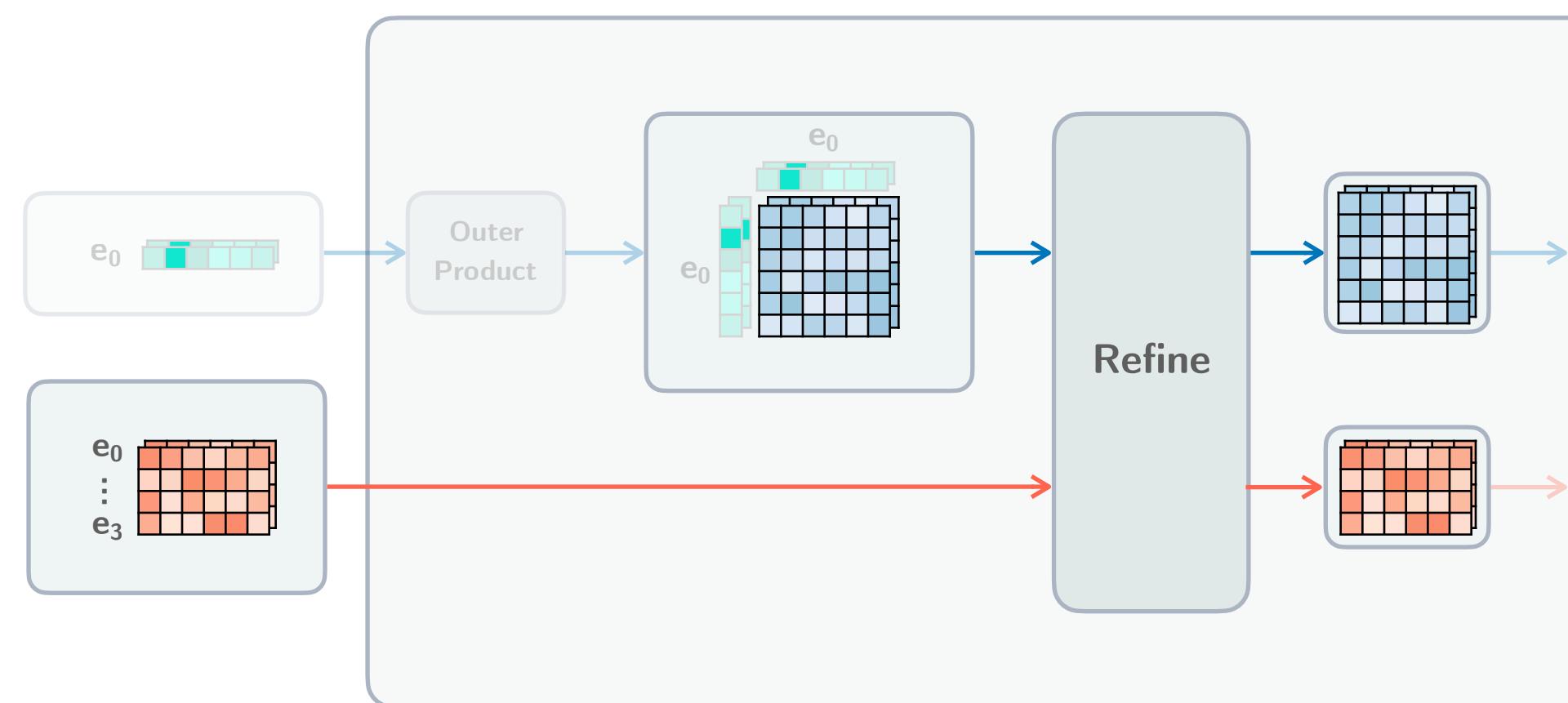


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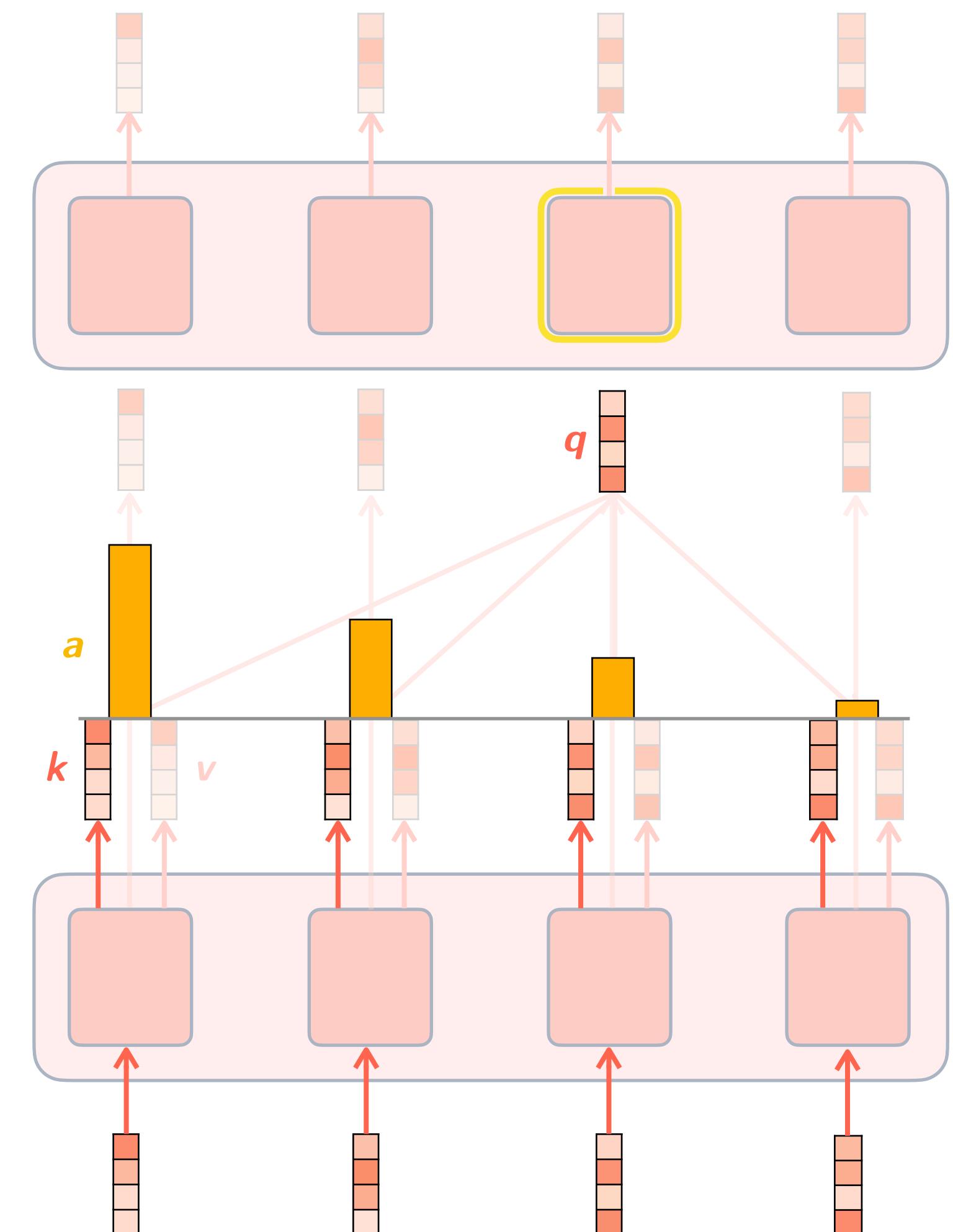
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



Self-Attention

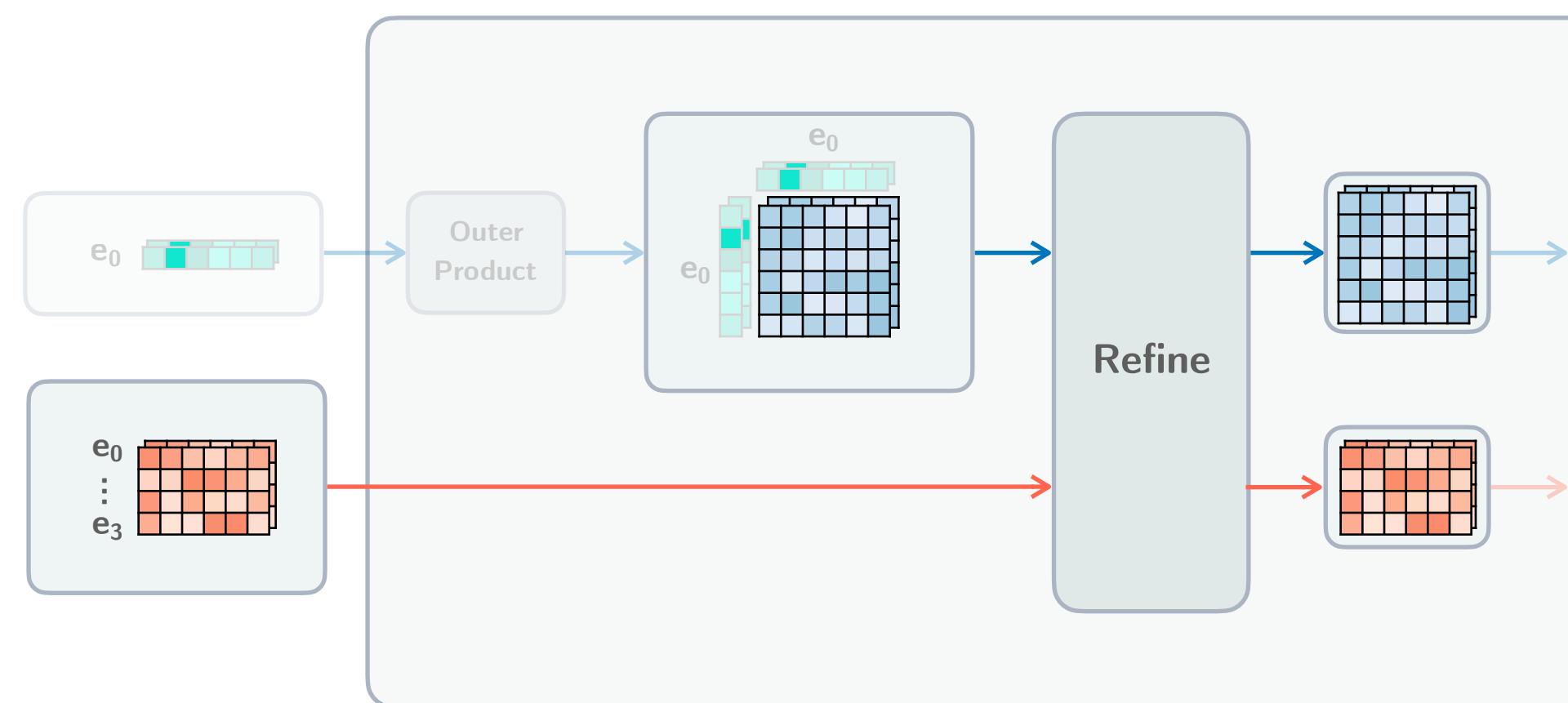


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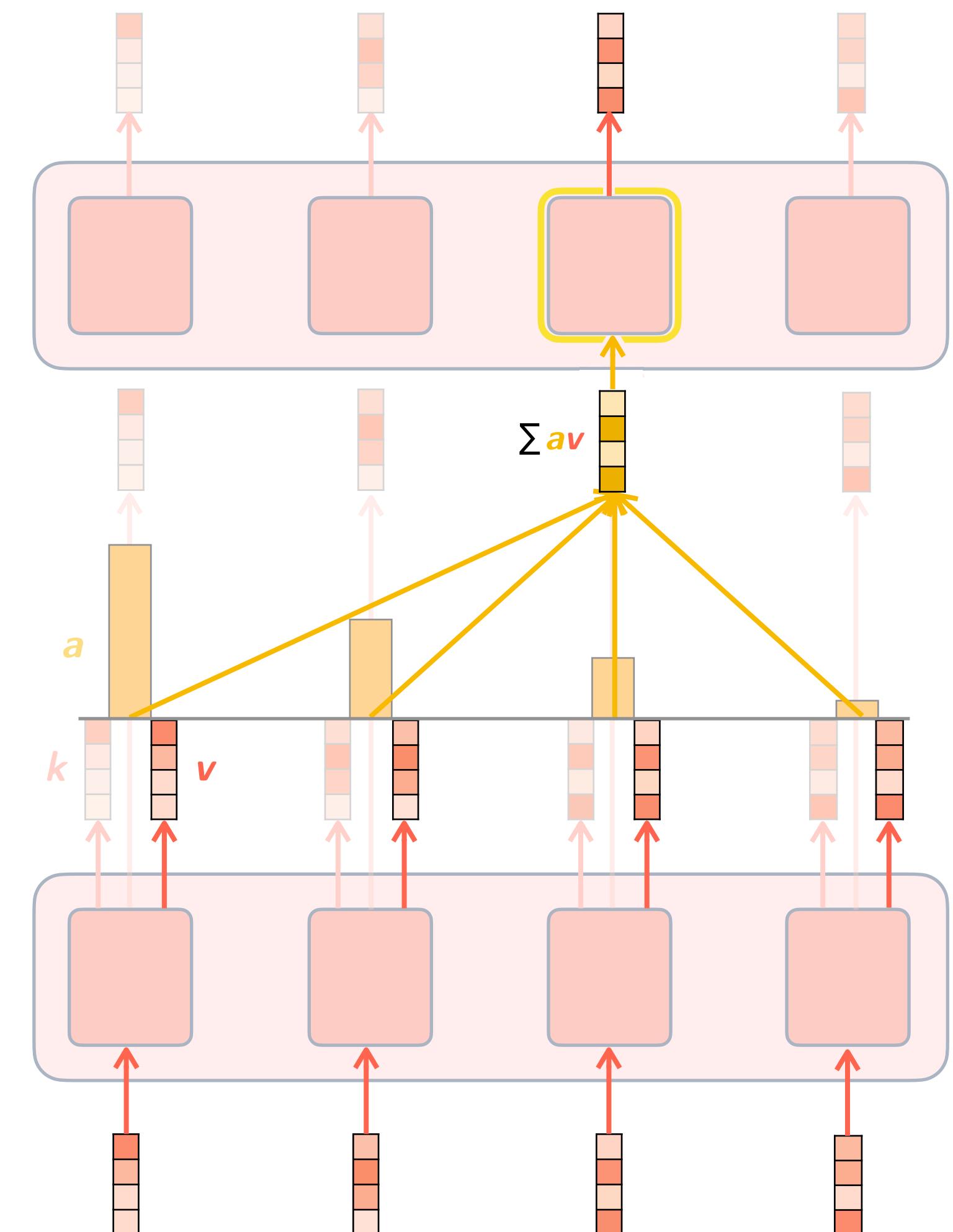
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



Self-Attention

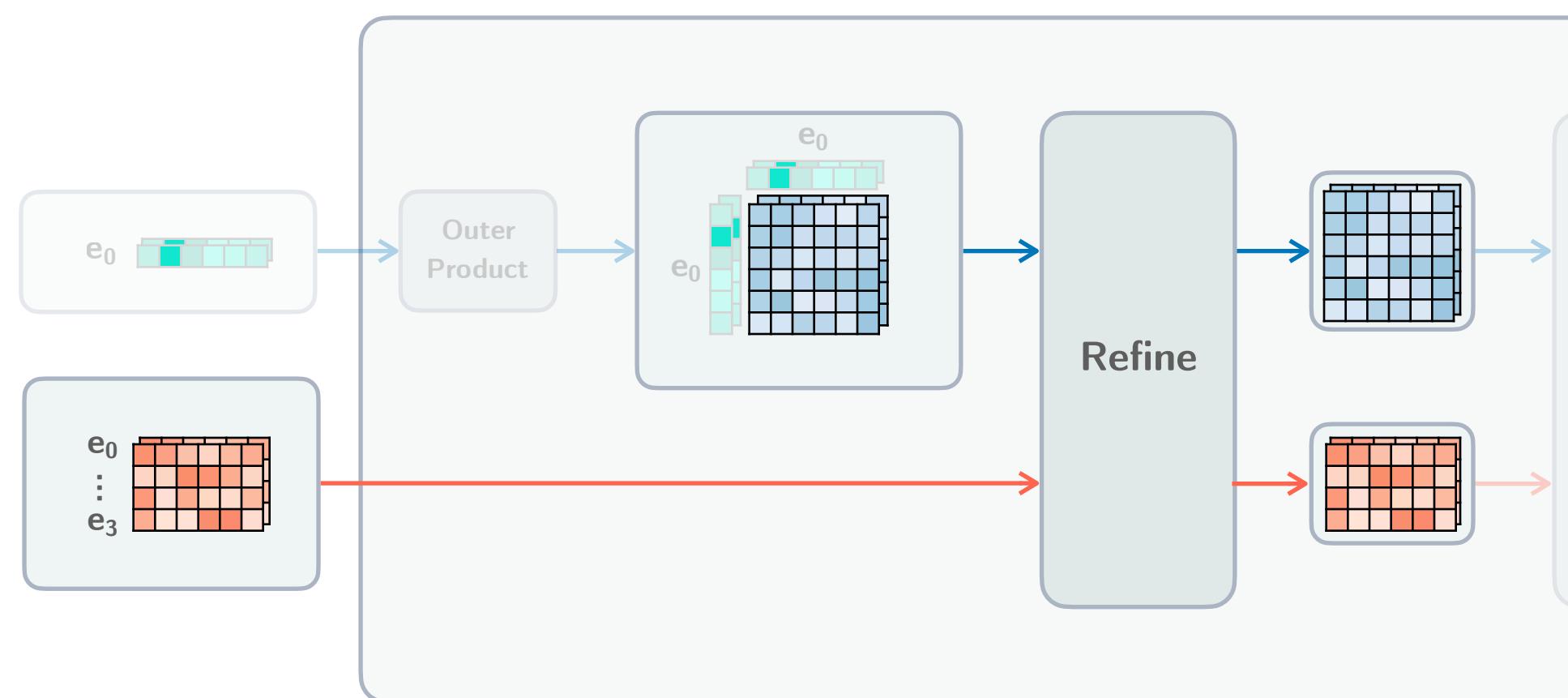


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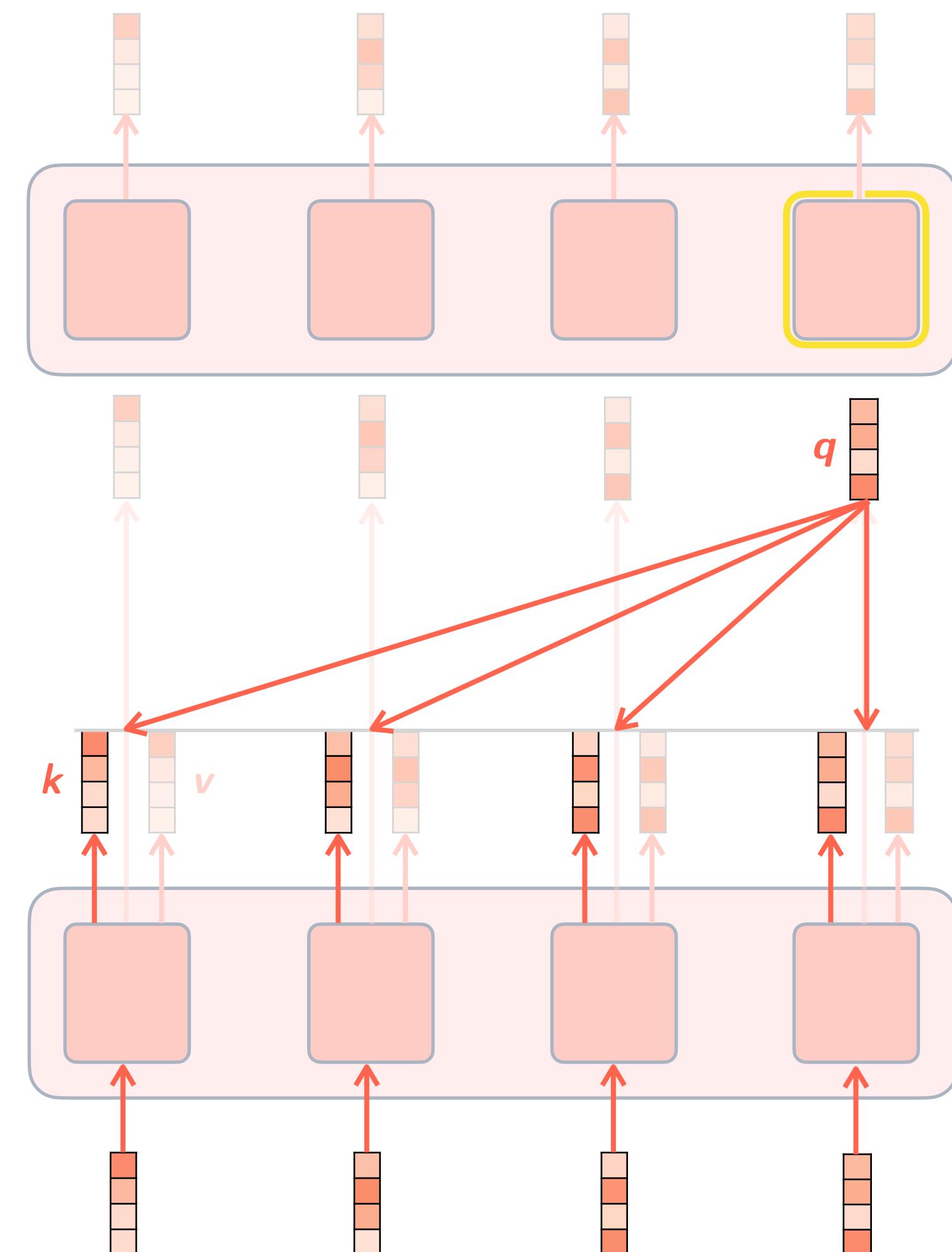
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



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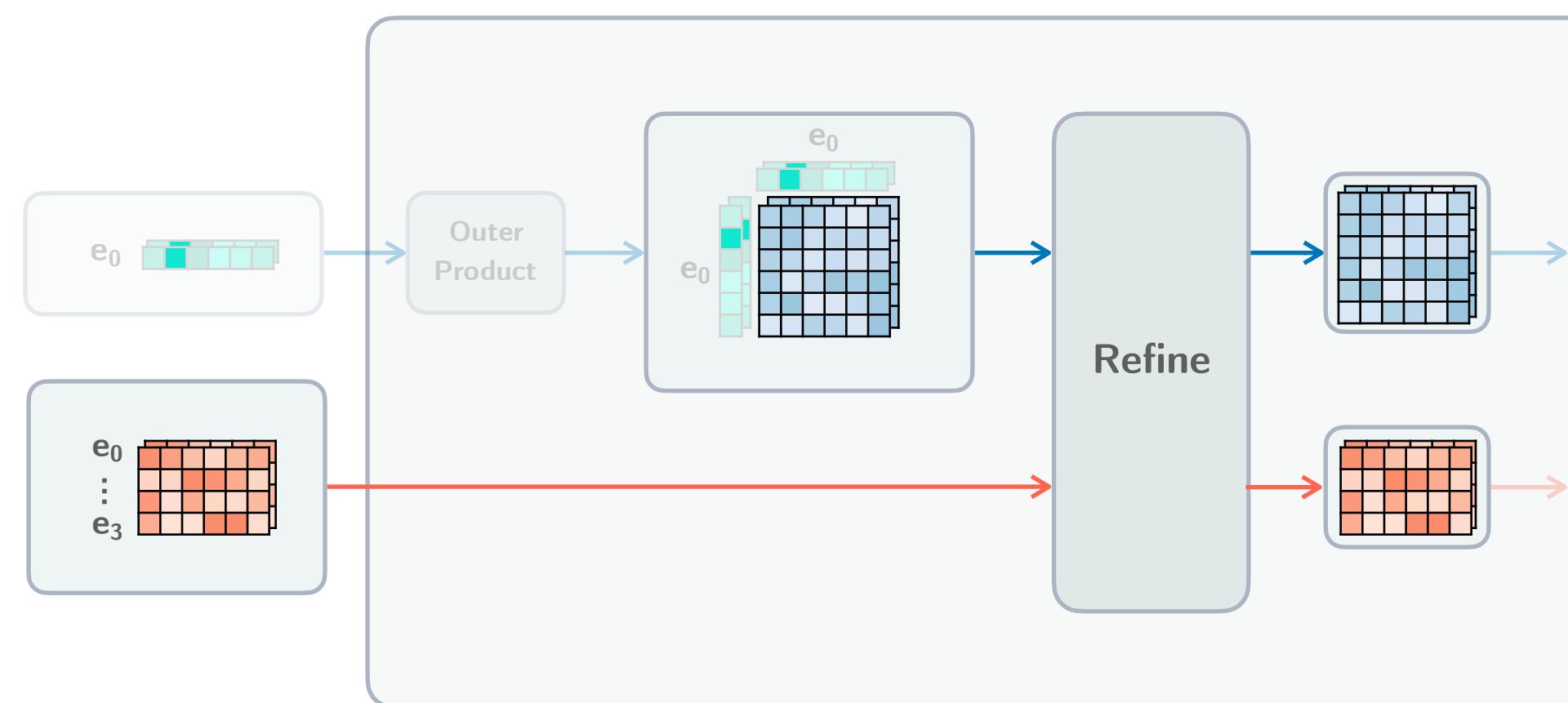


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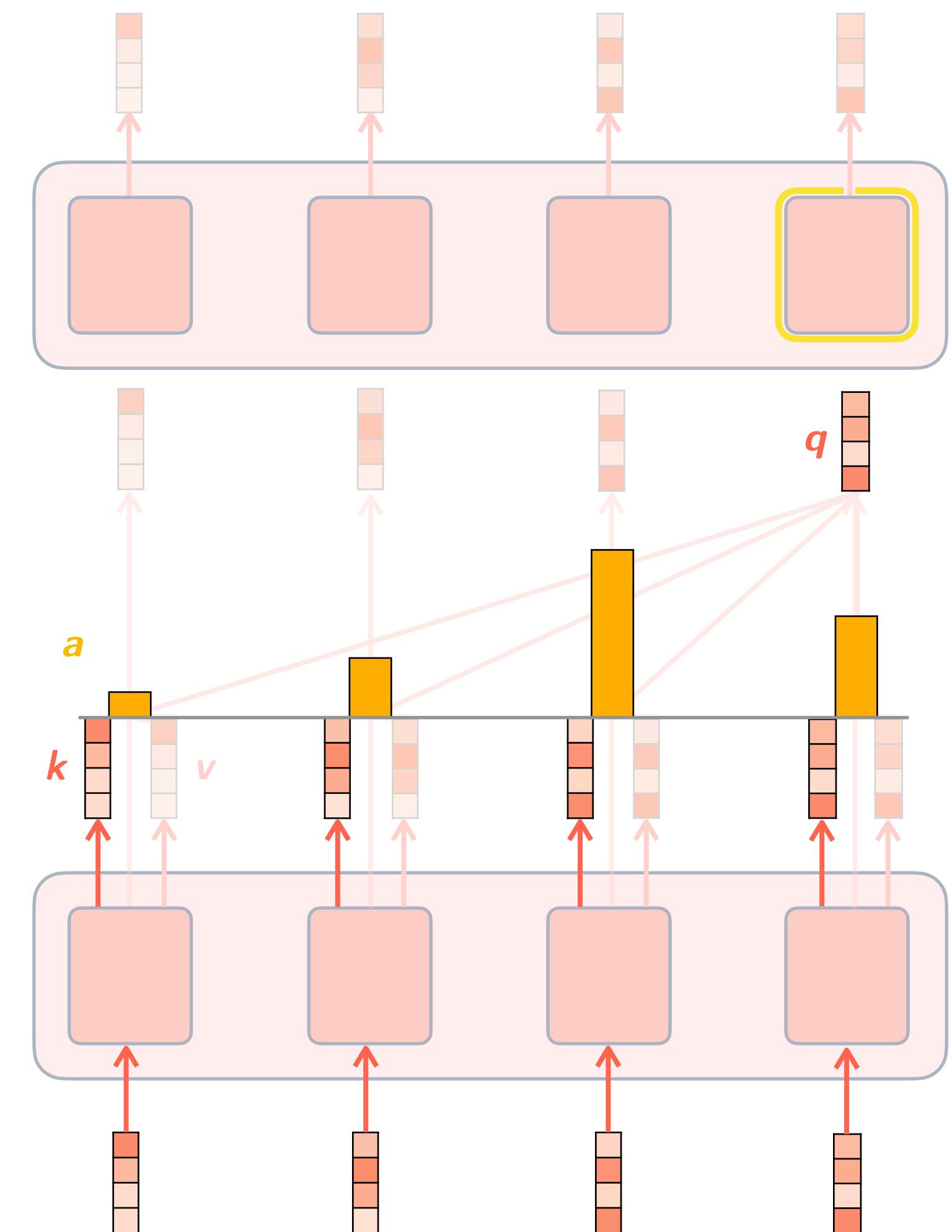
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Refining & Predicting

and contextualizing



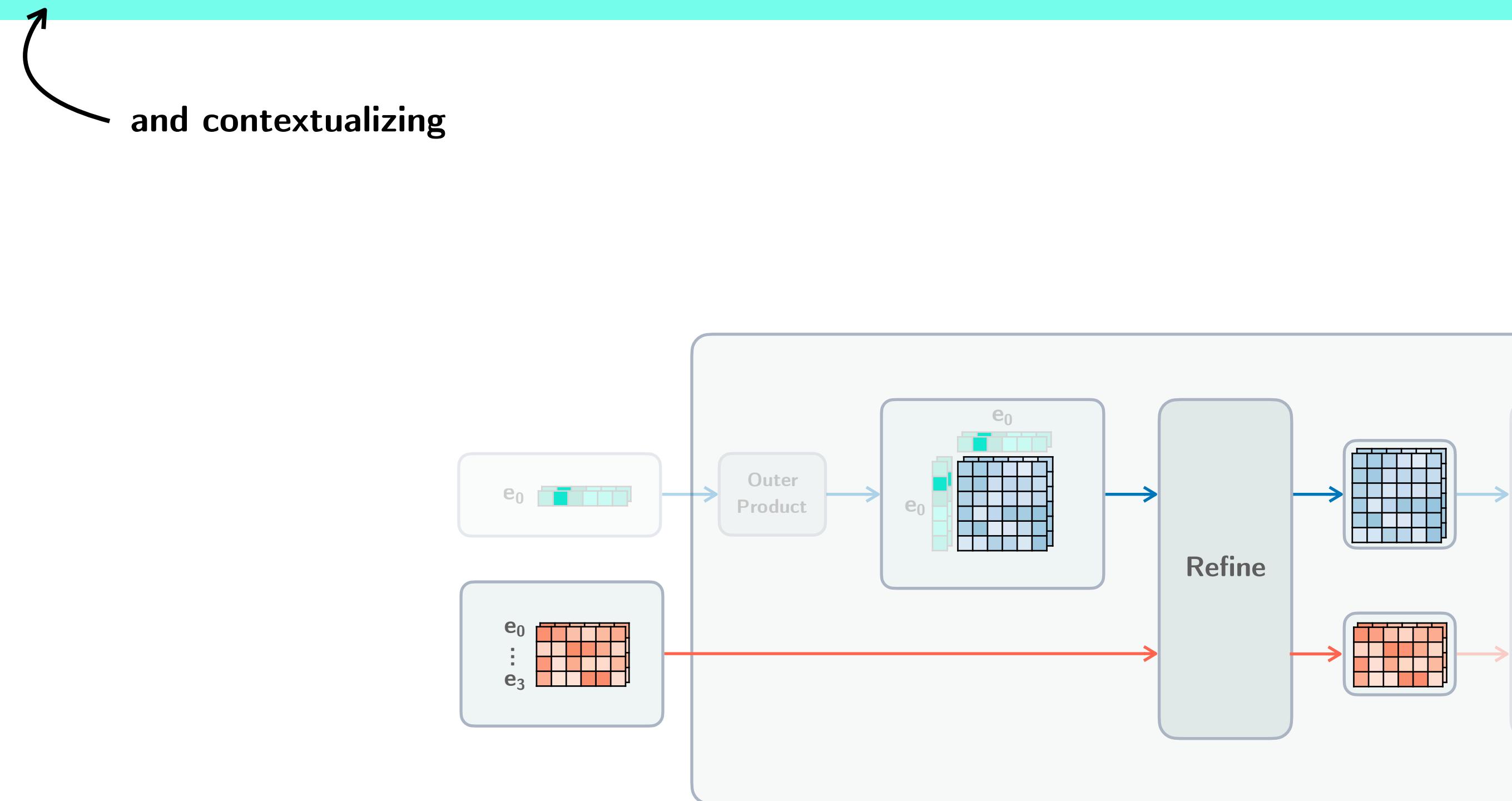
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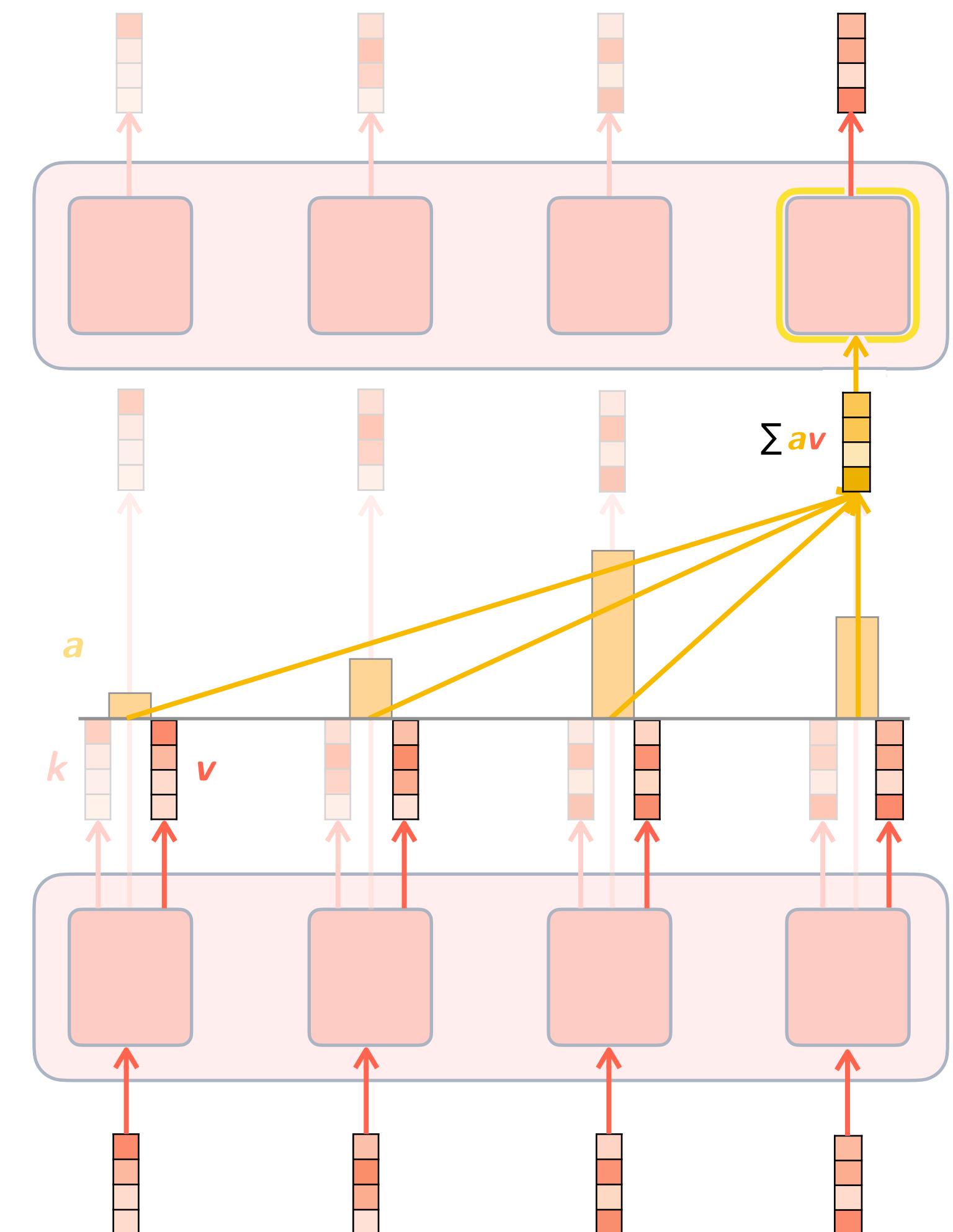
AlphaFold and Protein Structure Prediction

The Solution AlphaFold 2

Refining & Predicting



Self-Attention

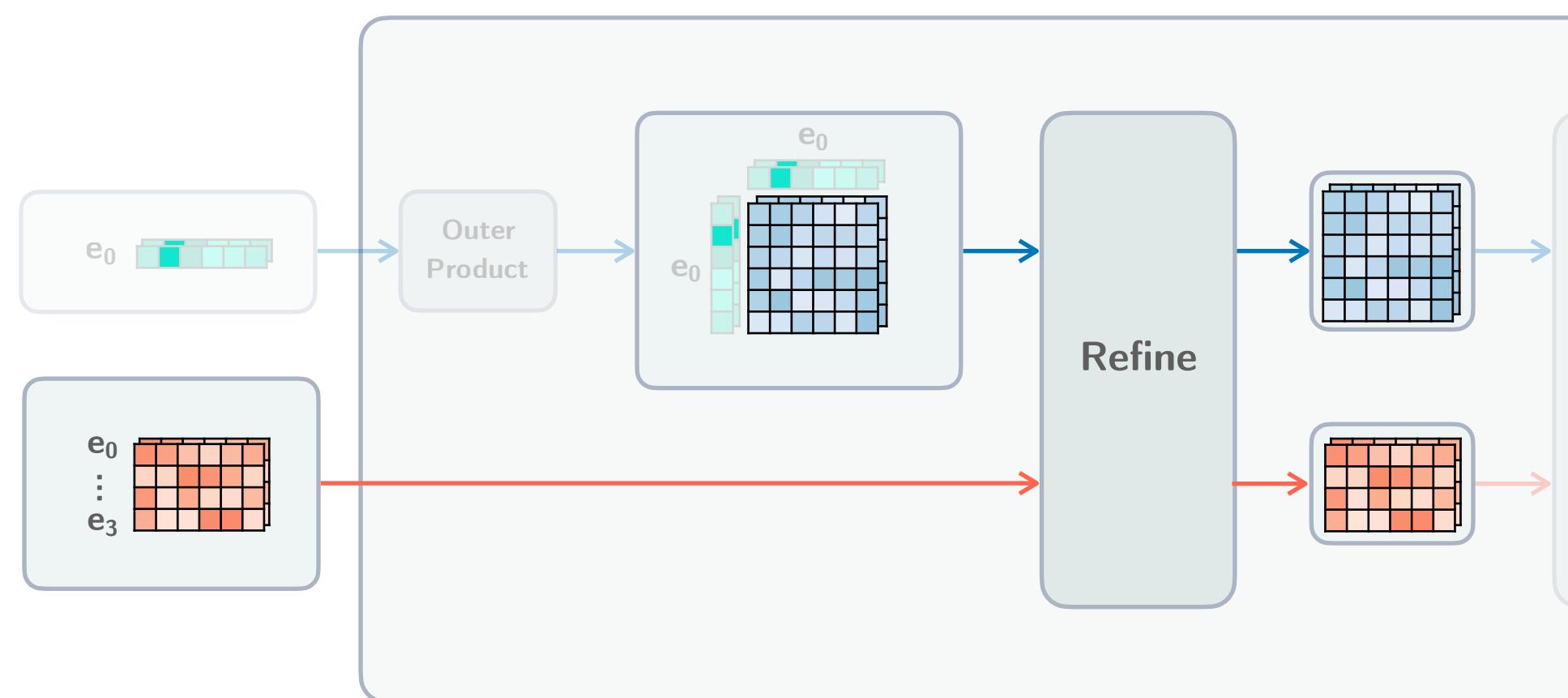


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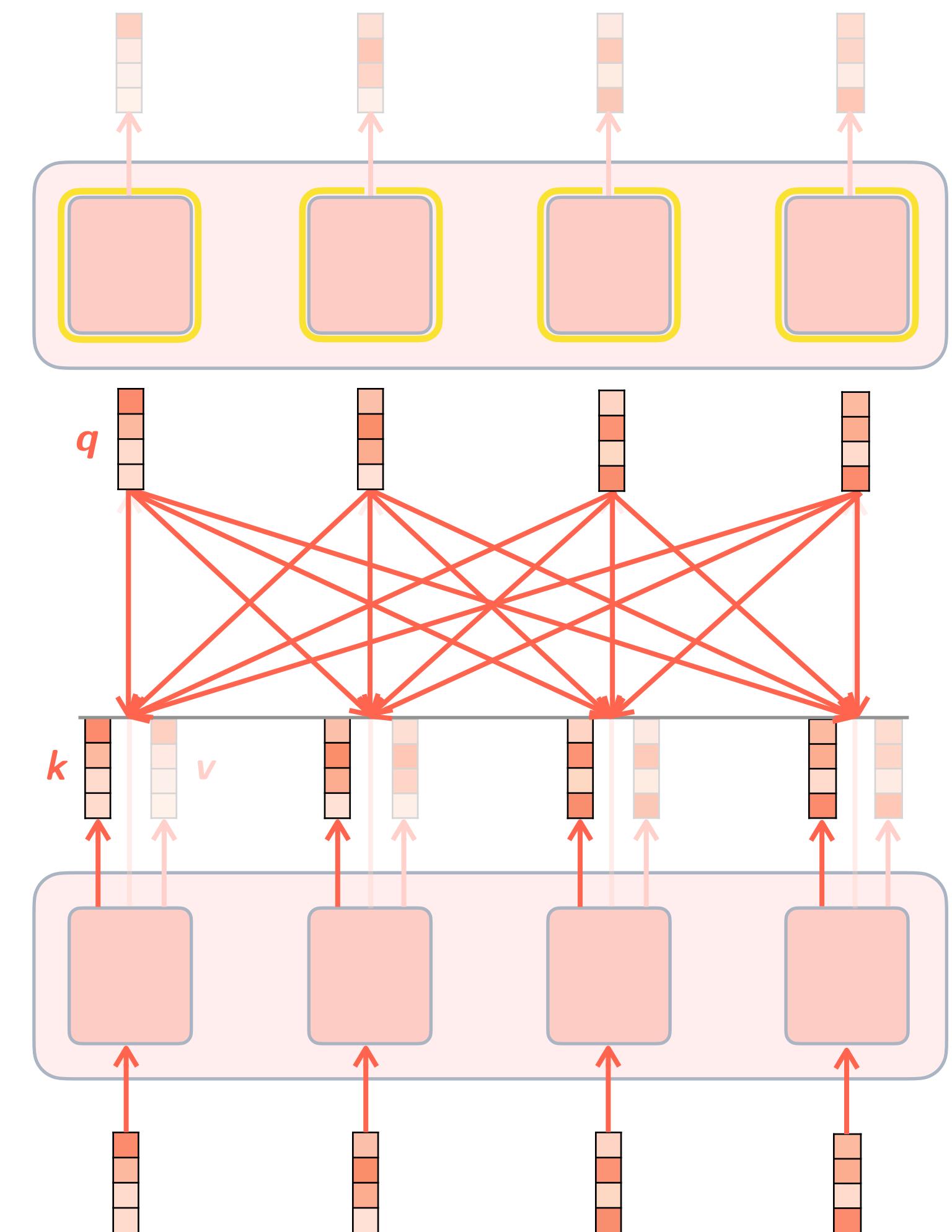
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Refining & Predicting

and contextualizing



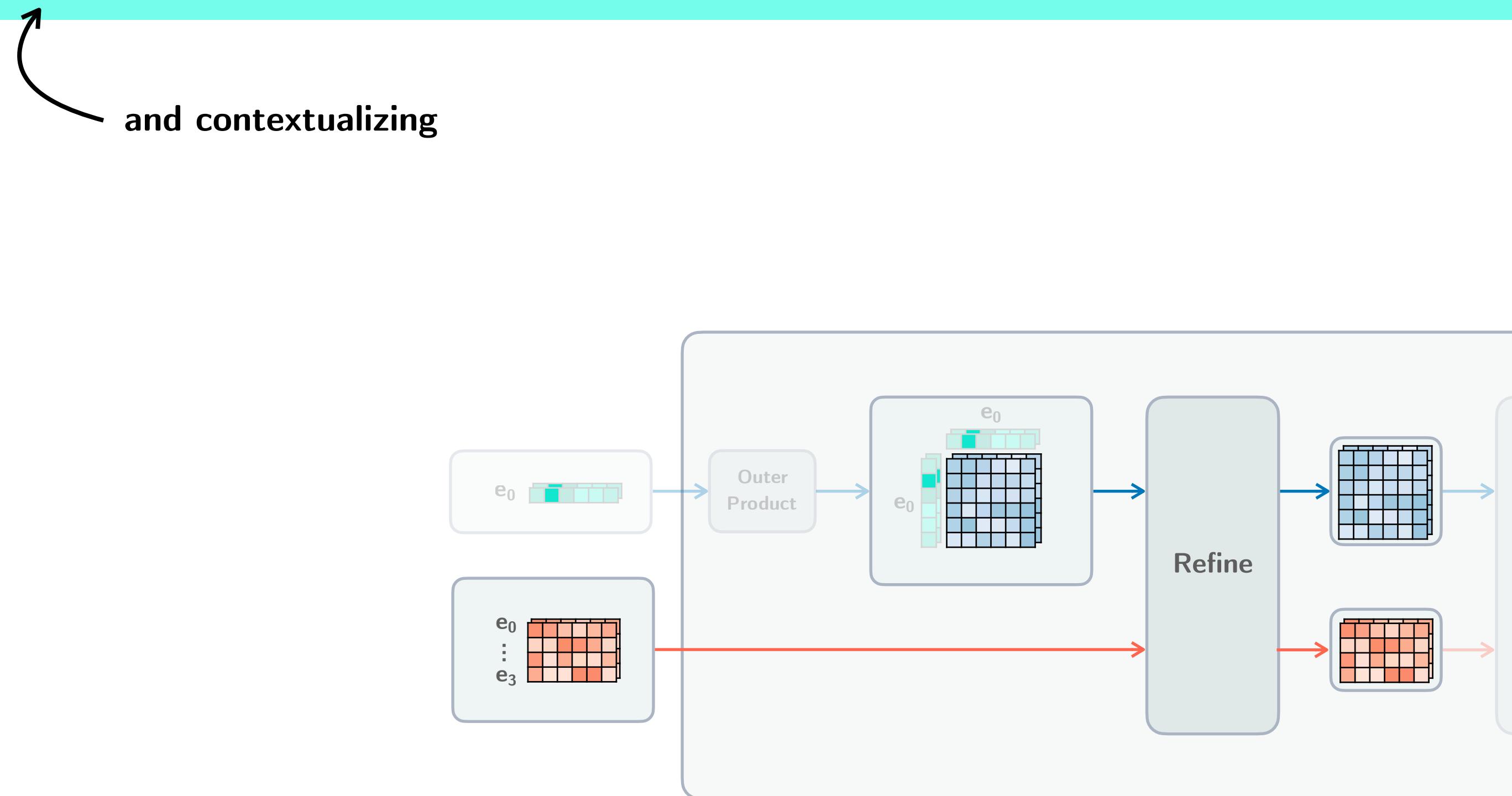
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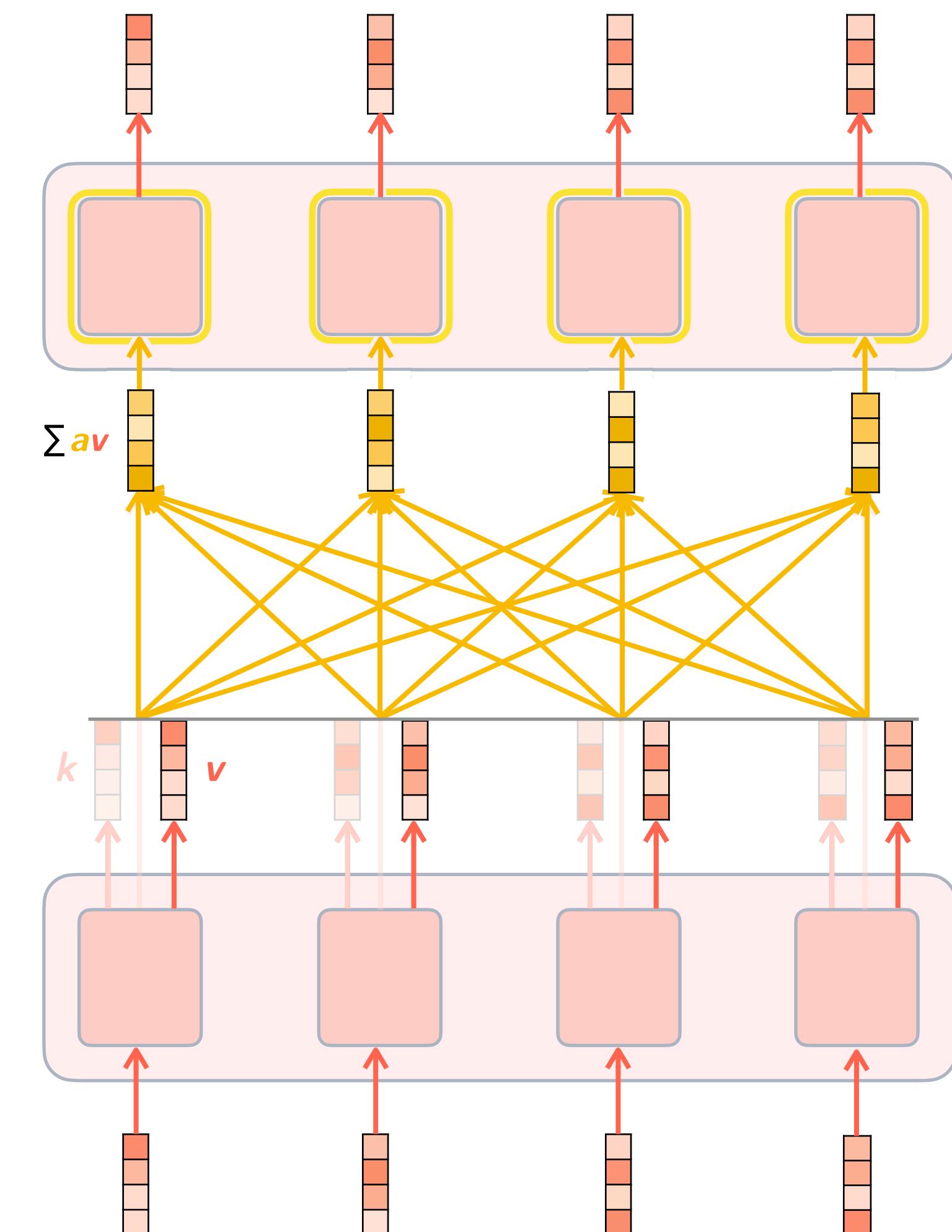
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Refining & Predicting



and contextualizing

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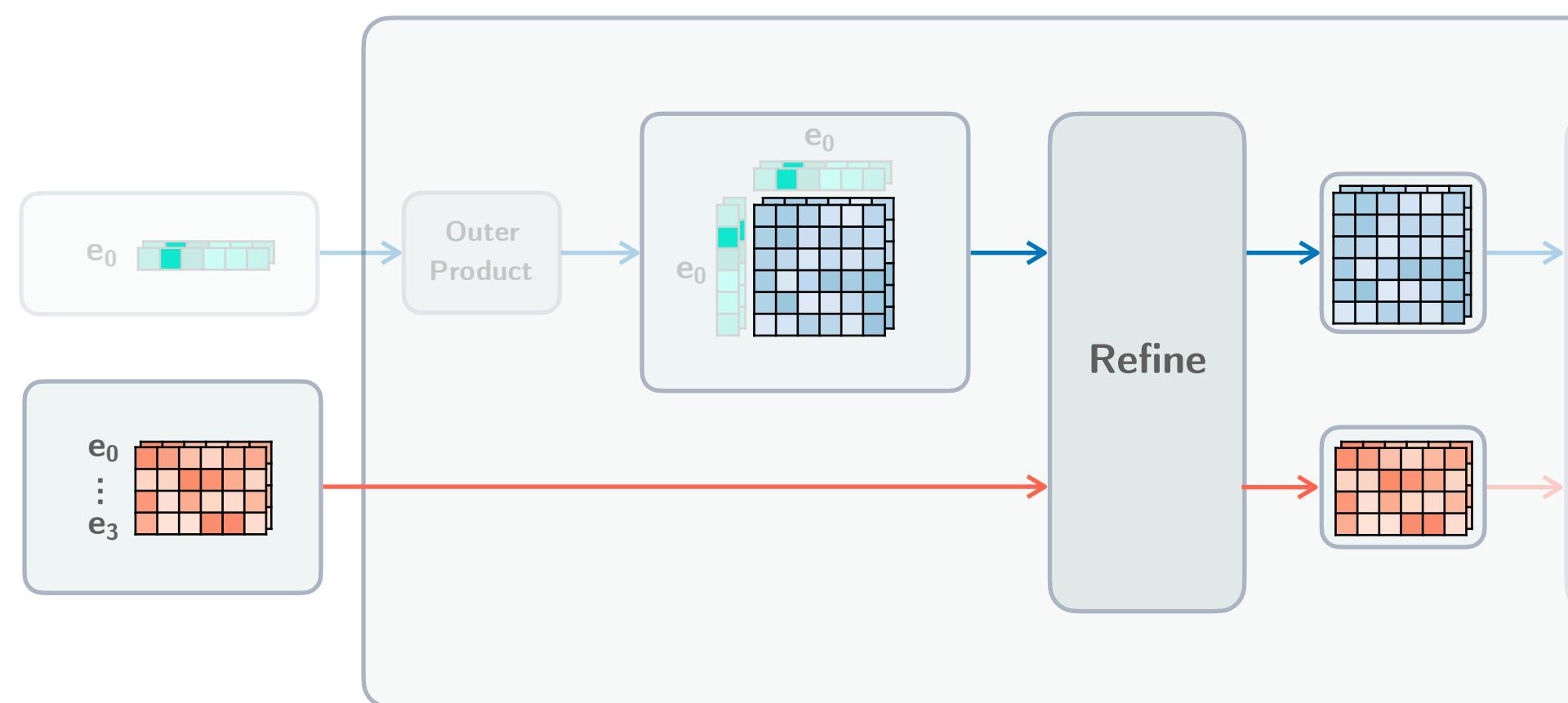


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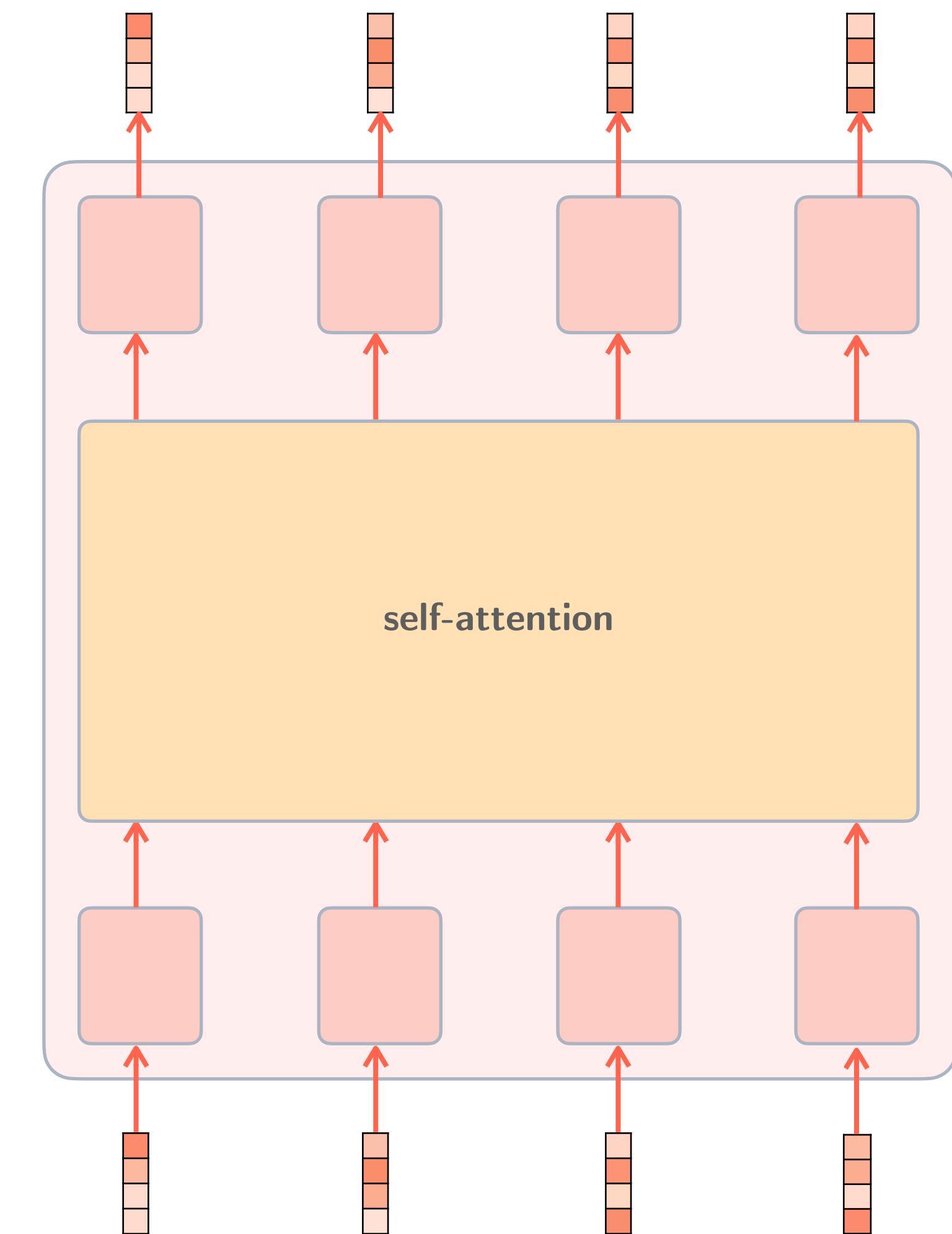
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



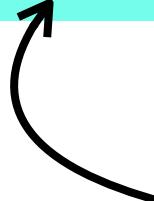
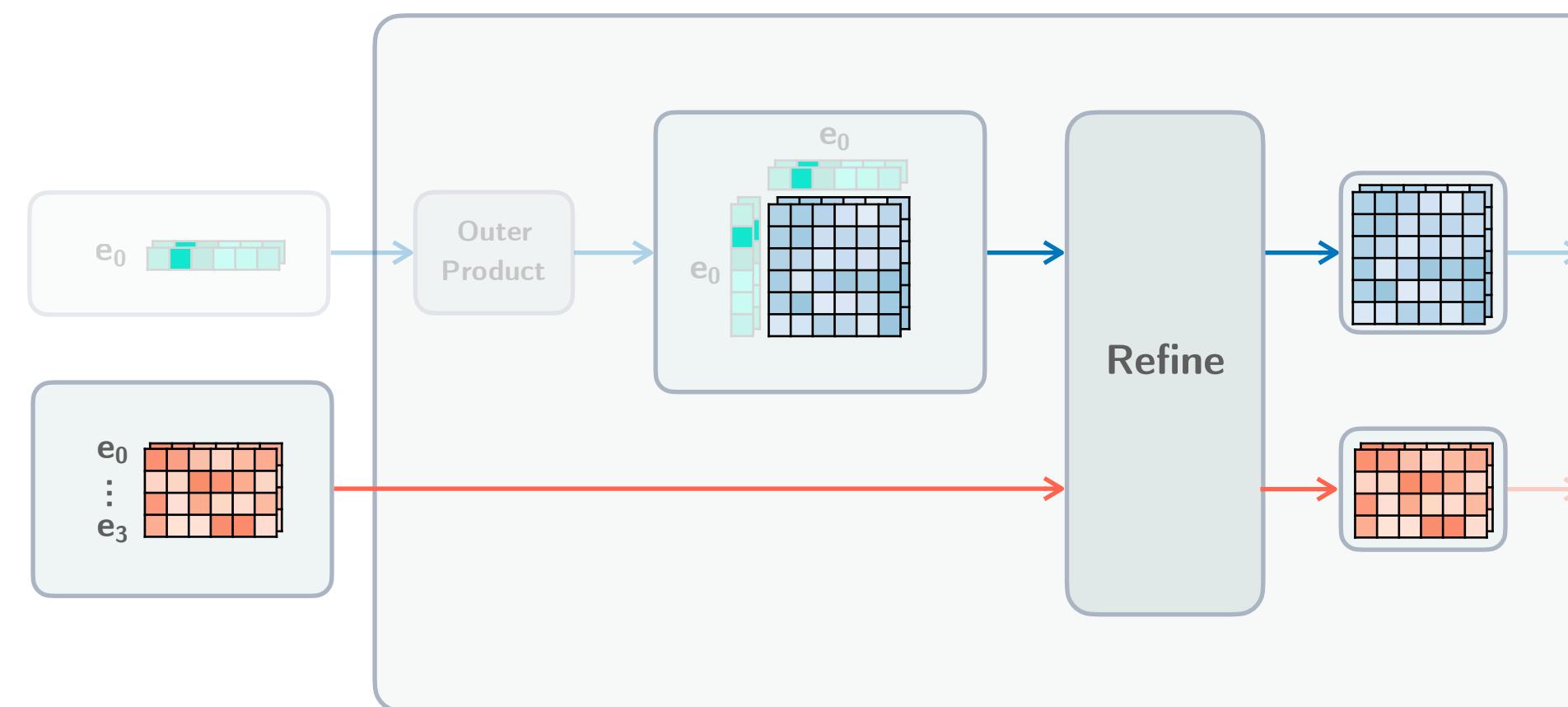
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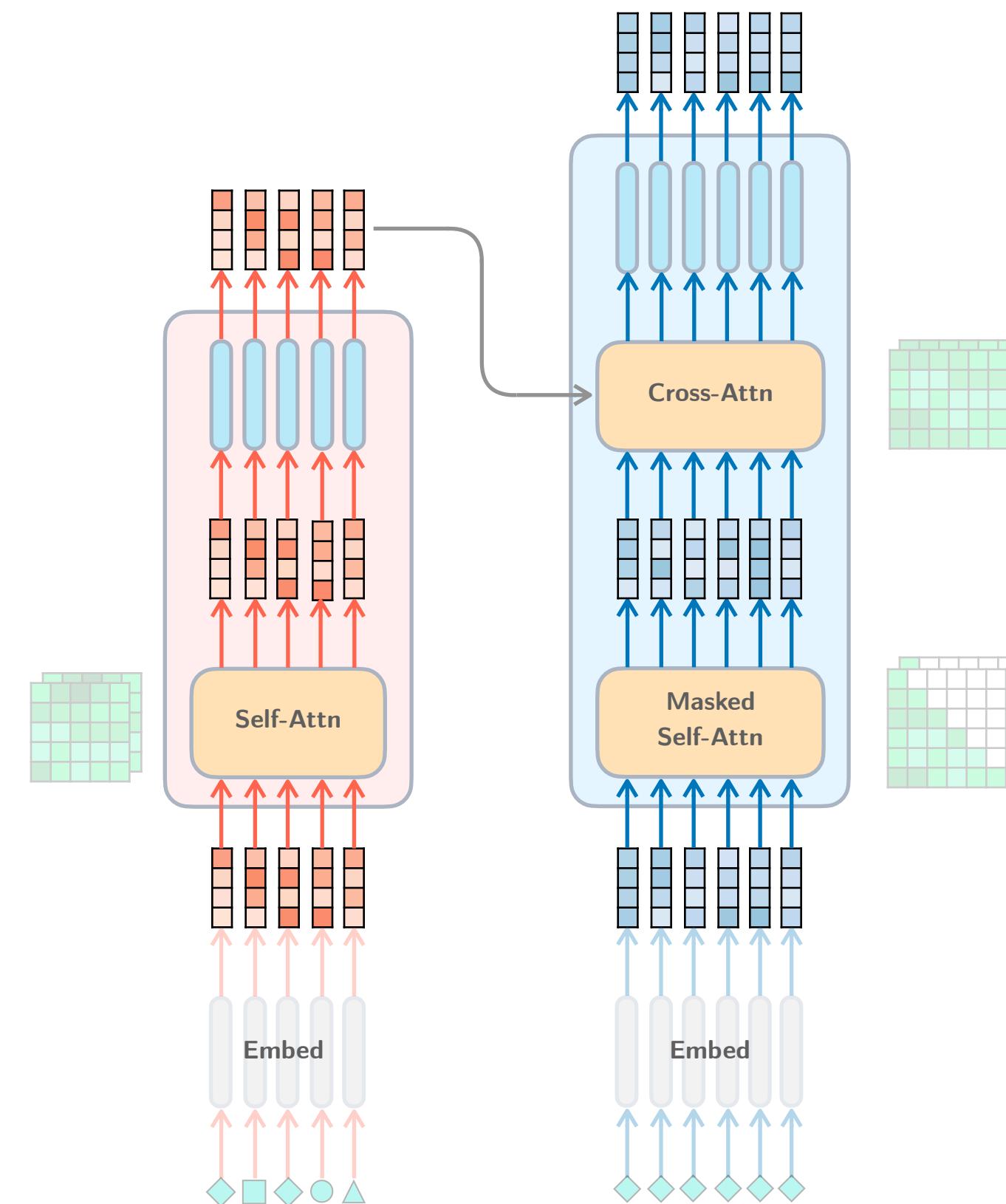
The Solution AlphaFold 2

Refining & Predicting

and contextualizing

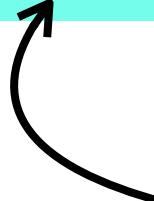
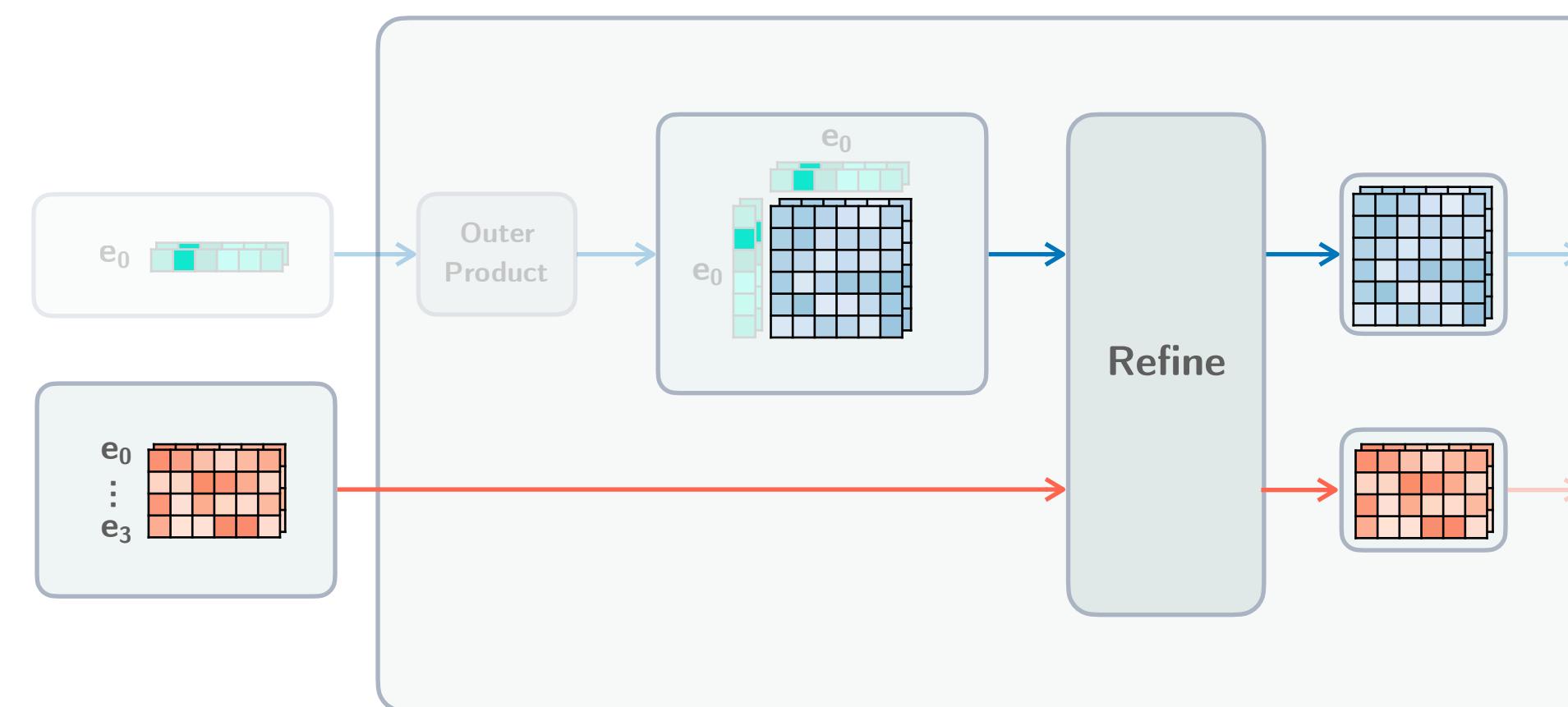
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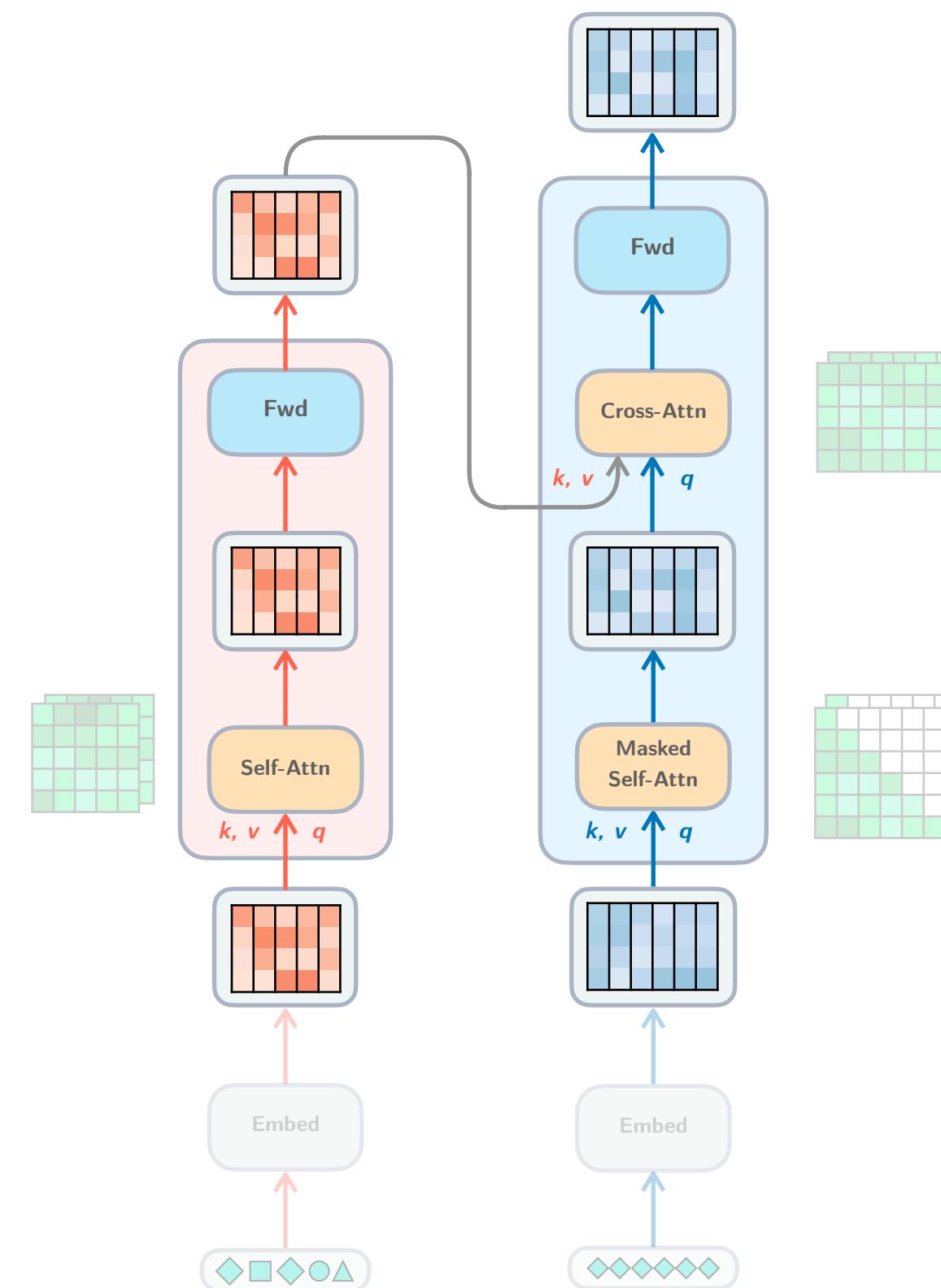
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Refining & Predicting

and contextualizing

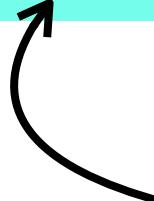
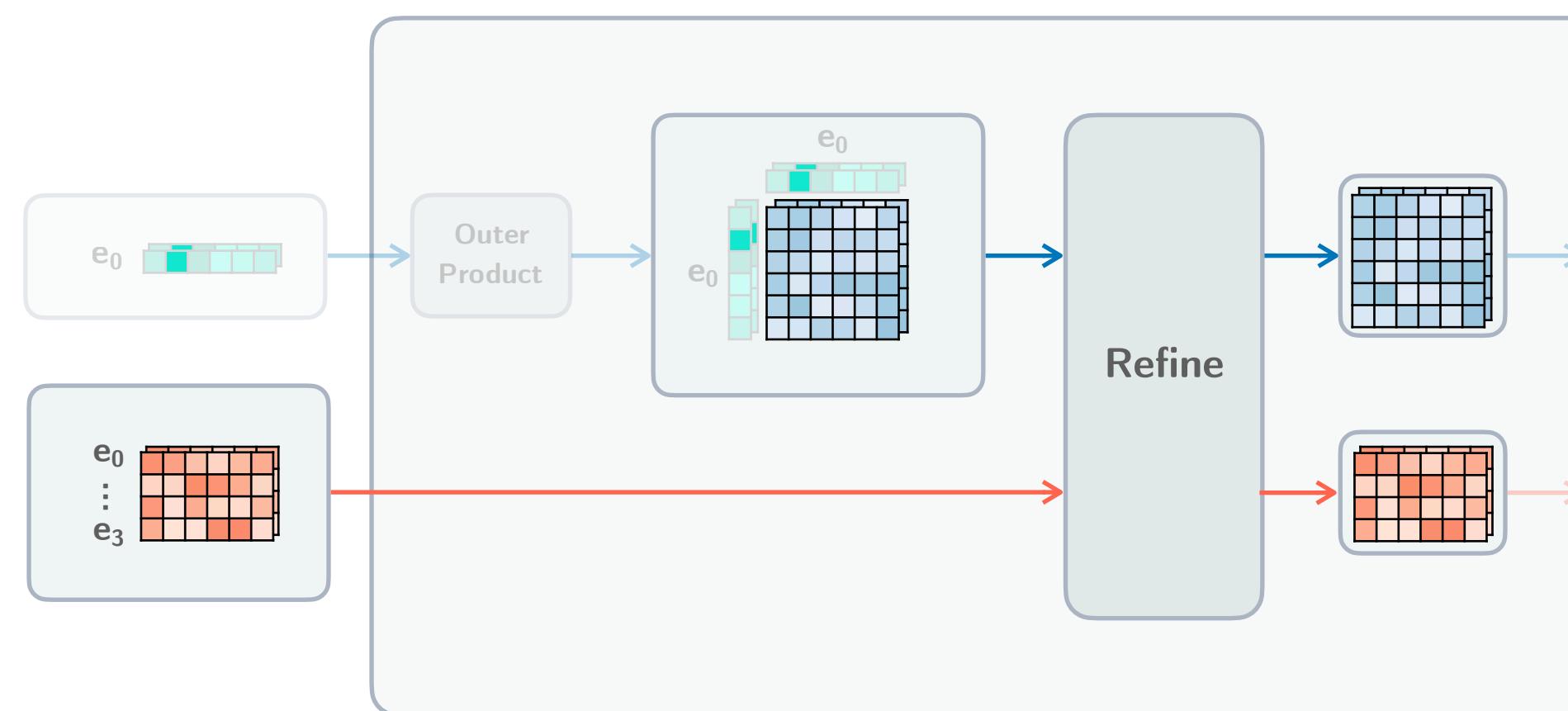
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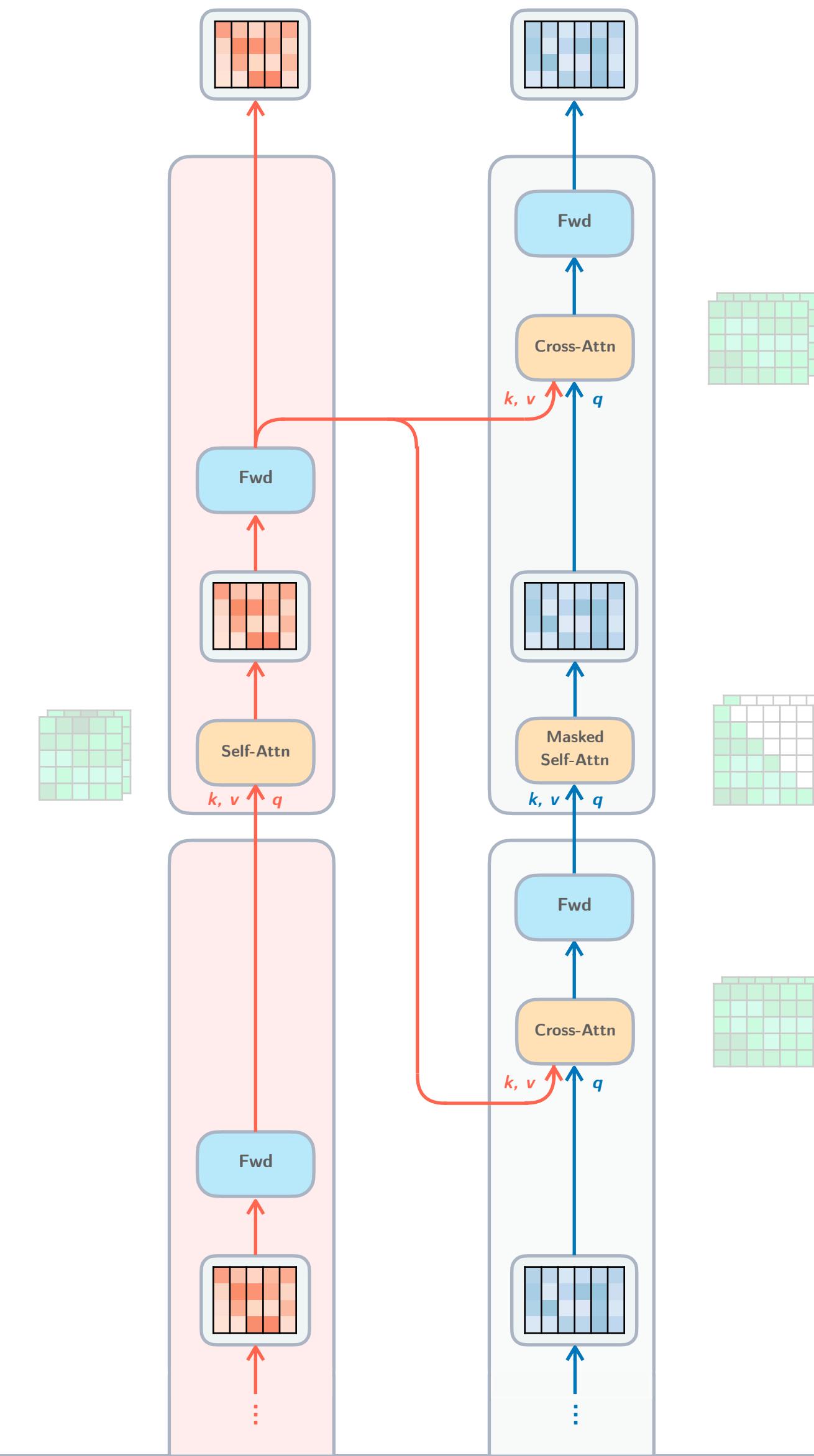
The Solution AlphaFold 2

Refining & Predicting

and contextualizing

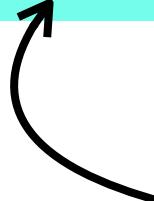
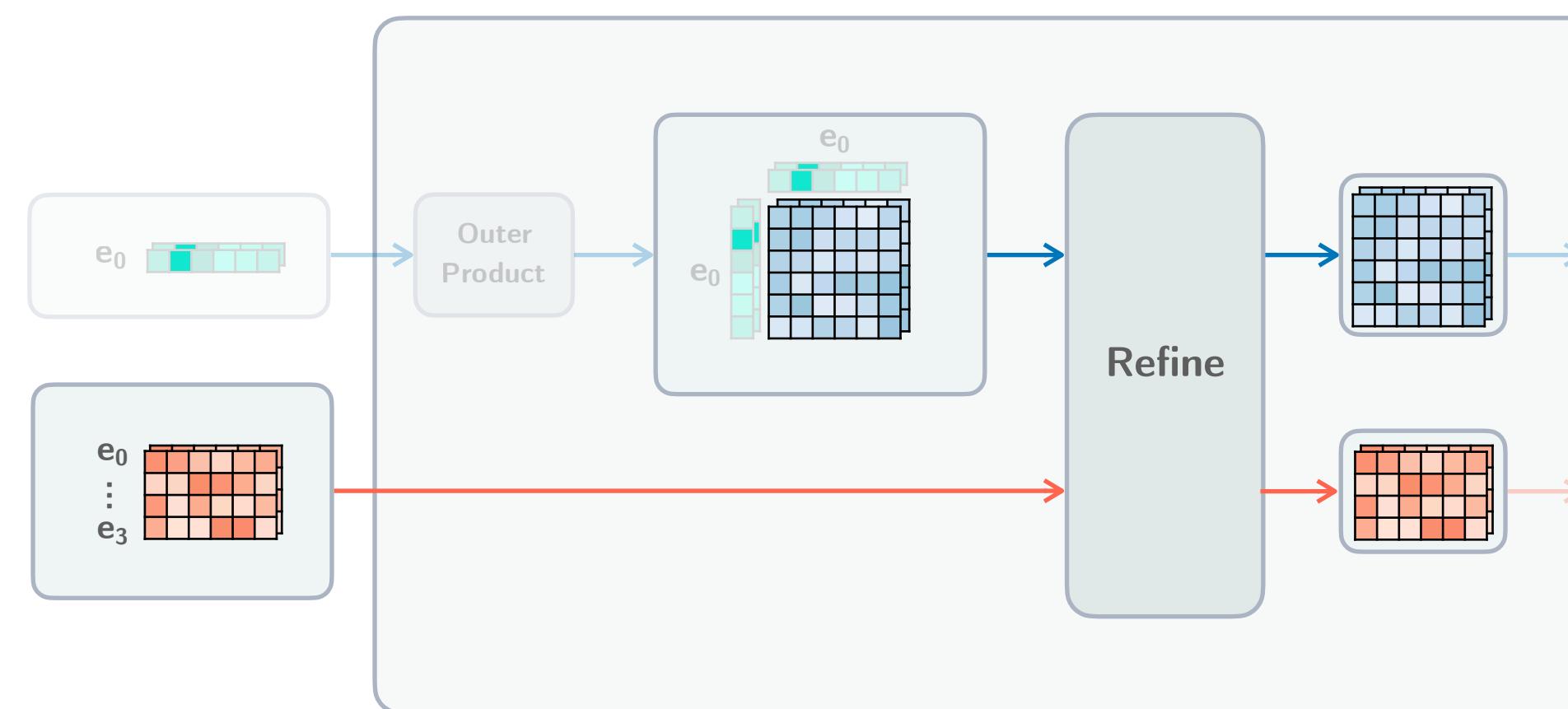
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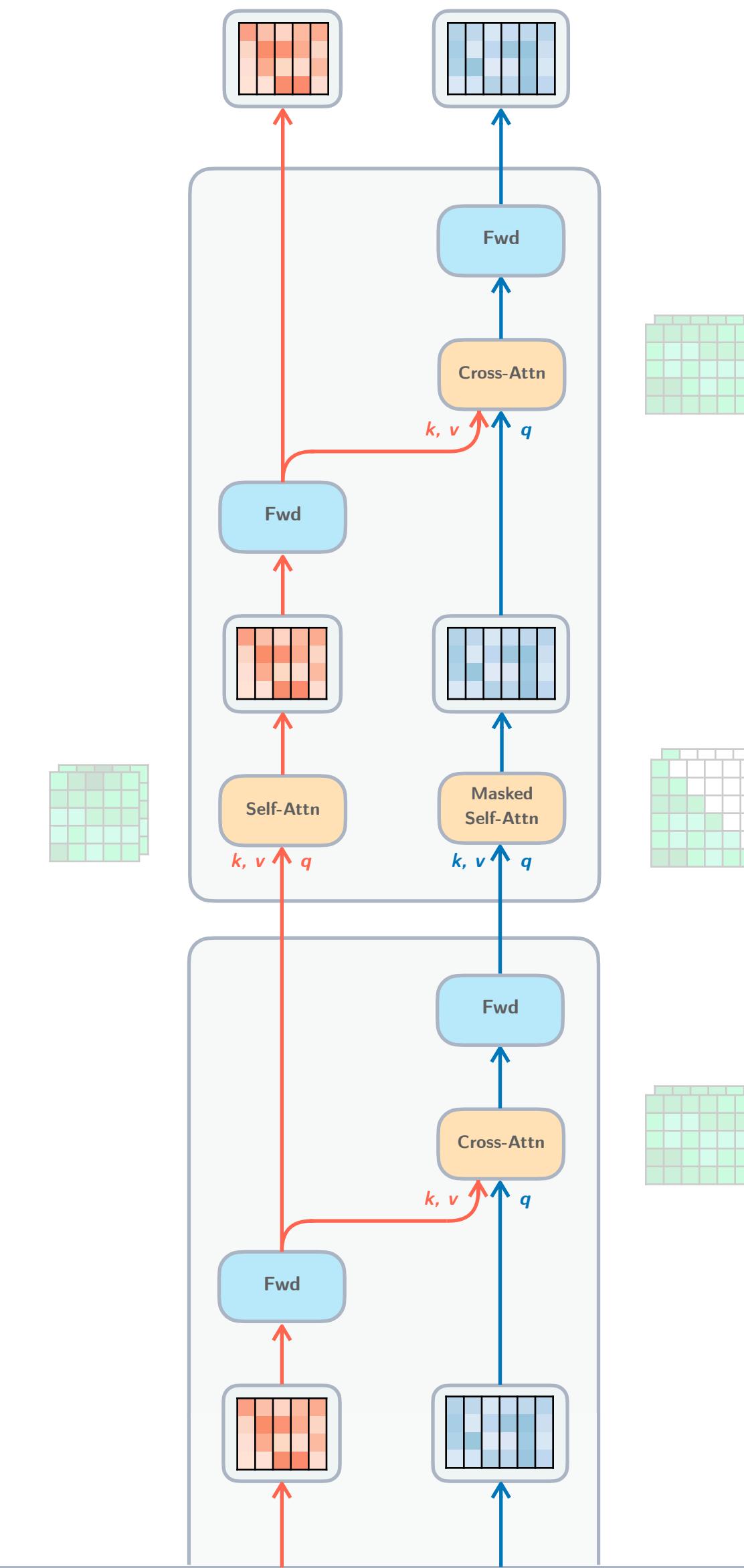
The Solution AlphaFold 2

Refining & Predicting

and contextualizing

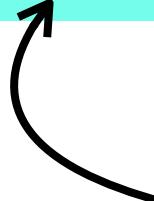
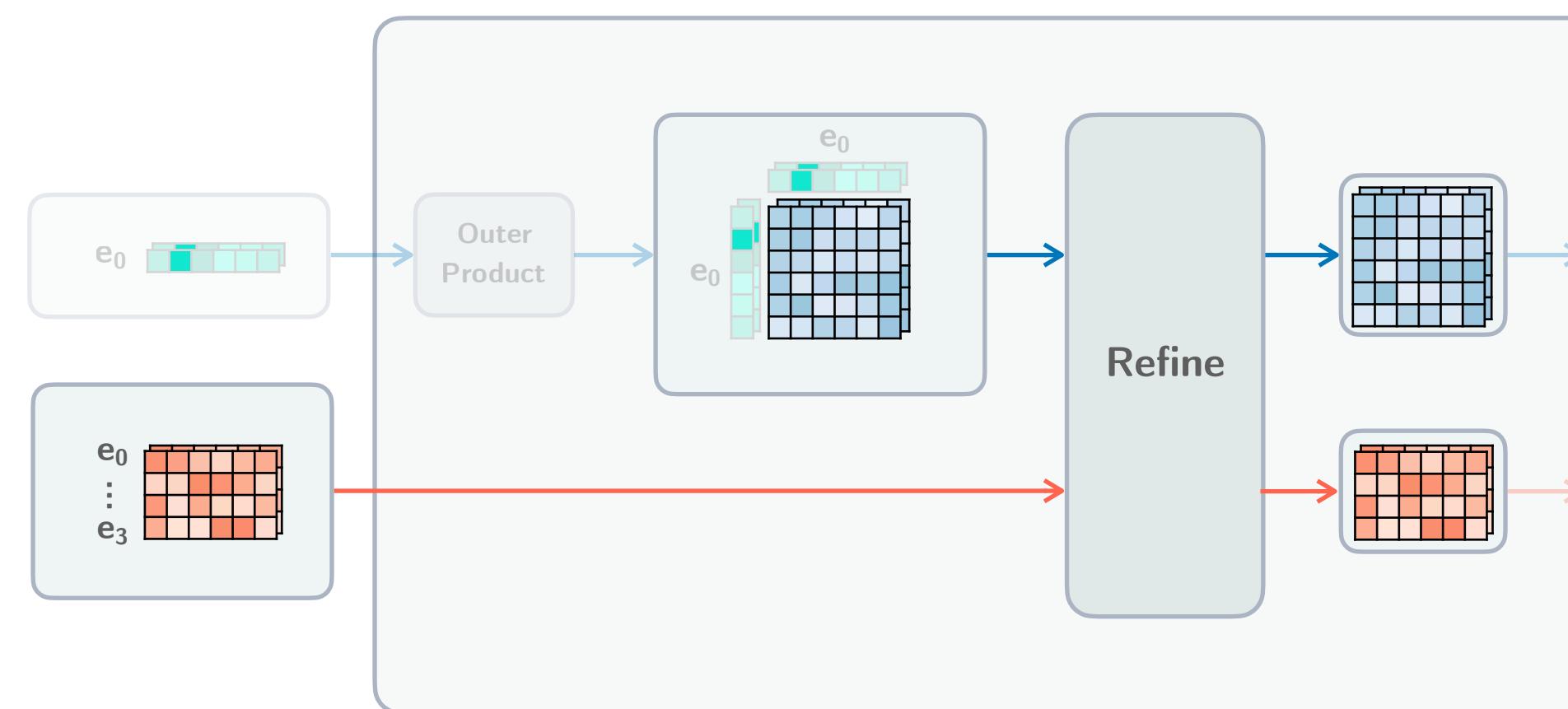
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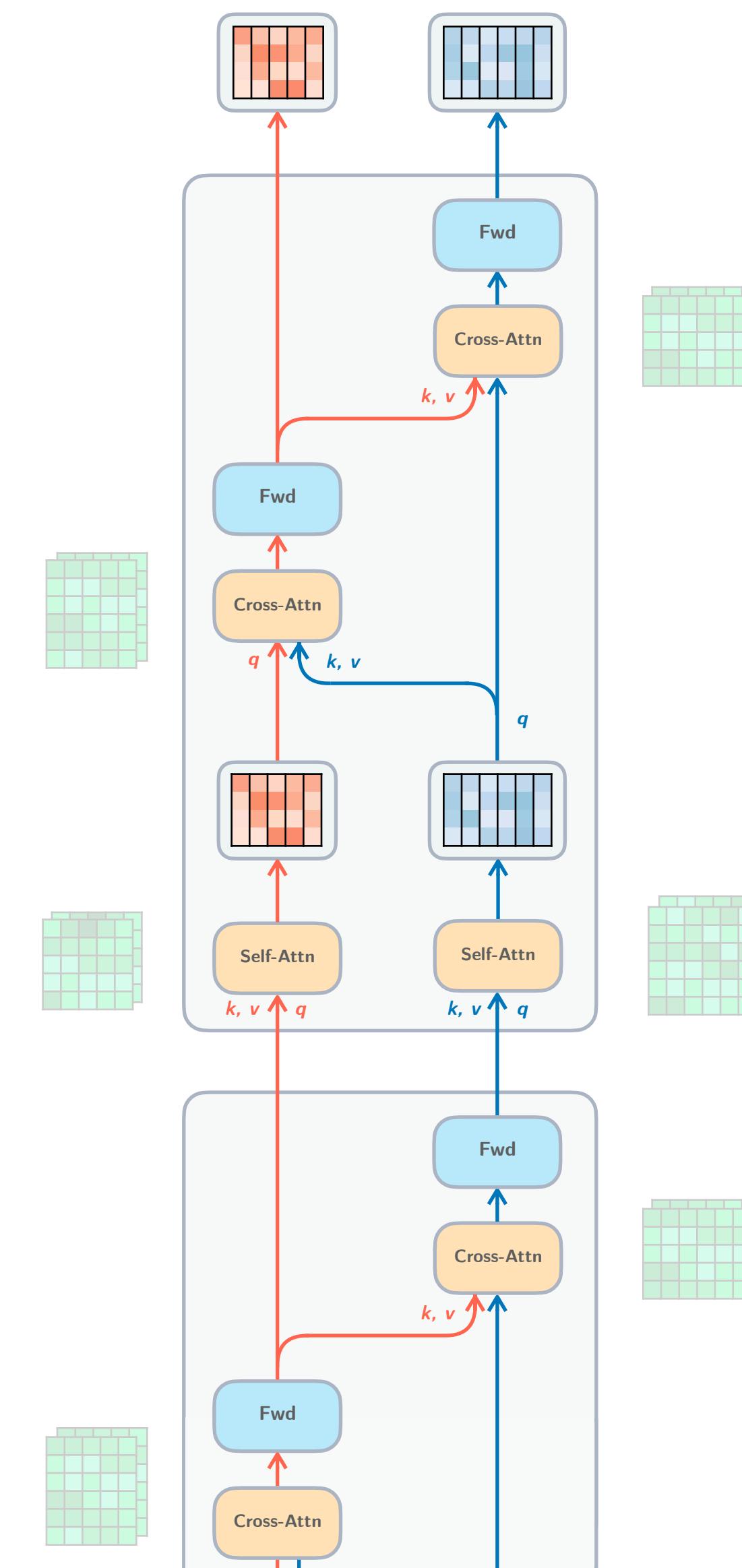
The Solution AlphaFold 2

Refining & Predicting

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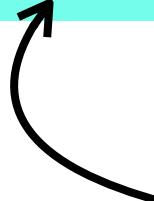
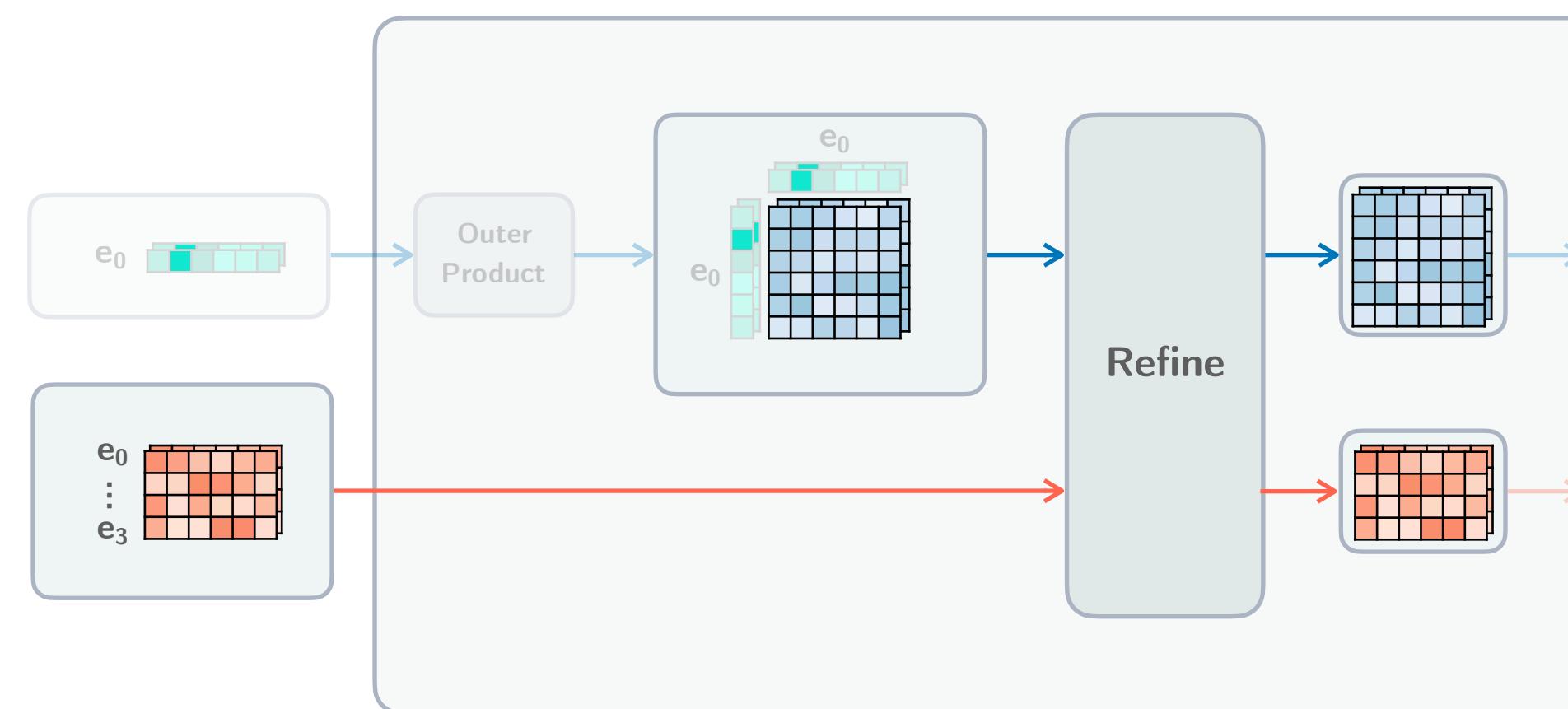
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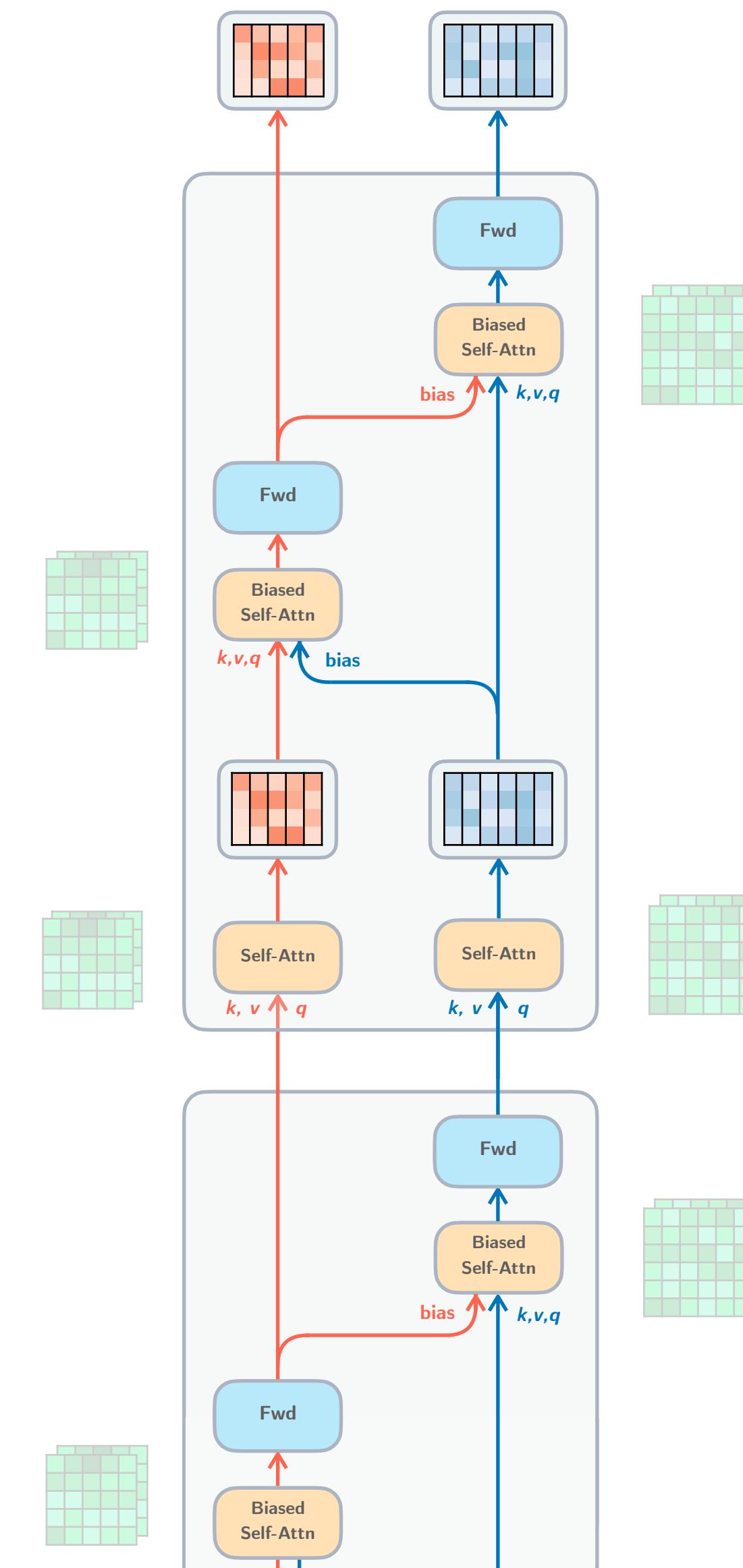
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and contextualizing

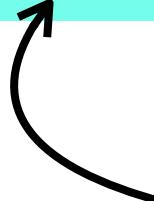
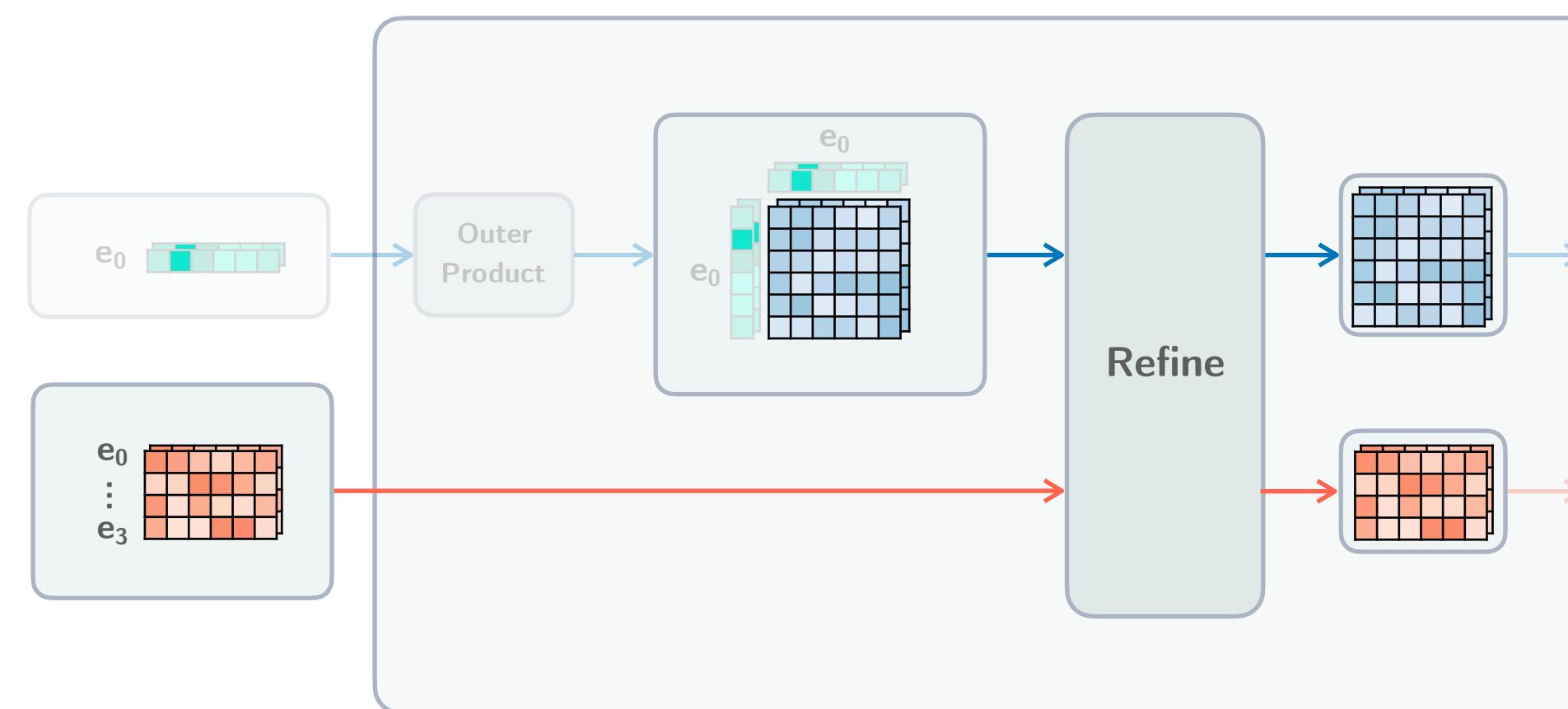
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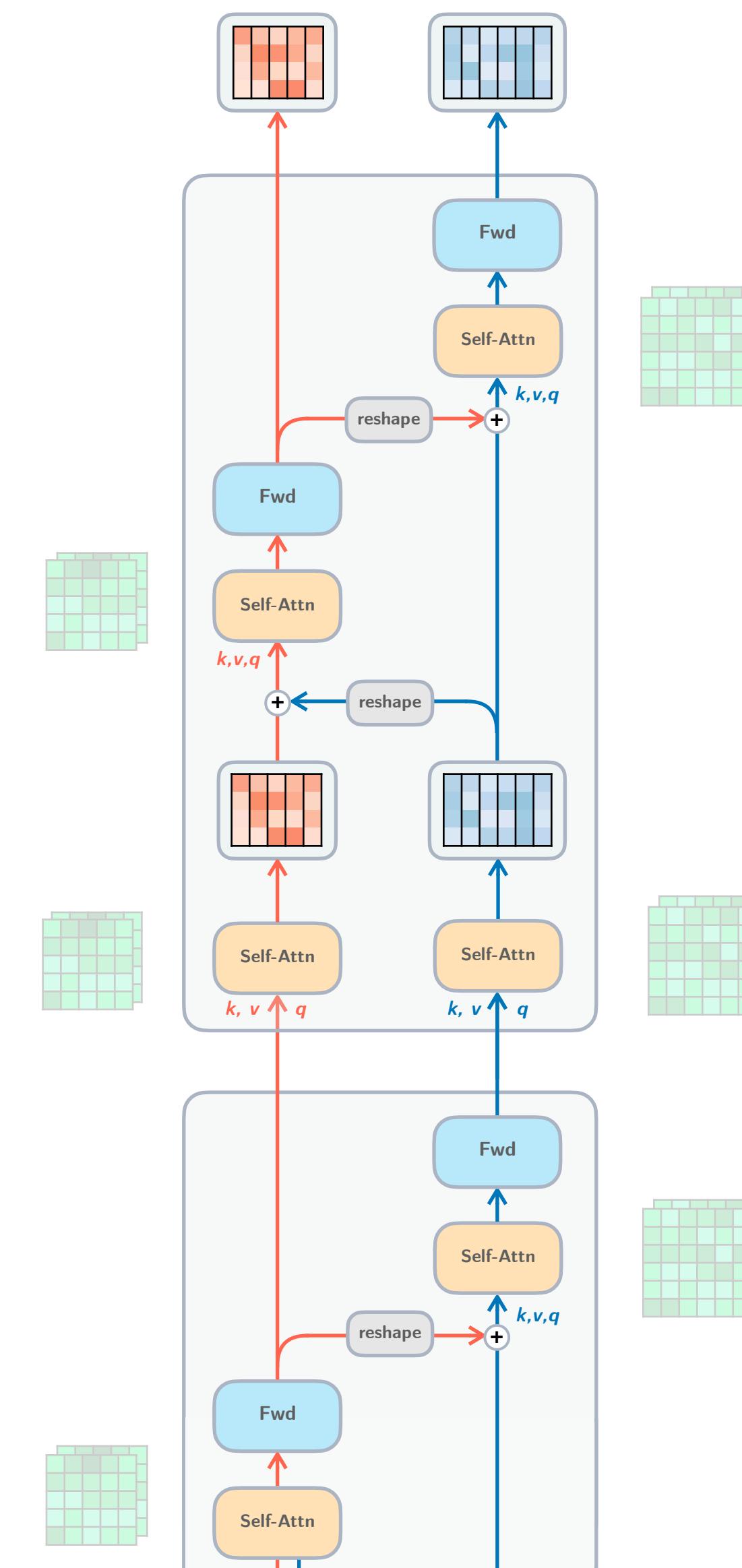
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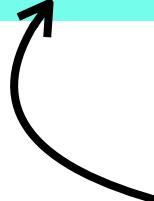
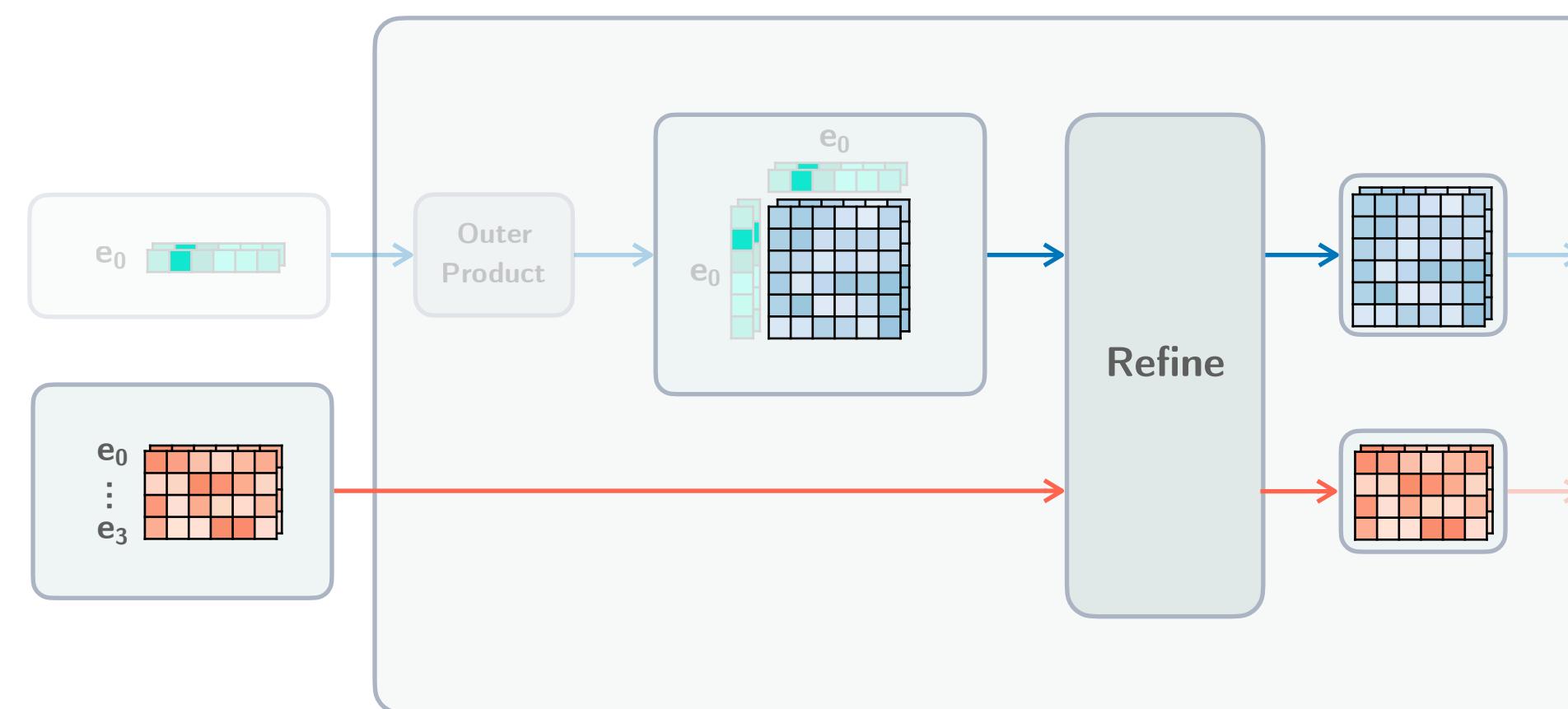
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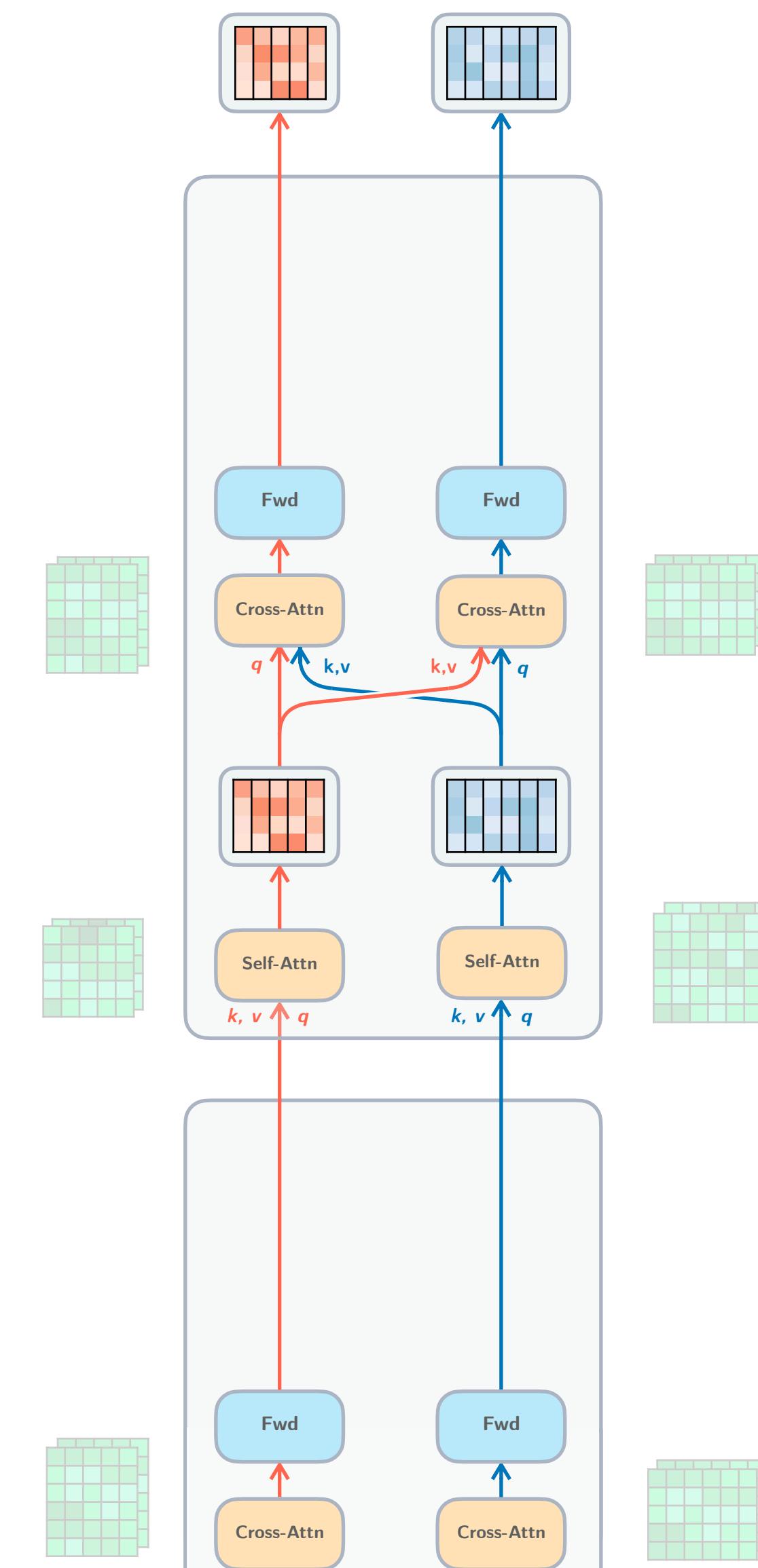
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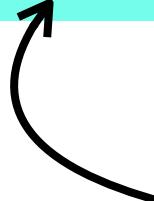
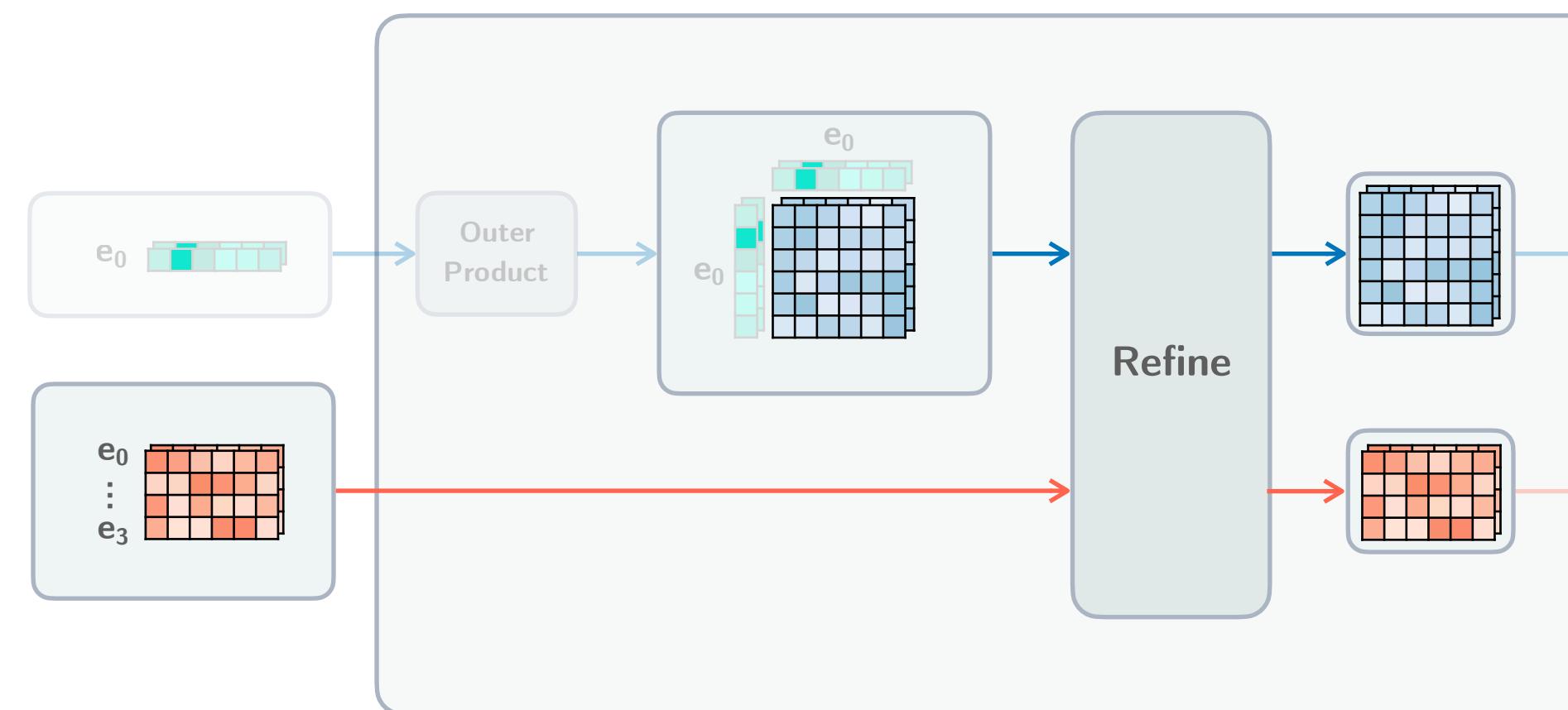
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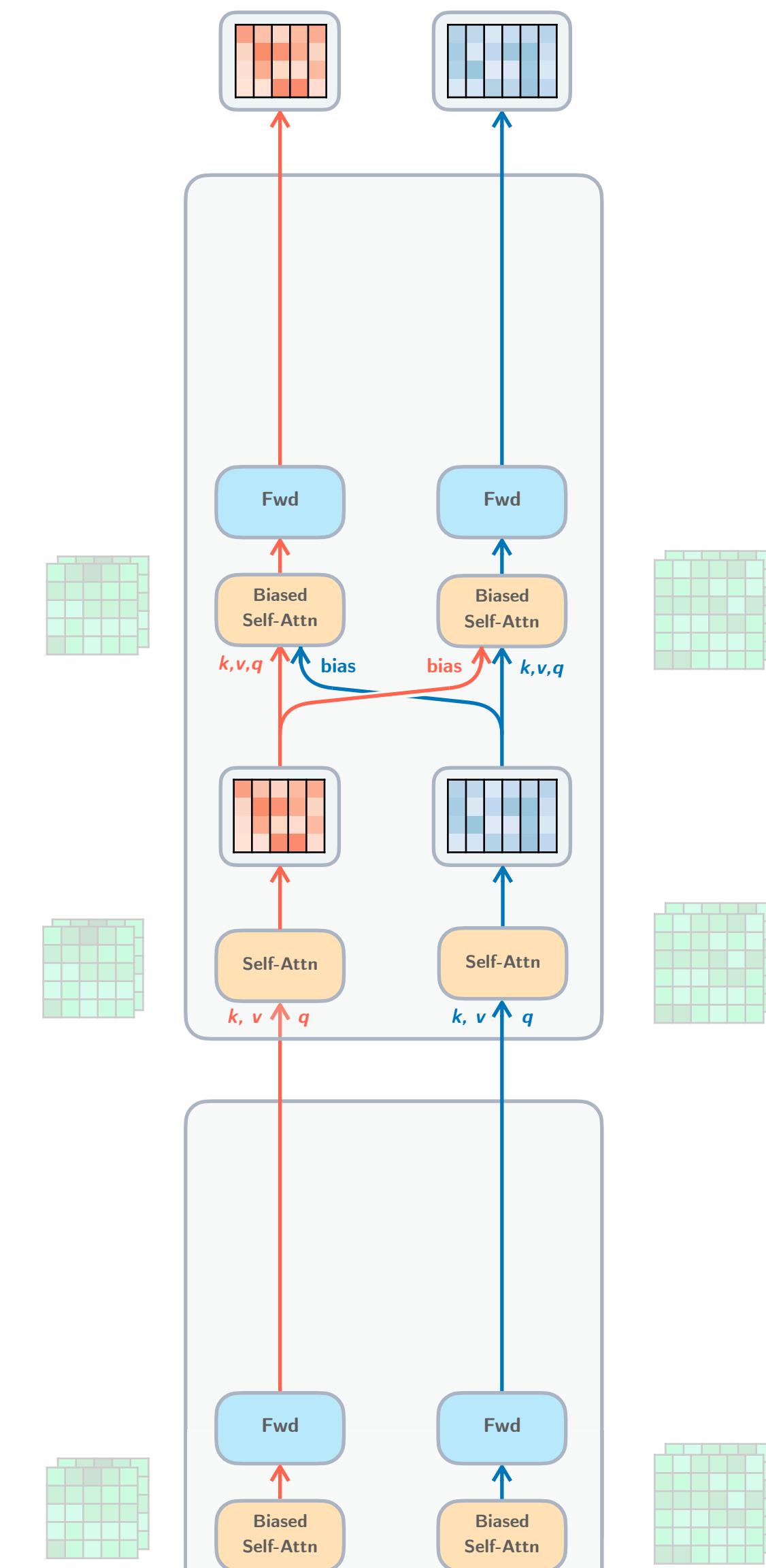
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Refining & Predicting

and contextualizing

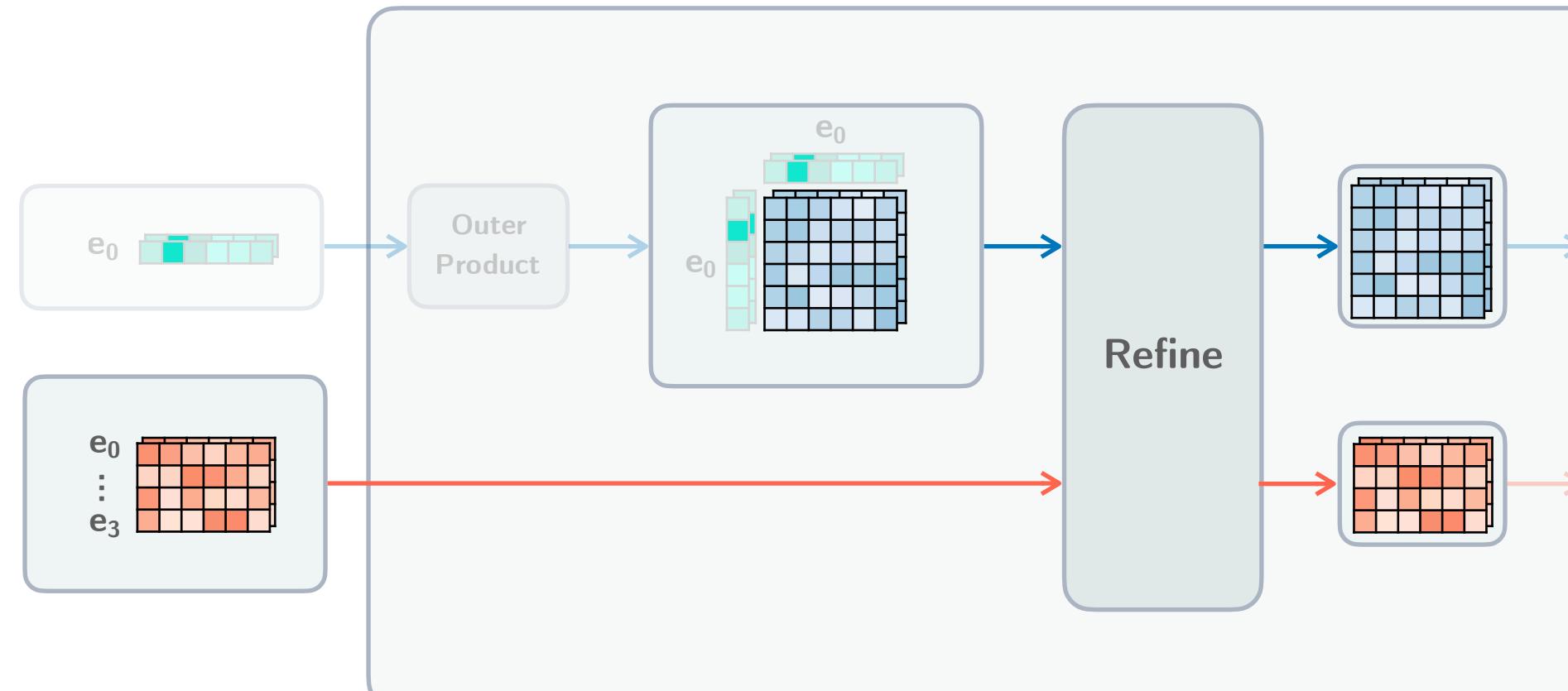
2-Lane Transformer



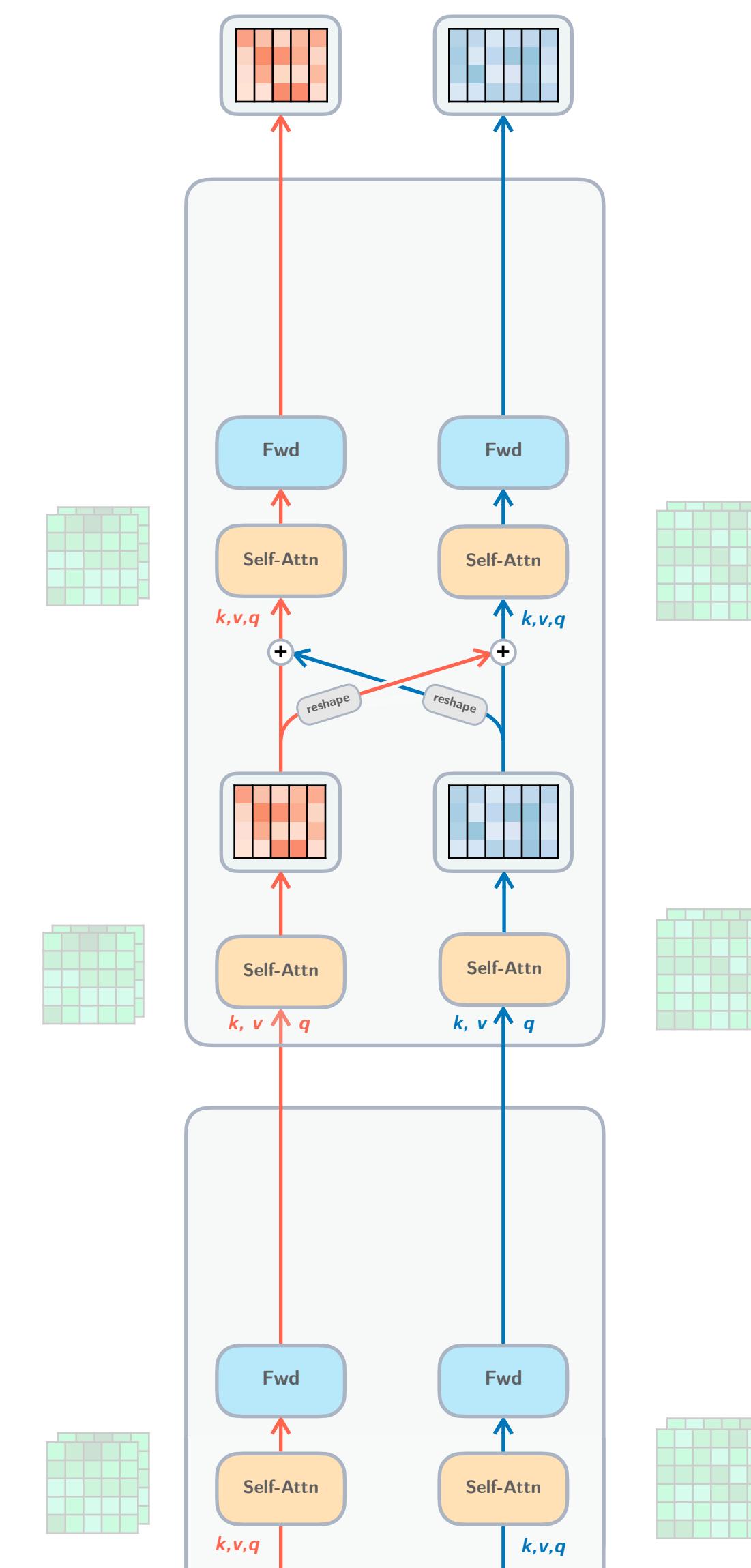
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



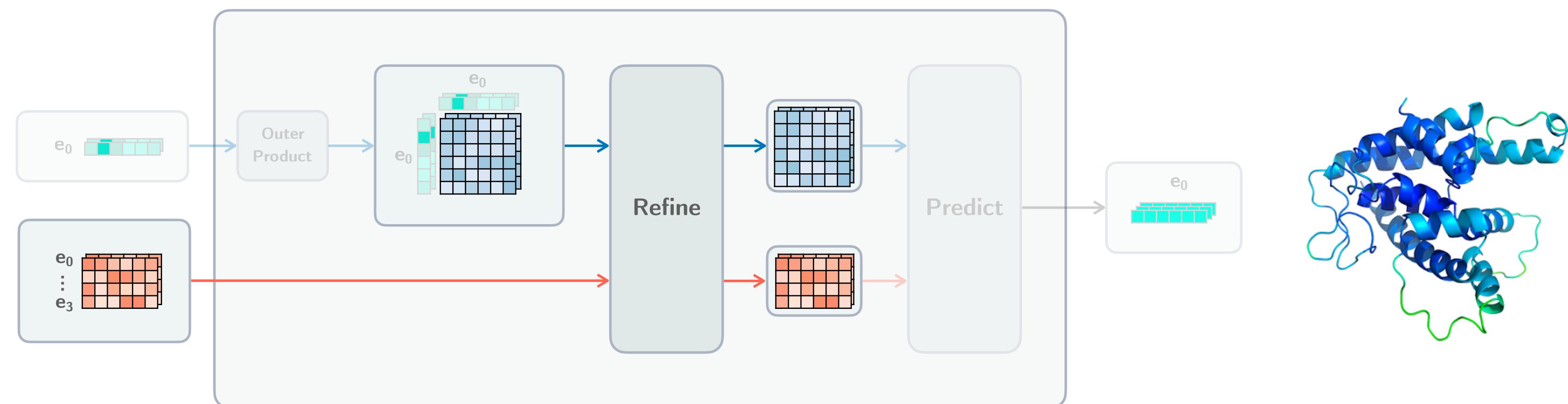
2-Lane Transformer



The Solution AlphaFold 2

Refining & Predicting

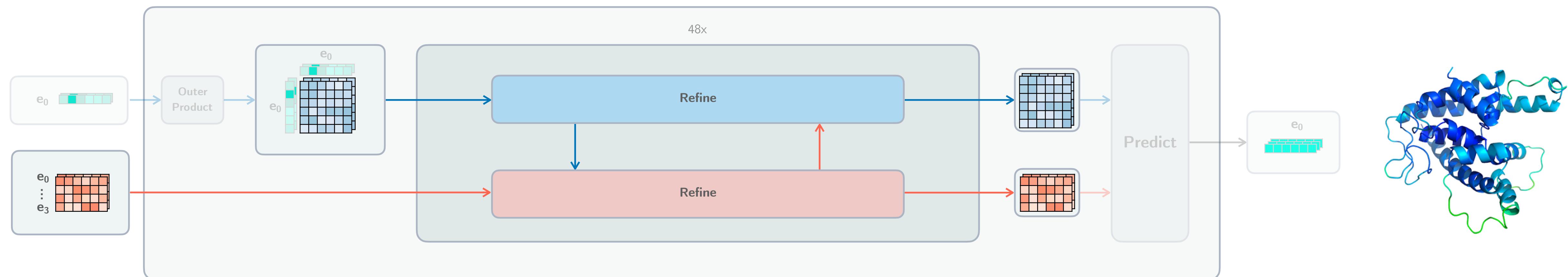
and contextualizing



The Solution AlphaFold 2

Refining & Predicting

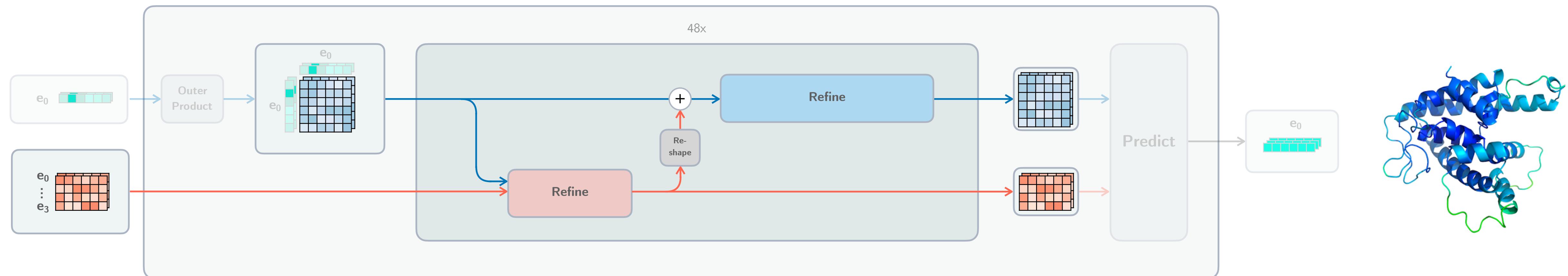
and contextualizing



The Solution AlphaFold 2

Refining & Predicting

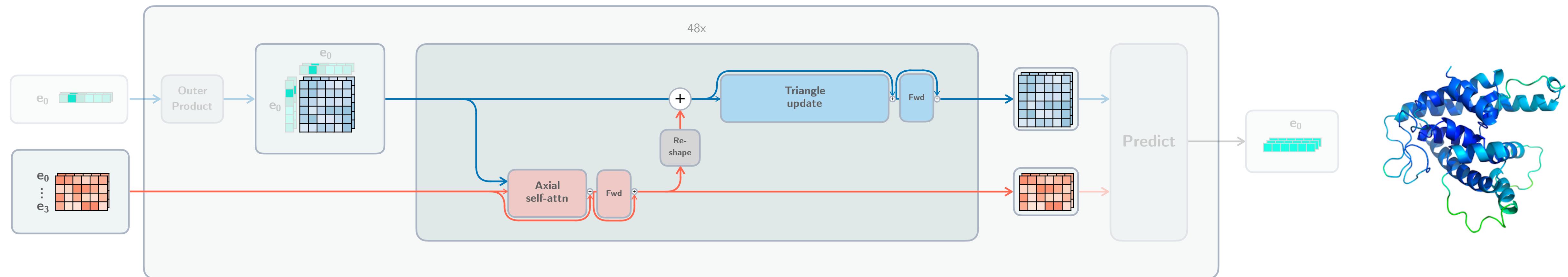
and contextualizing

The Solution AlphaFold 2

Refining & Predicting

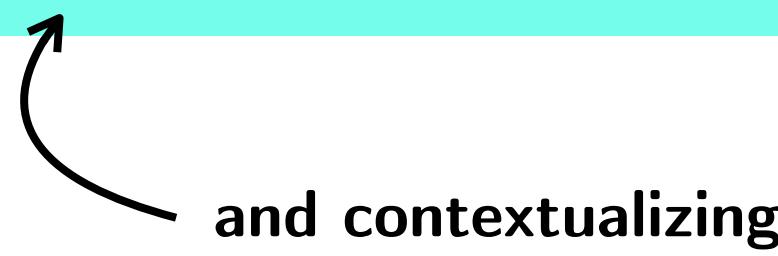
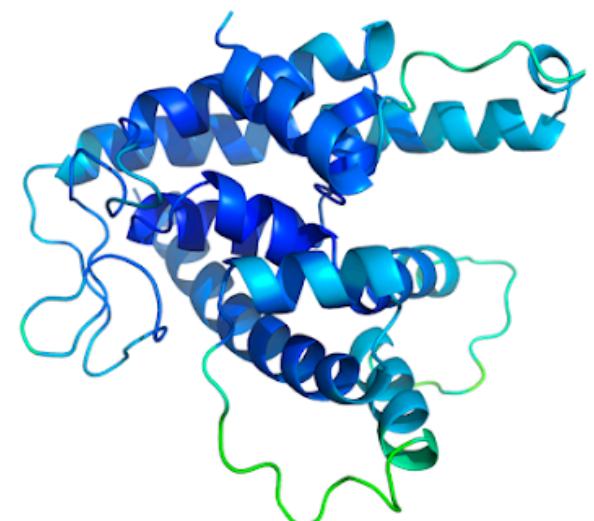
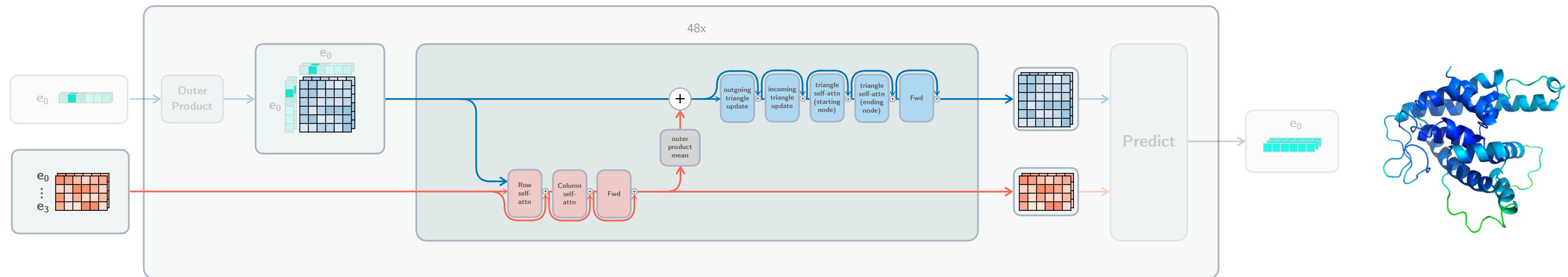
and contextualizing

The Solution AlphaFold 2

Refining & Predicting

and contextualizing

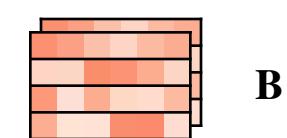
The Solution AlphaFold 2

Refining & Predicting

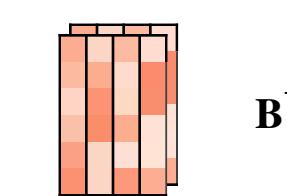
and contextualizing

Row-wise vs column-wise self-attention

$$\mathbf{B} = f(\mathbf{A}^T)^T$$



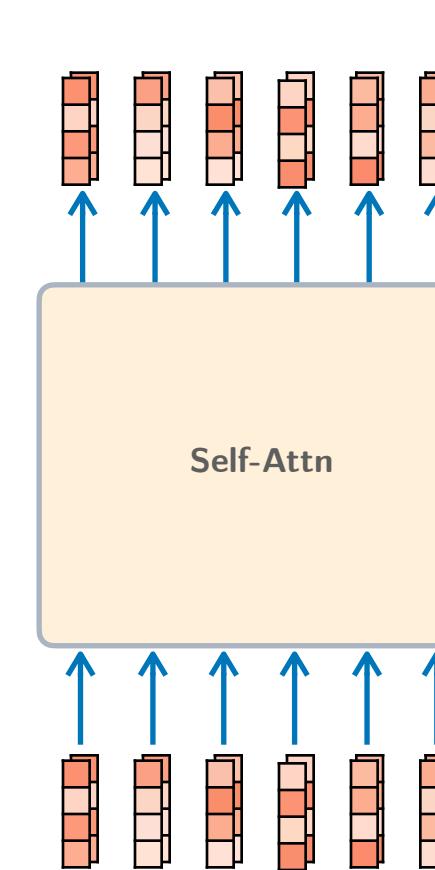
$$\mathbf{B} = f(\mathbf{A})$$



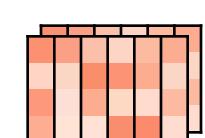
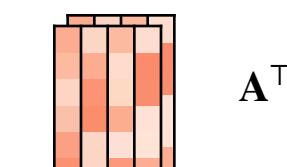
$$\mathbf{B}$$



Self-Attn



Self-Attn



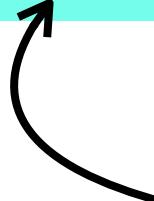
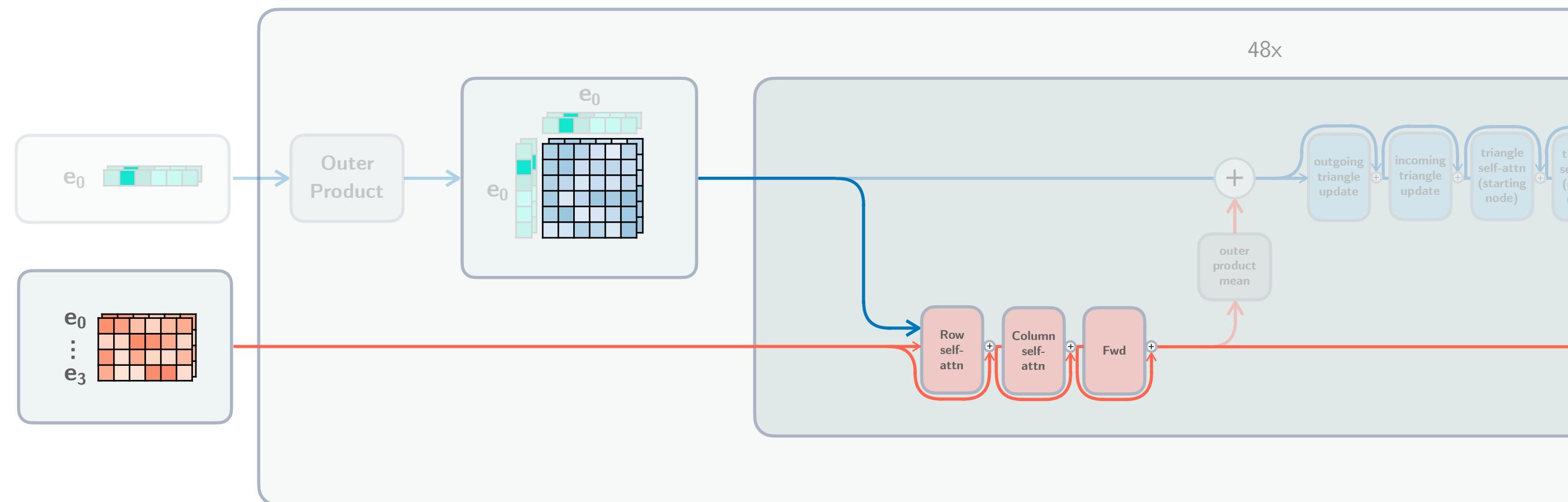
$$\mathbf{A}^T$$

$$\mathbf{A}$$

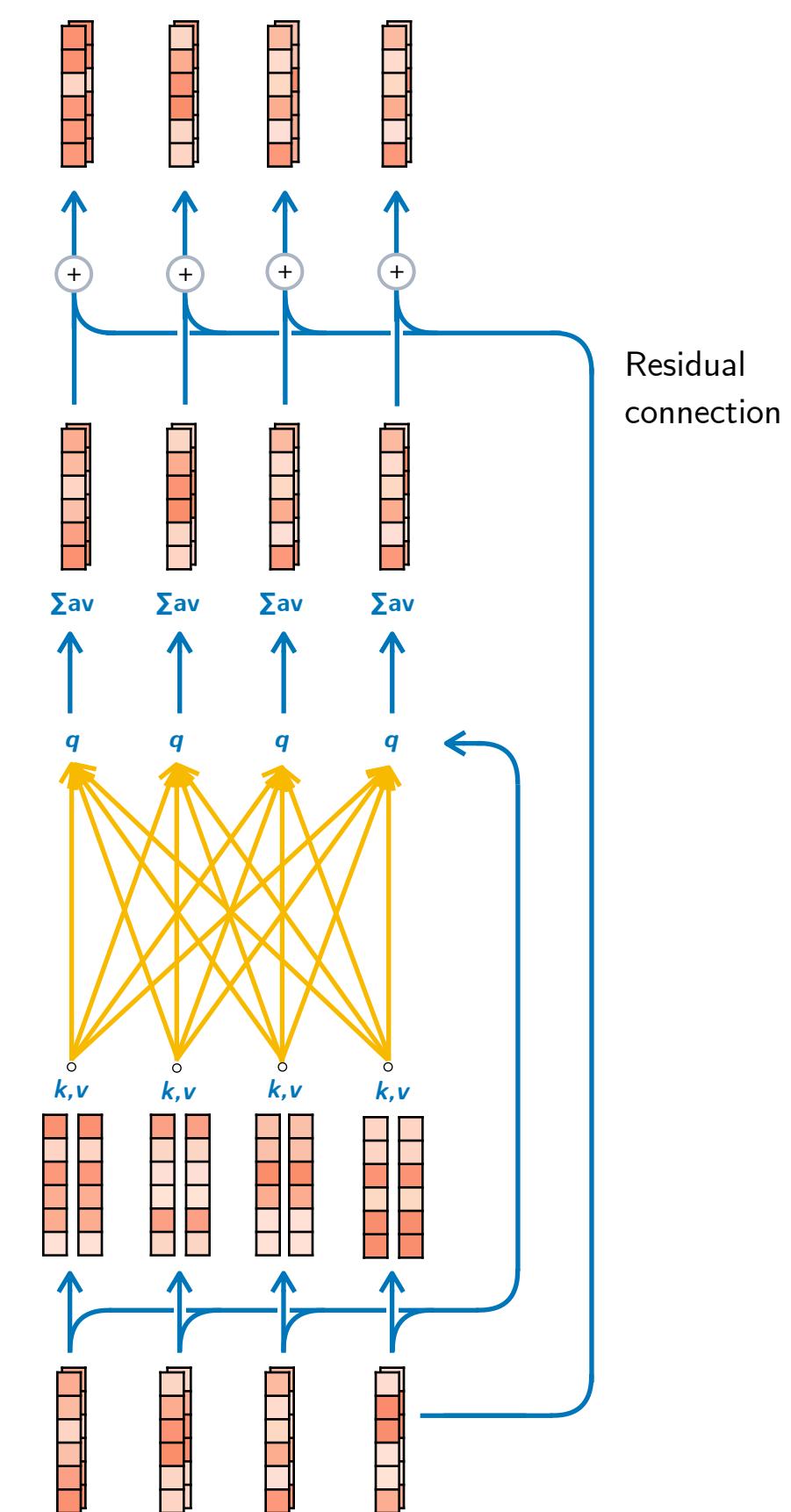
The Solution AlphaFold 2

Refining & Predicting

and contextualizing

Self-attention

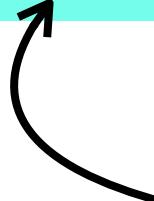
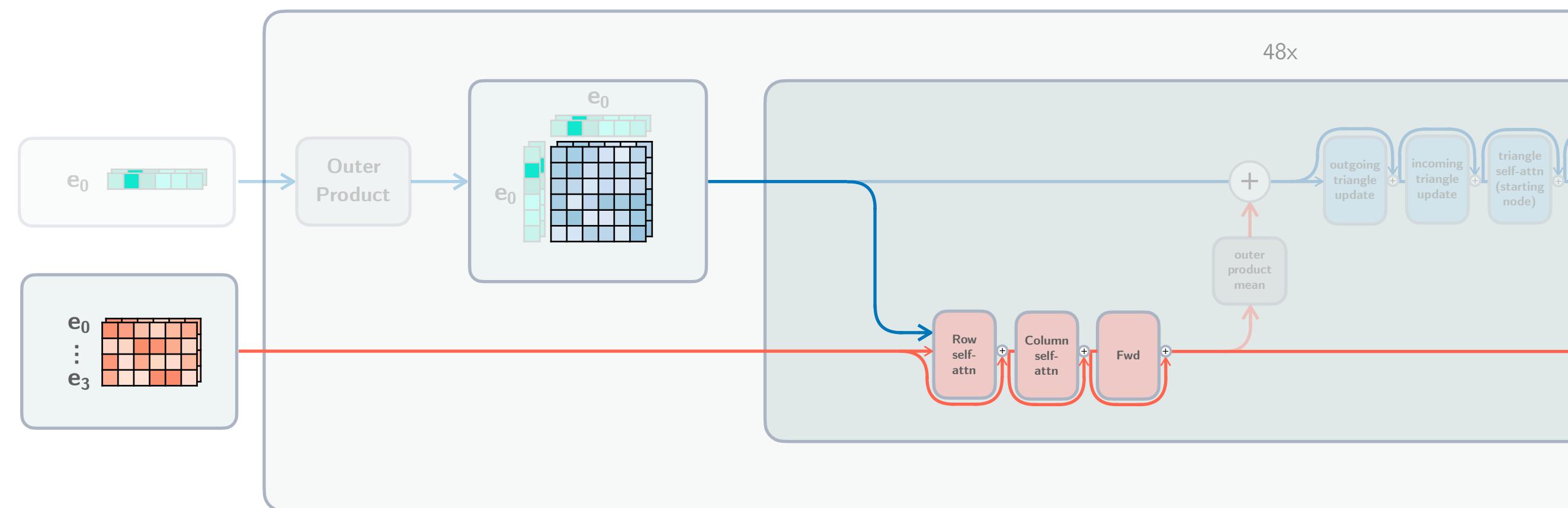


Linear layers to compute keys, values, queries not shown.

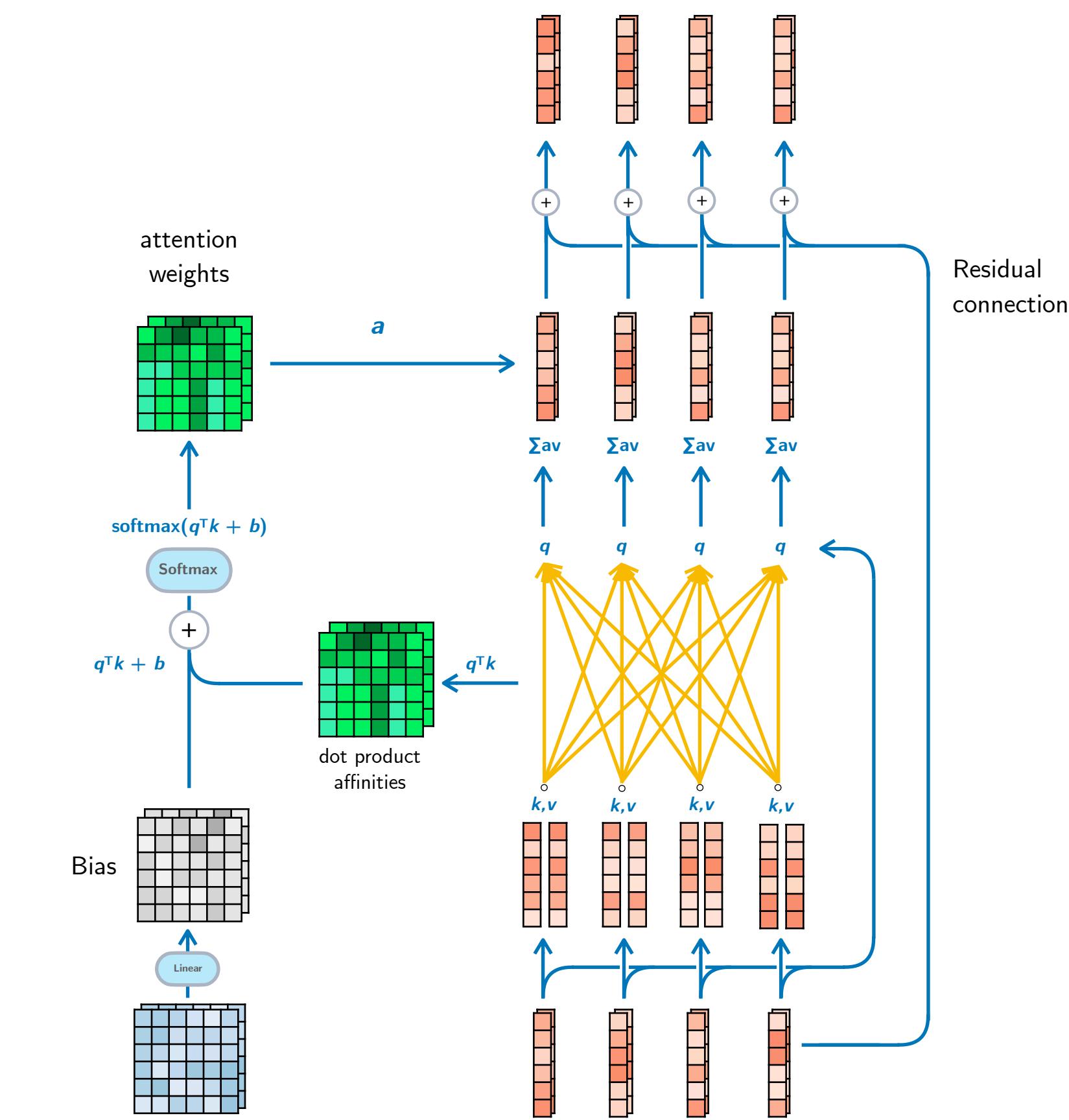
The Solution AlphaFold 2

Refining & Predicting

and contextualizing

Biased self-attention

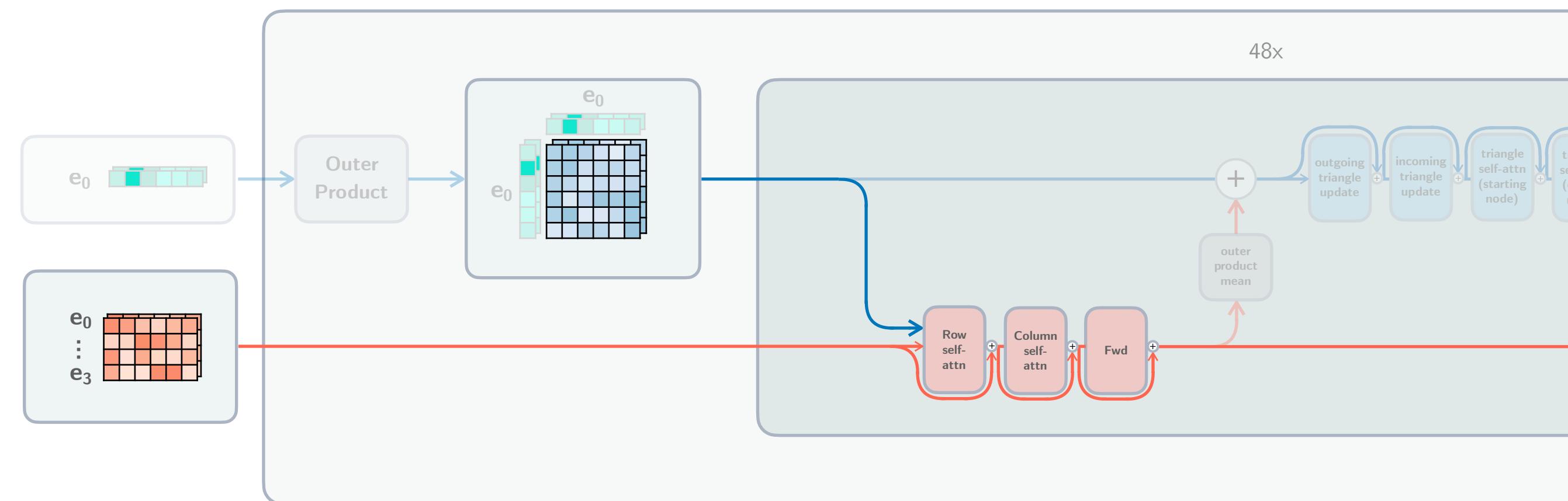


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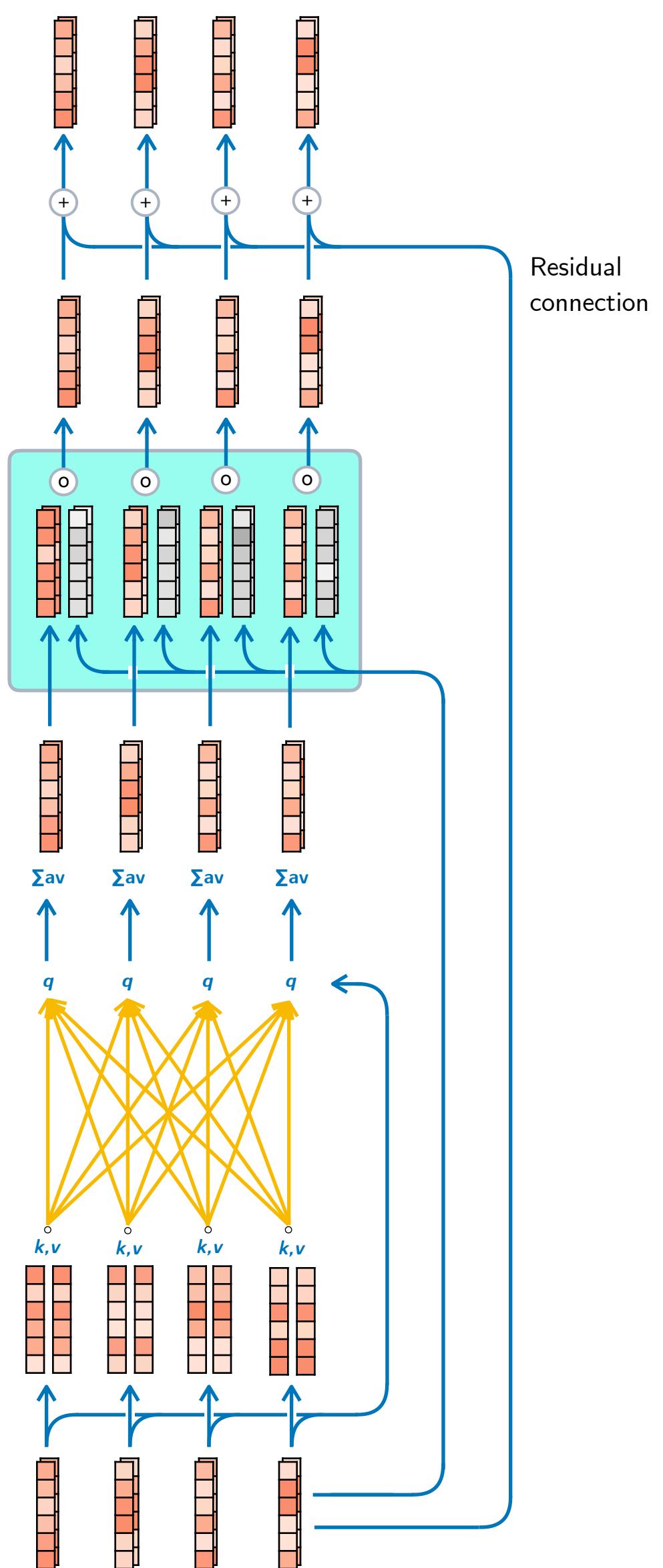
The Solution AlphaFold 2

Refining & Predicting

and contextualizing

Gated self-attention

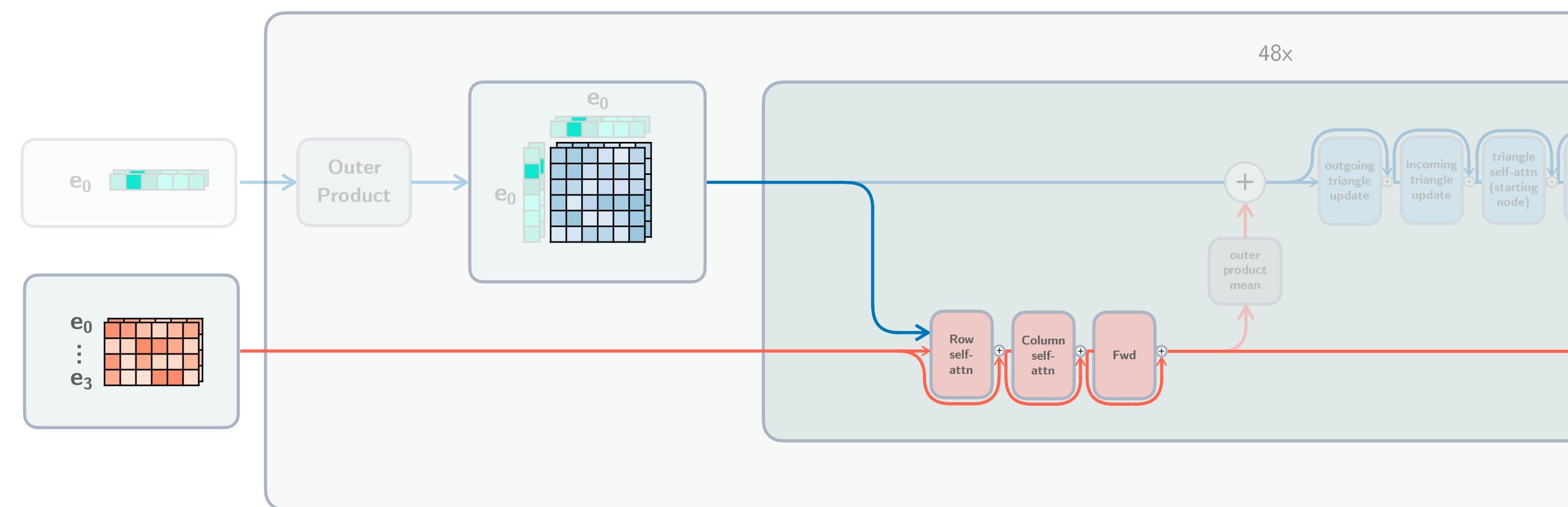


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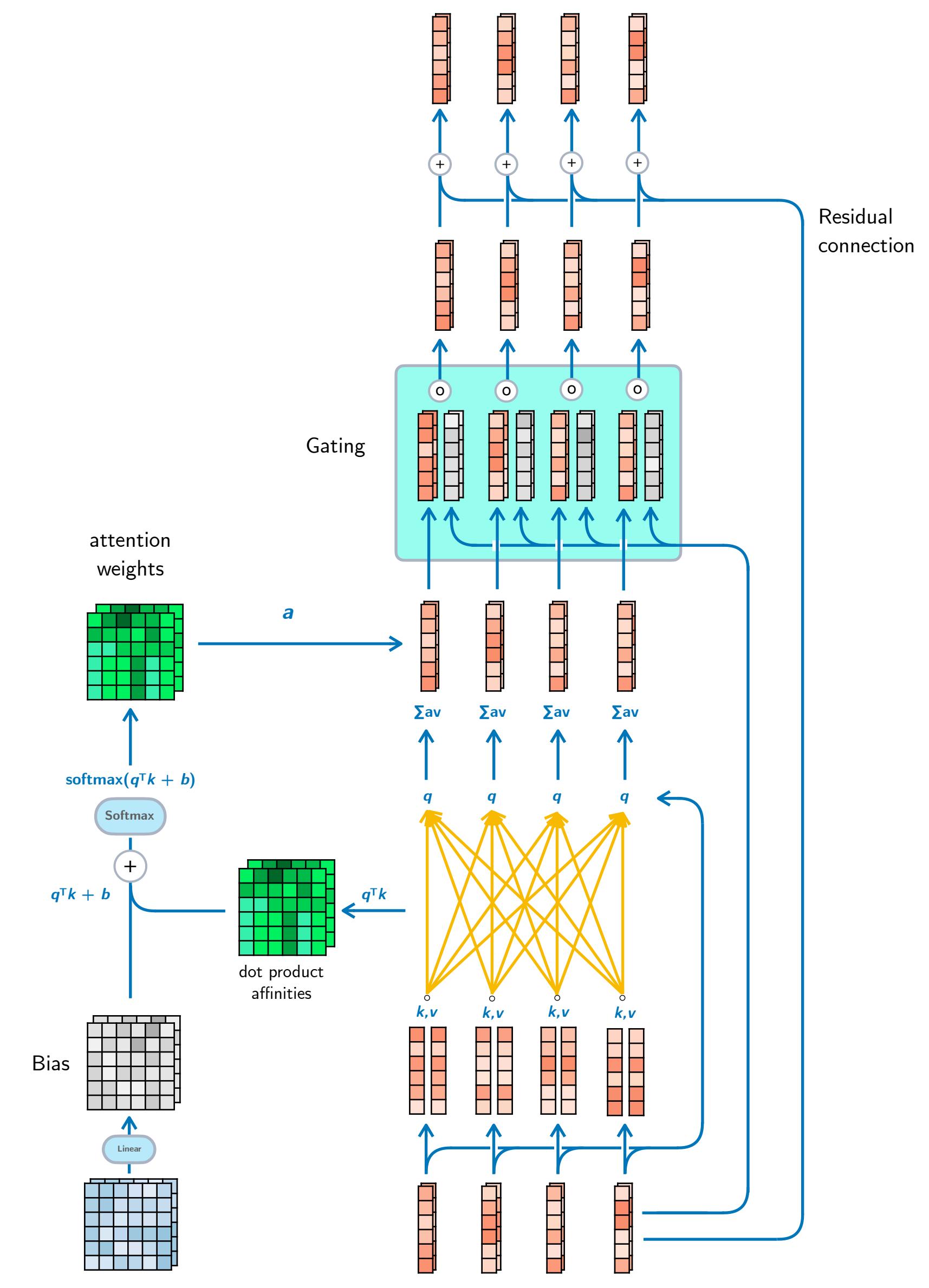
The Solution AlphaFold 2

Refining & Predicting

and contextualizing

Gated biased self-attention



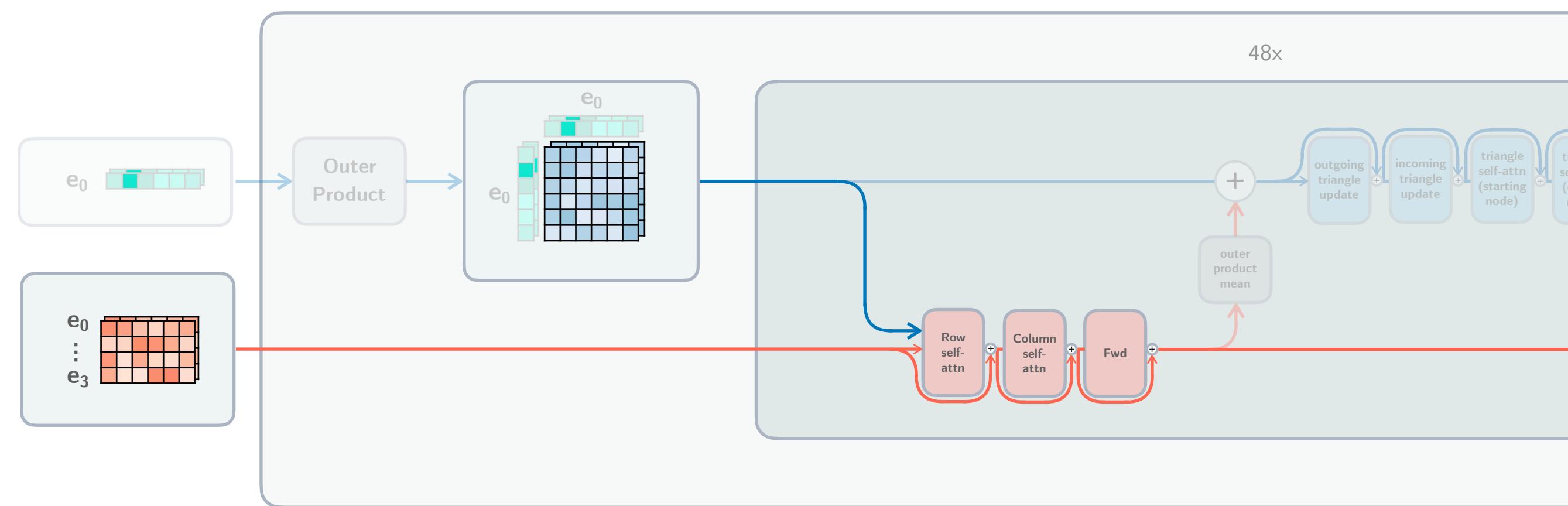
Linear layers to compute keys, values, queries not shown.

AlphaFold and Protein Structure Prediction

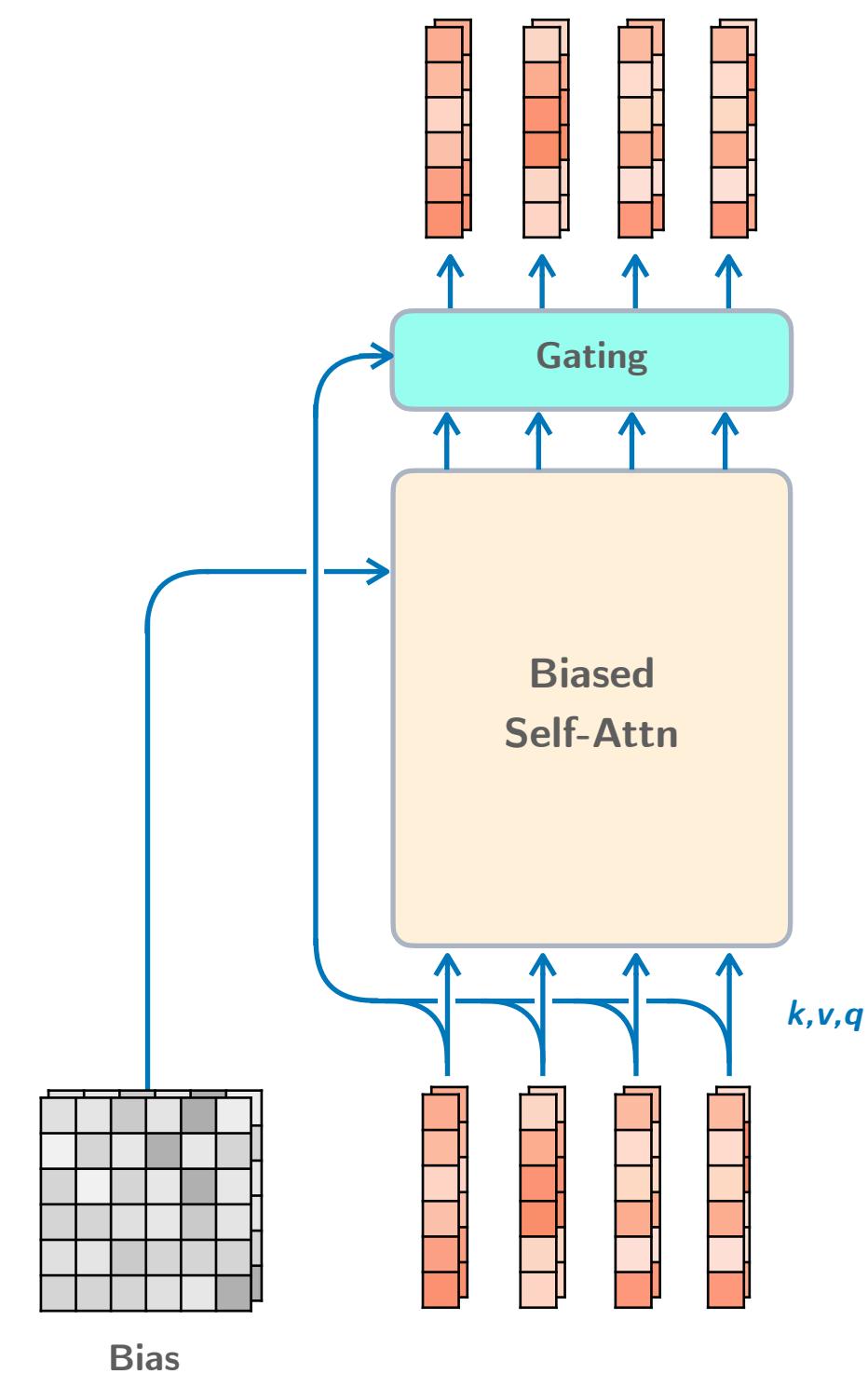
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



Gated biased self-attention



Residual connection skipped for simplicity.

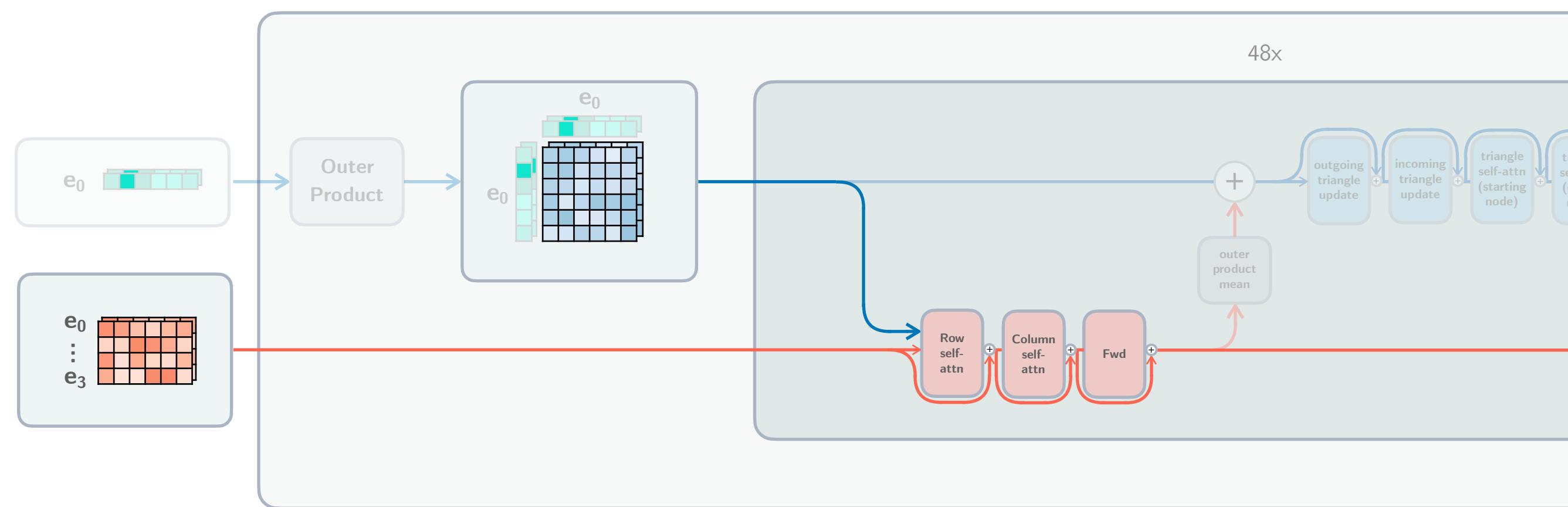
Linear layers to compute keys, values, queries not shown.

AlphaFold and Protein Structure Prediction

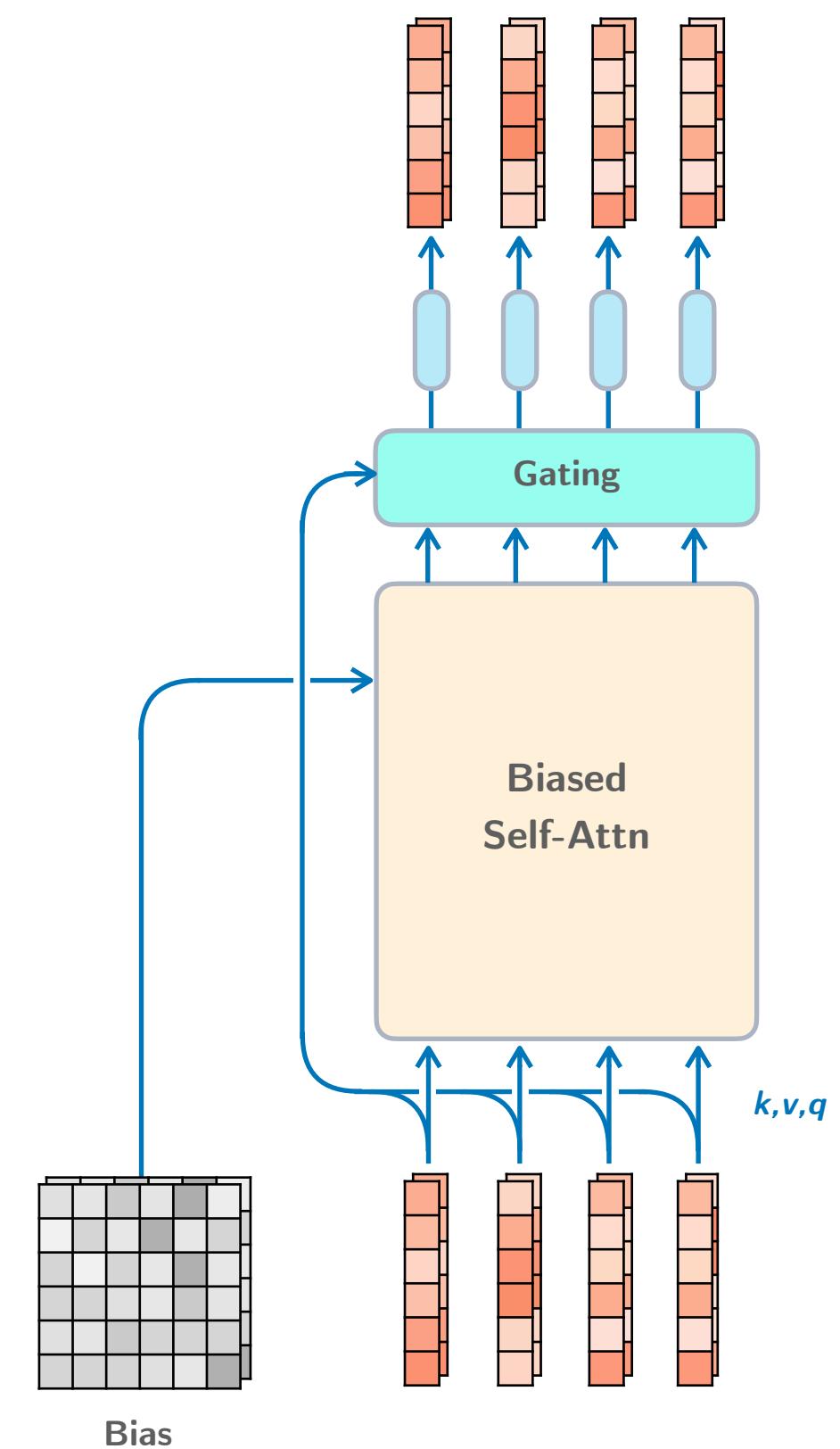
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



Gated biased self-attention



Residual connection skipped for simplicity.

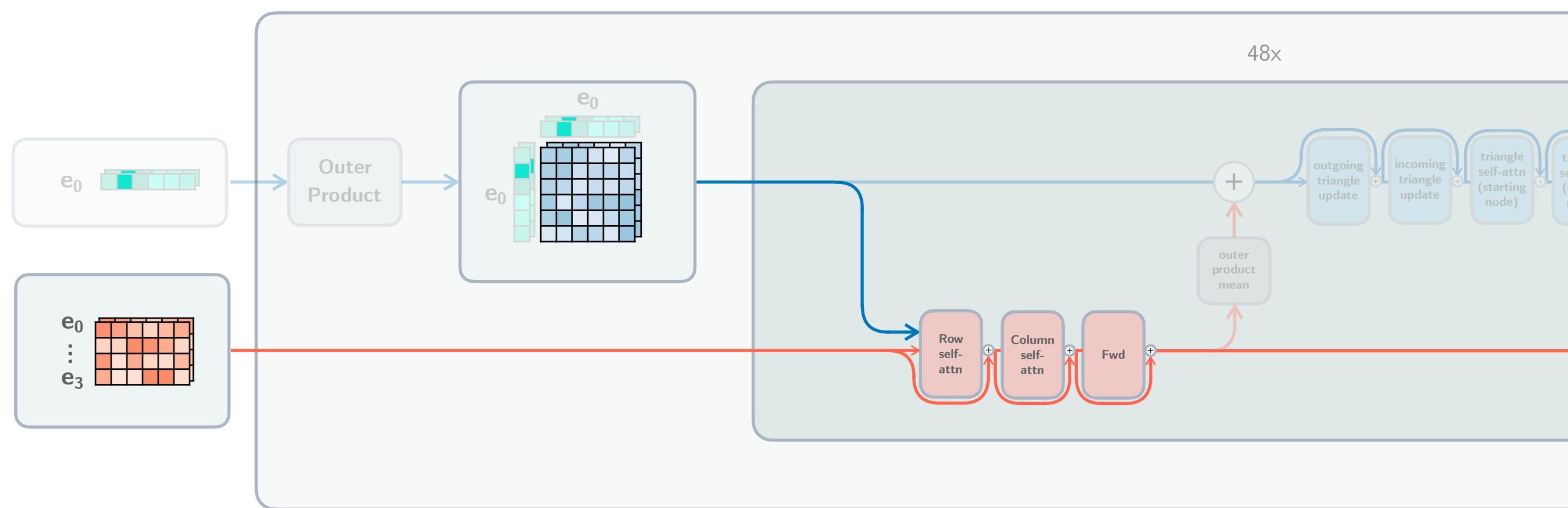
Linear layers to compute keys, values, queries not shown.

AlphaFold and Protein Structure Prediction

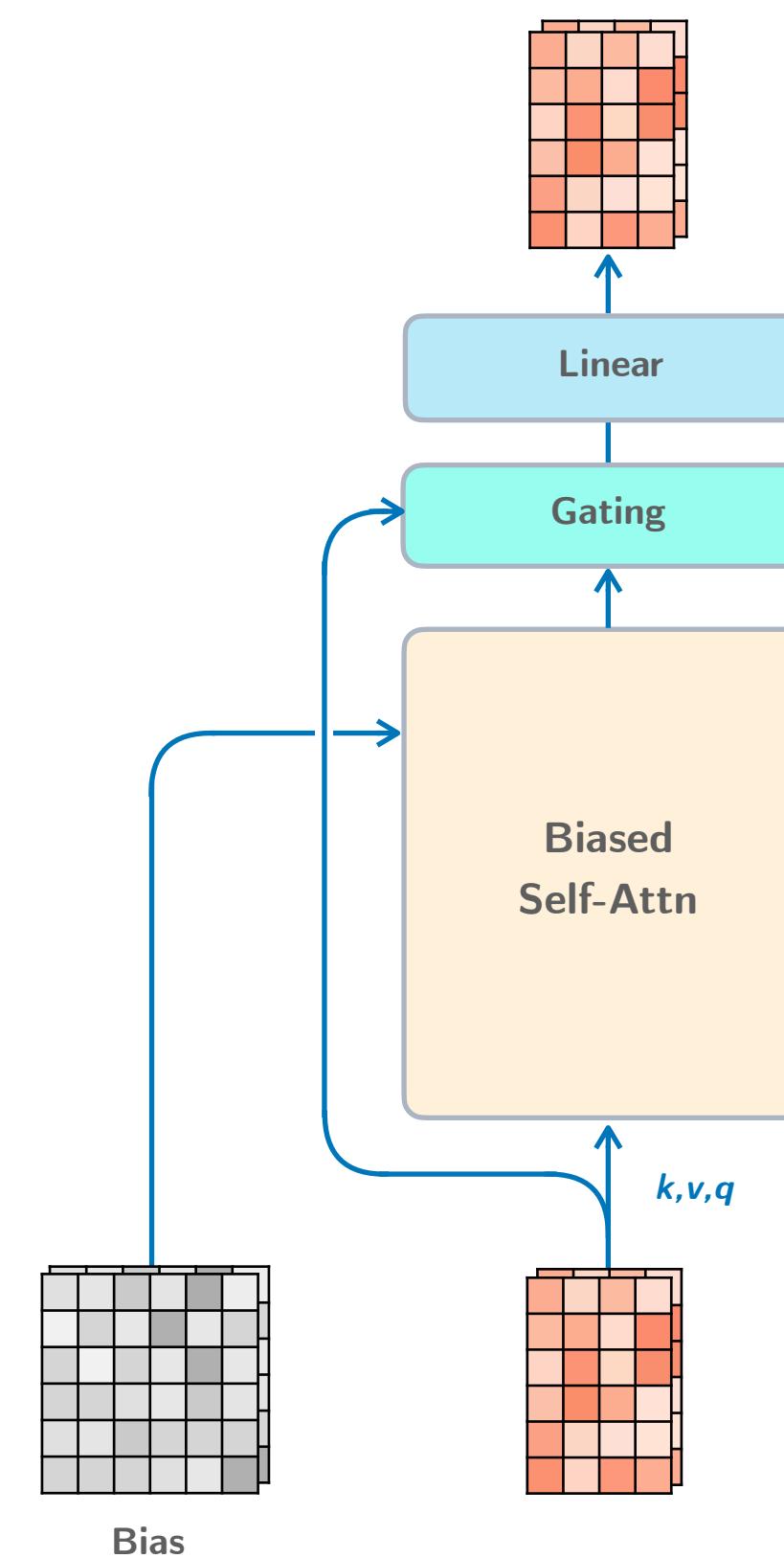
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



Gated biased self-attention



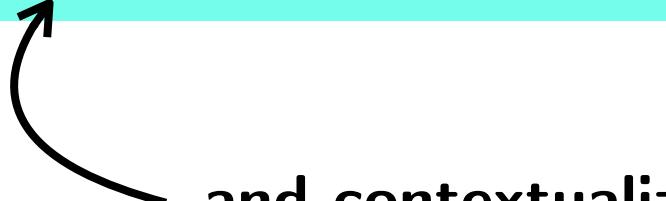
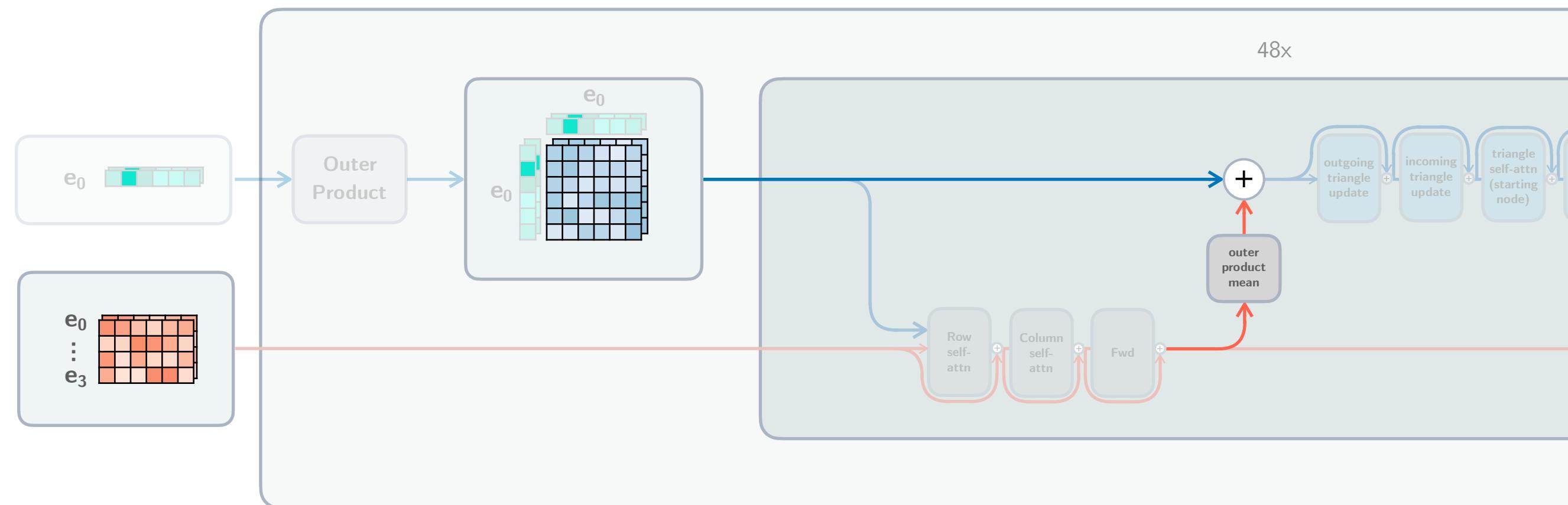
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Linear layers to compute keys, values, queries not shown.

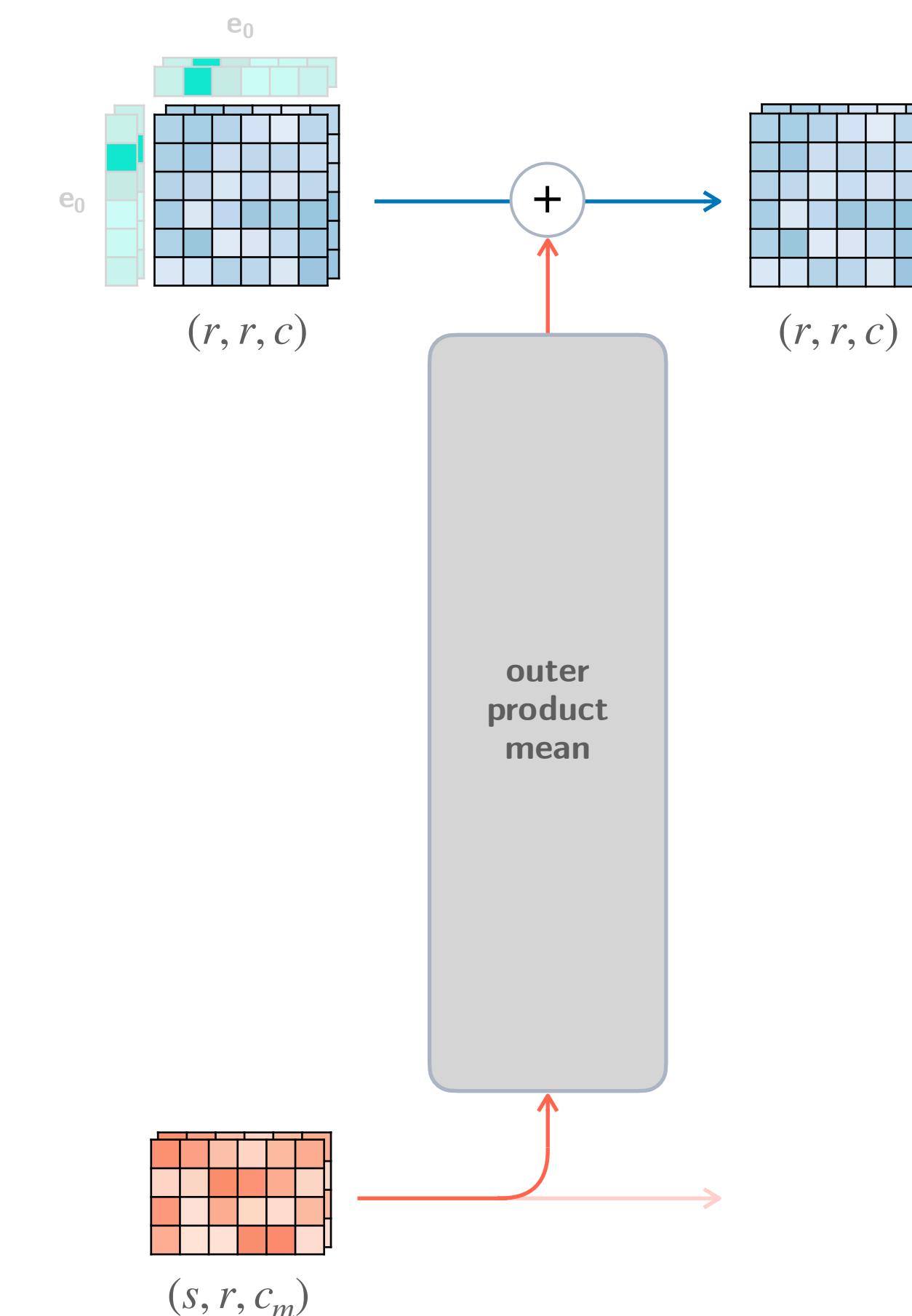
The Solution AlphaFold 2

Refining & Predicting

and contextualizing

Outer product mean

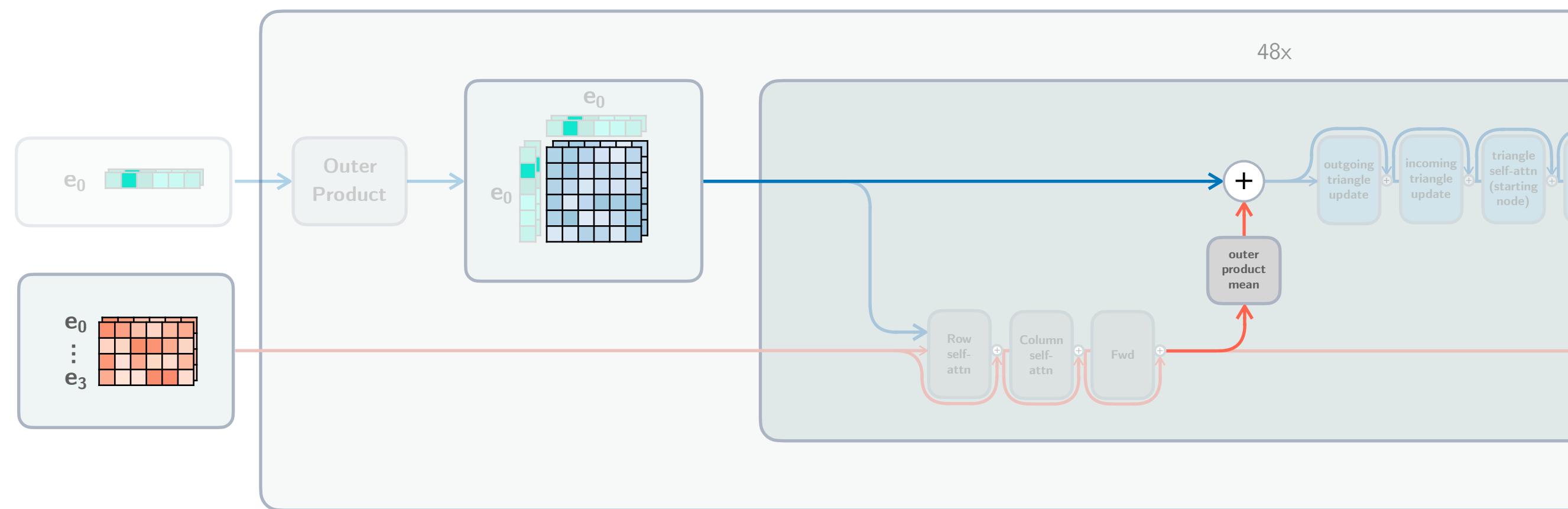


AlphaFold and Protein Structure Prediction

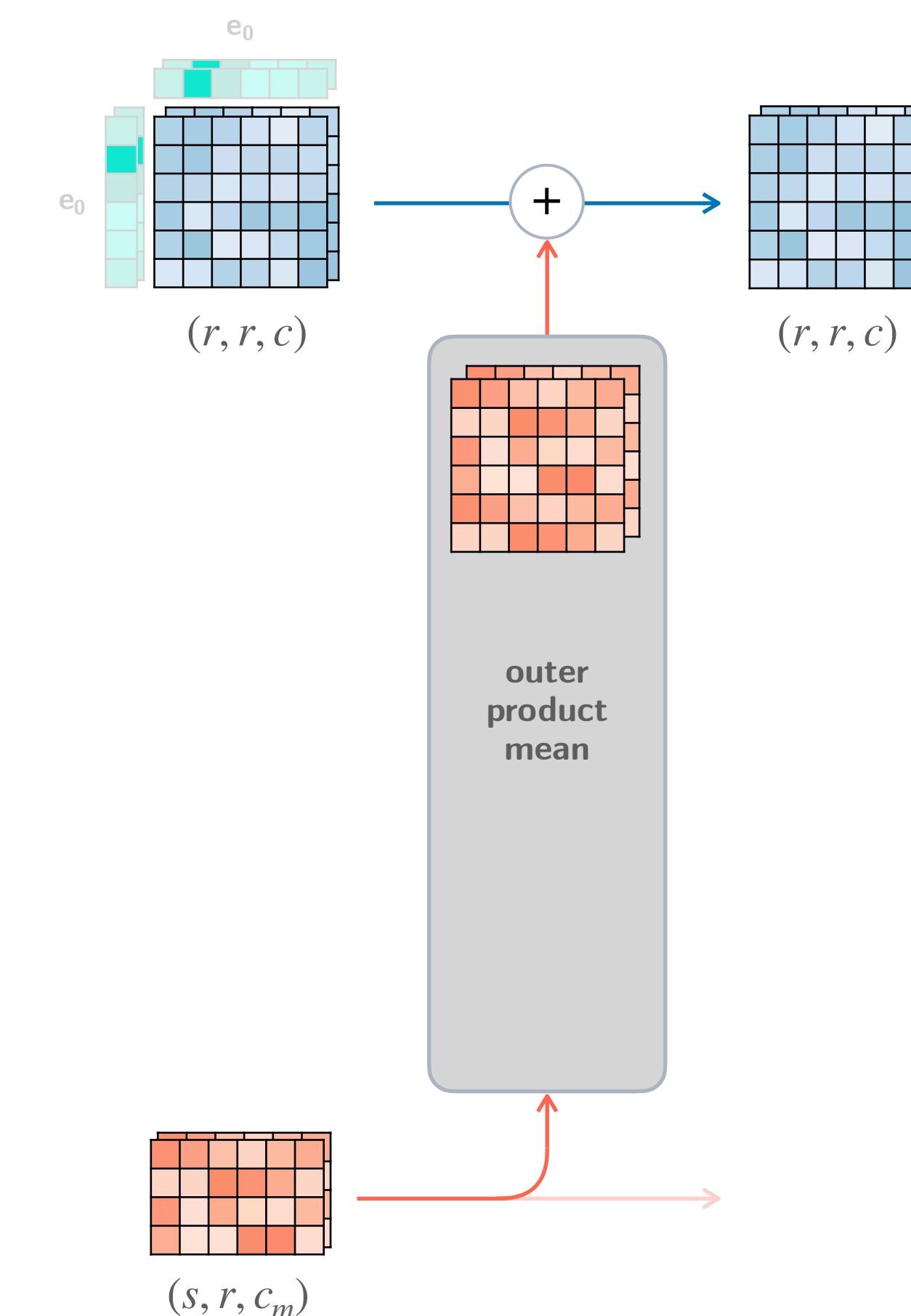
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



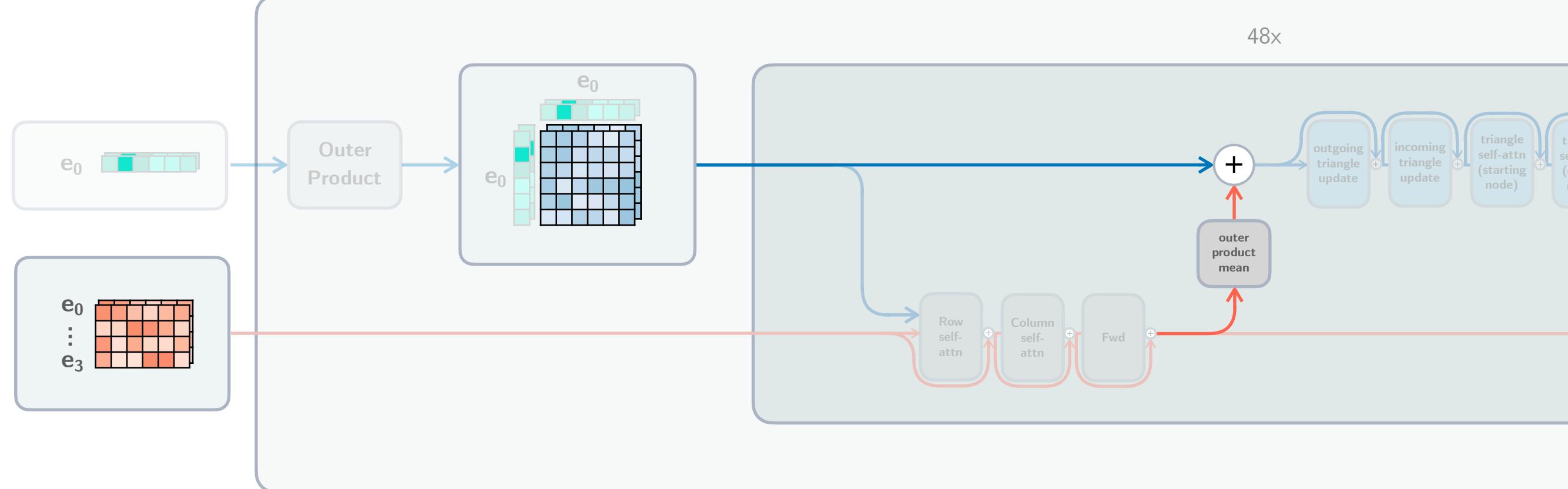
Outer product mean



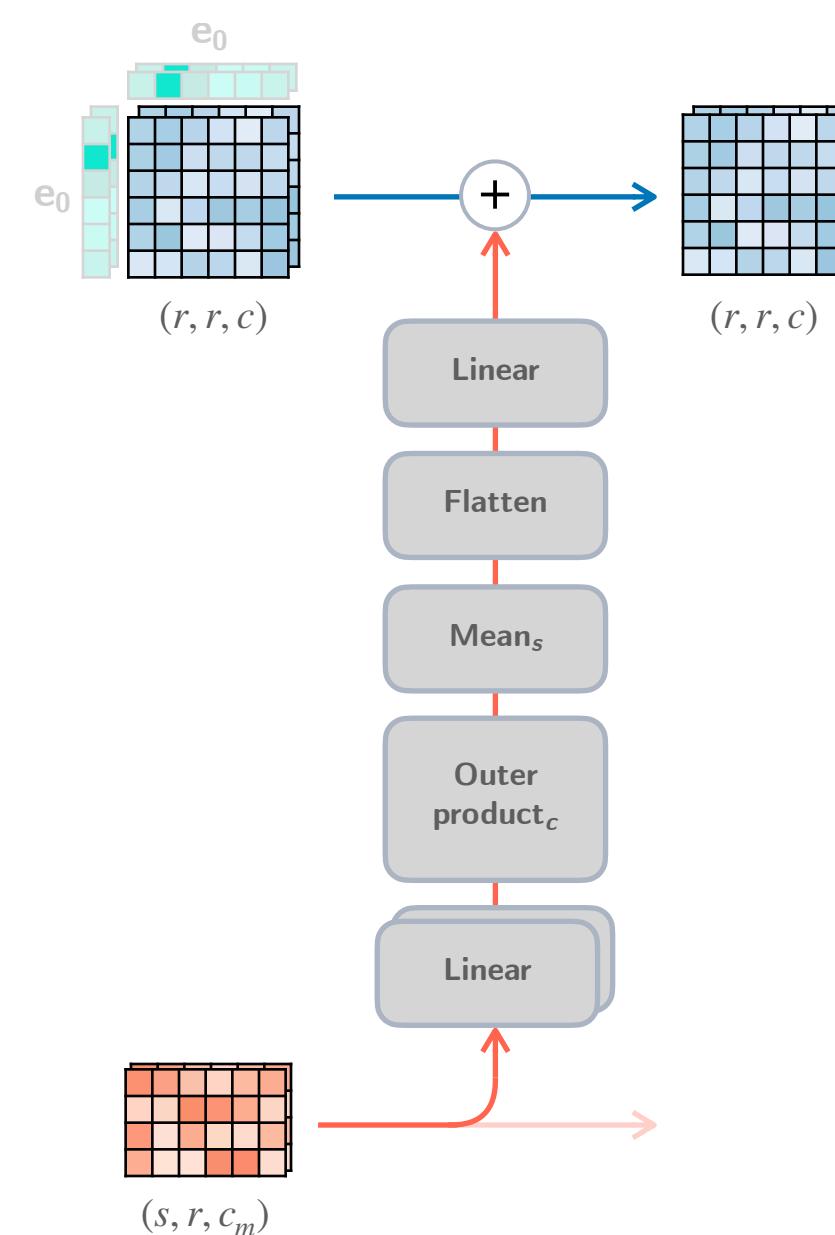
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



Outer product mean

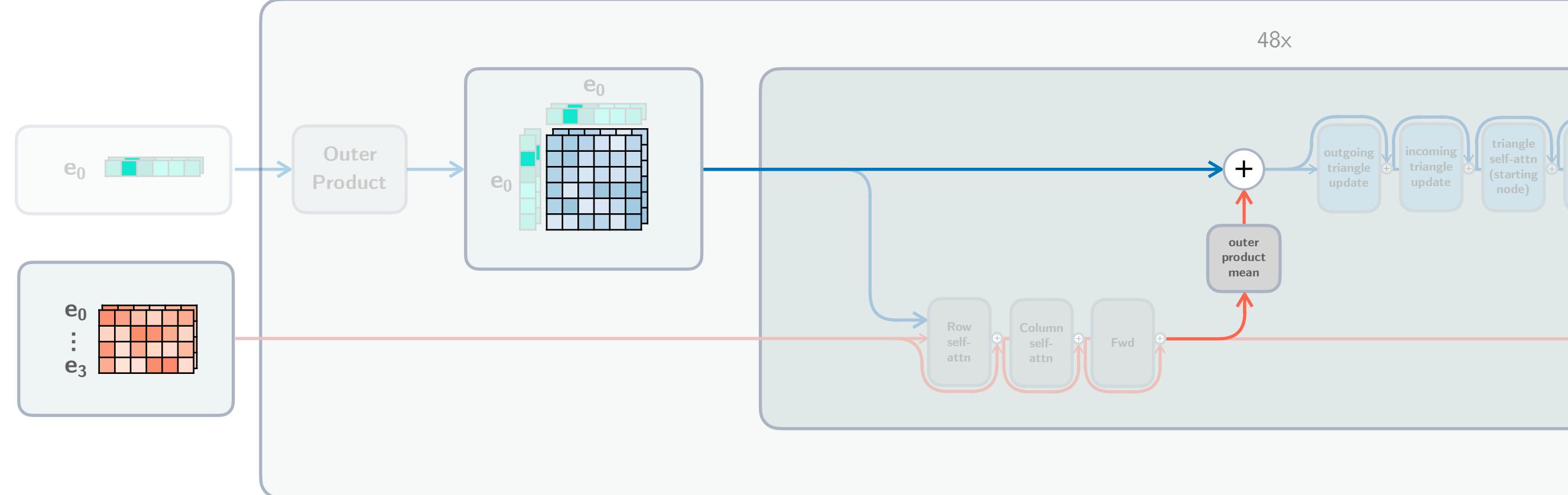


AlphaFold and Protein Structure Prediction

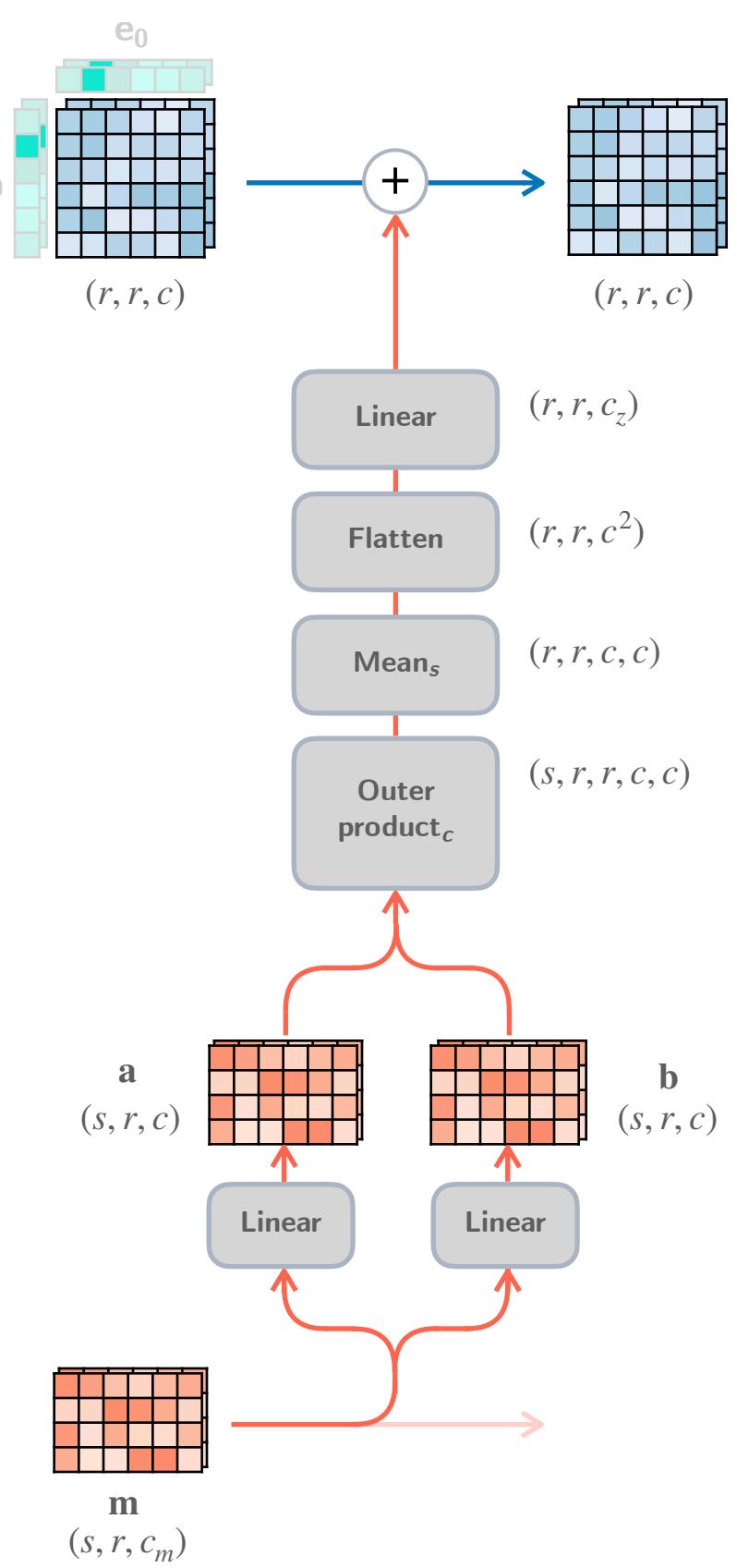
The Solution AlphaFold 2

Refining & Predicting

and contextualizing



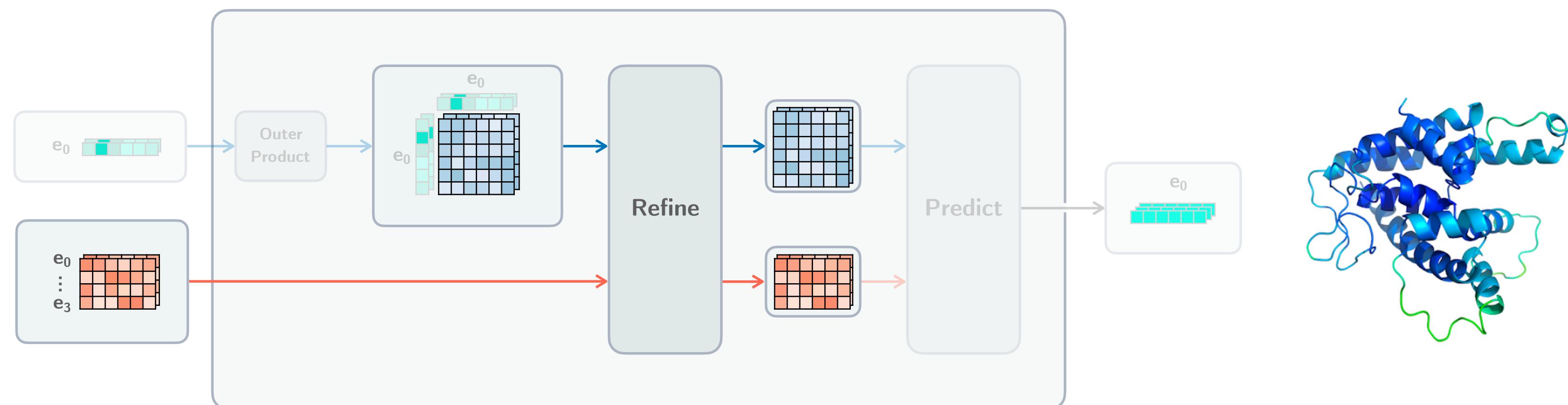
Outer product mean



The Solution AlphaFold 2

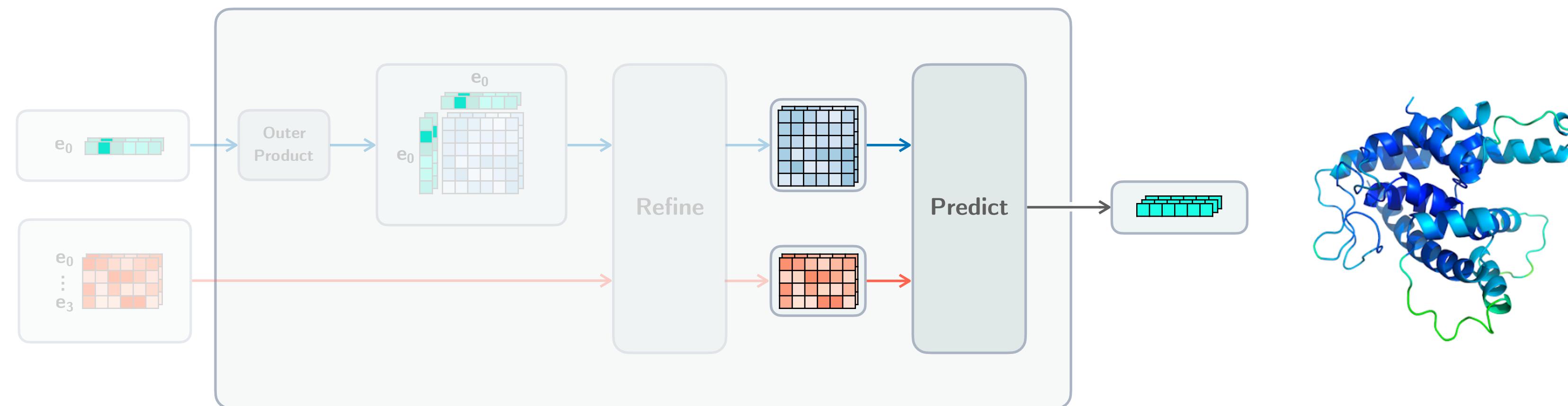
Refining & Predicting

and contextualizing



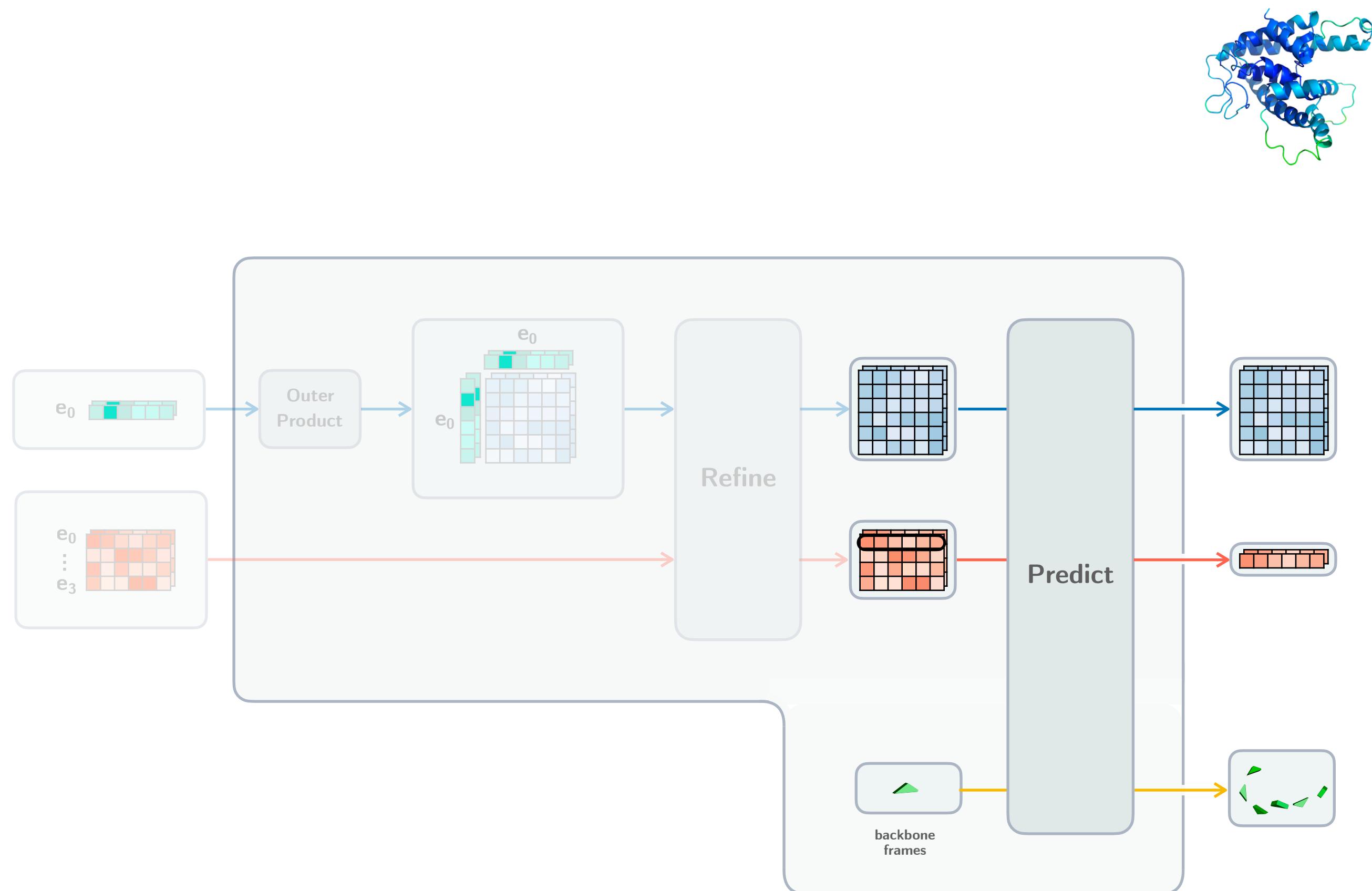
The Solution AlphaFold 2

Refining & Predicting



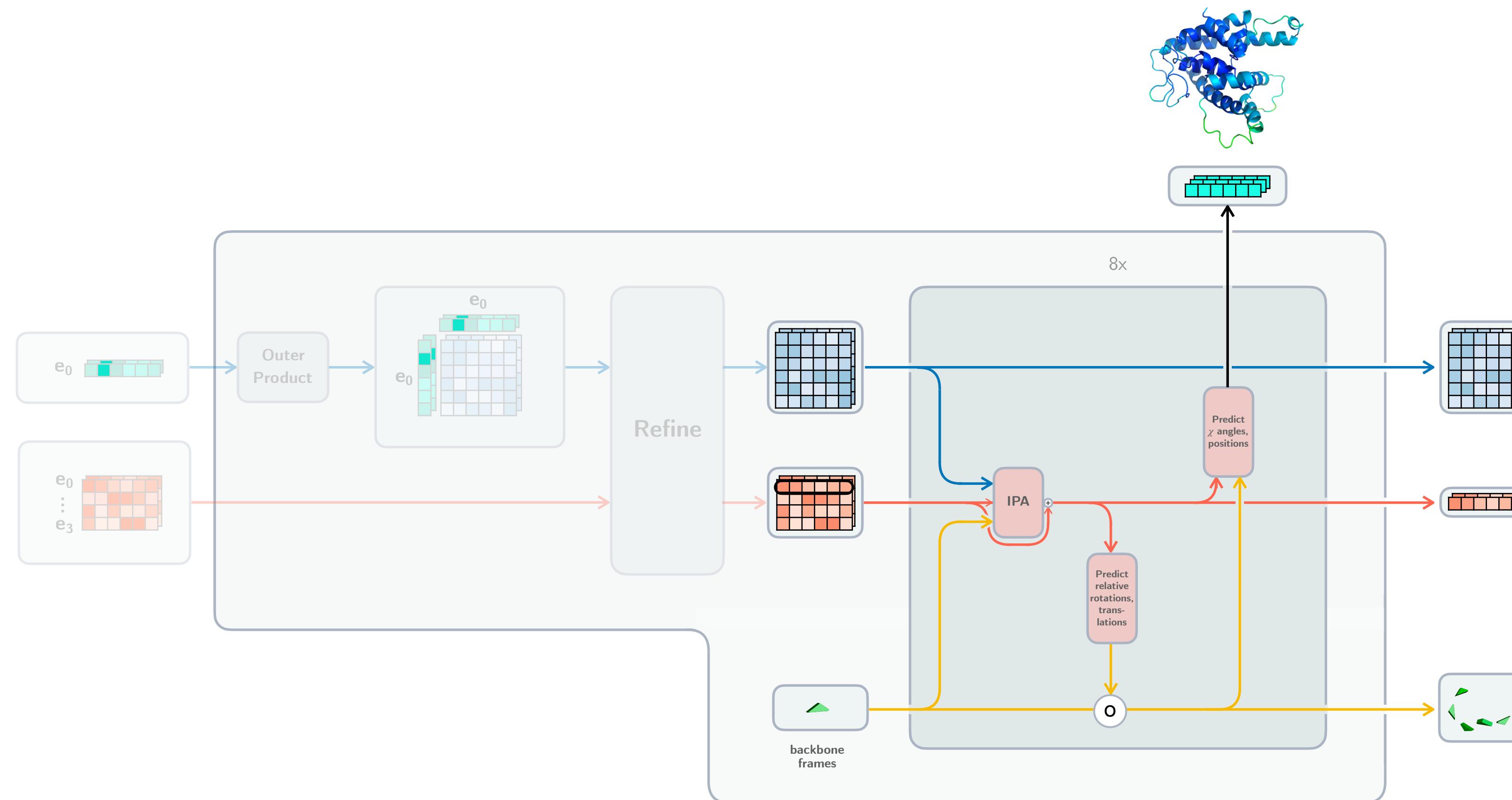
The Solution AlphaFold 2

Refining & Predicting



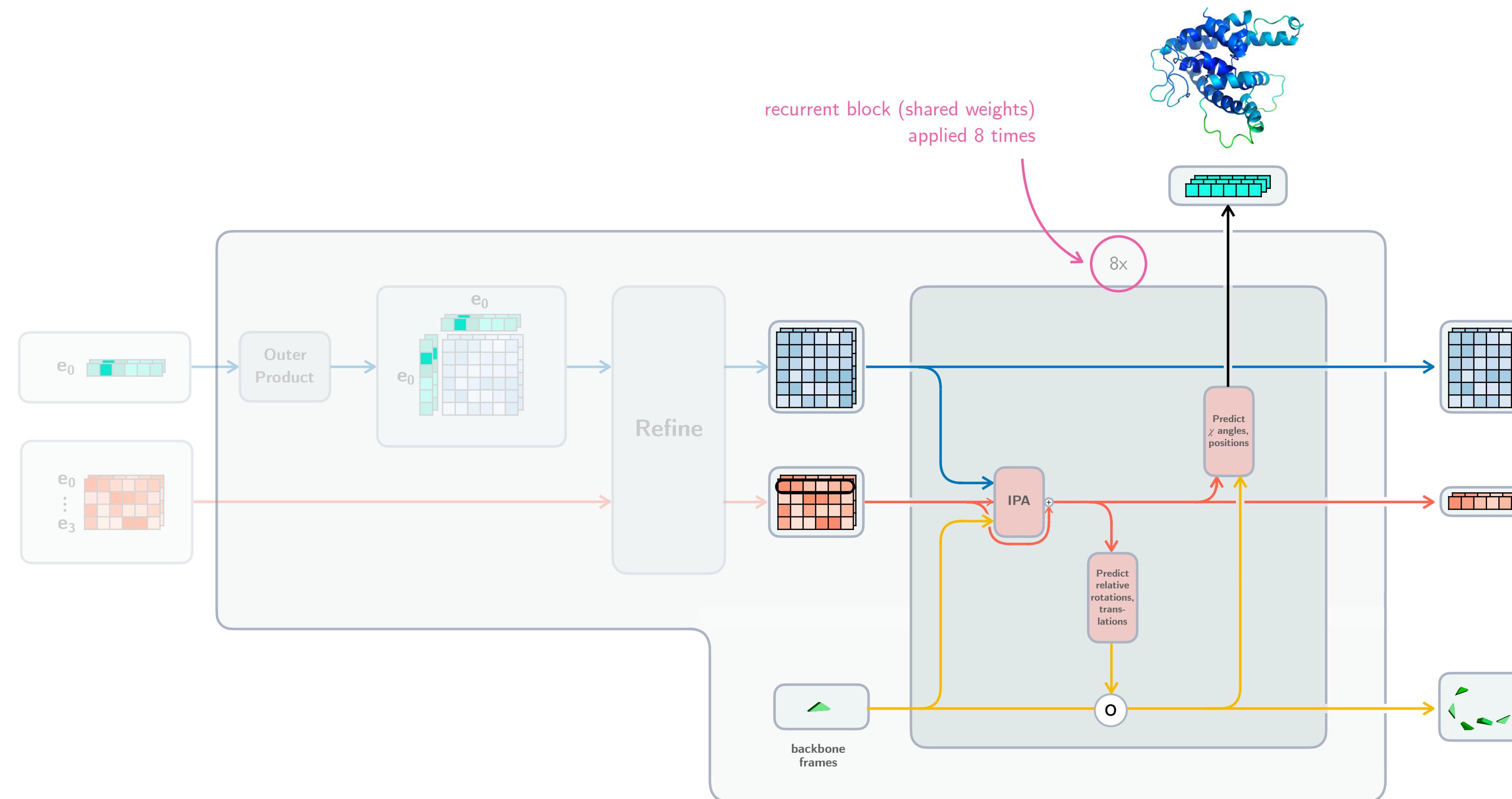
The Solution AlphaFold 2

Refining & Predicting



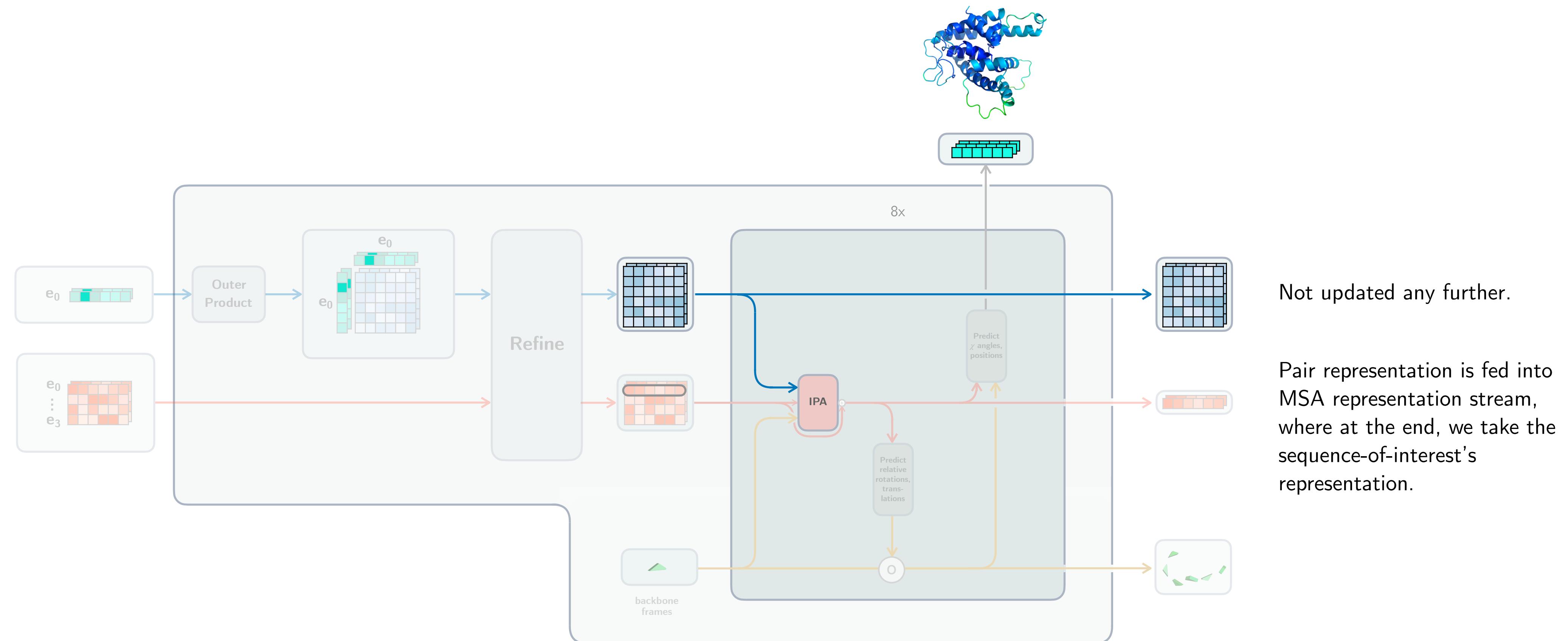
The Solution AlphaFold 2

Refining & Predicting



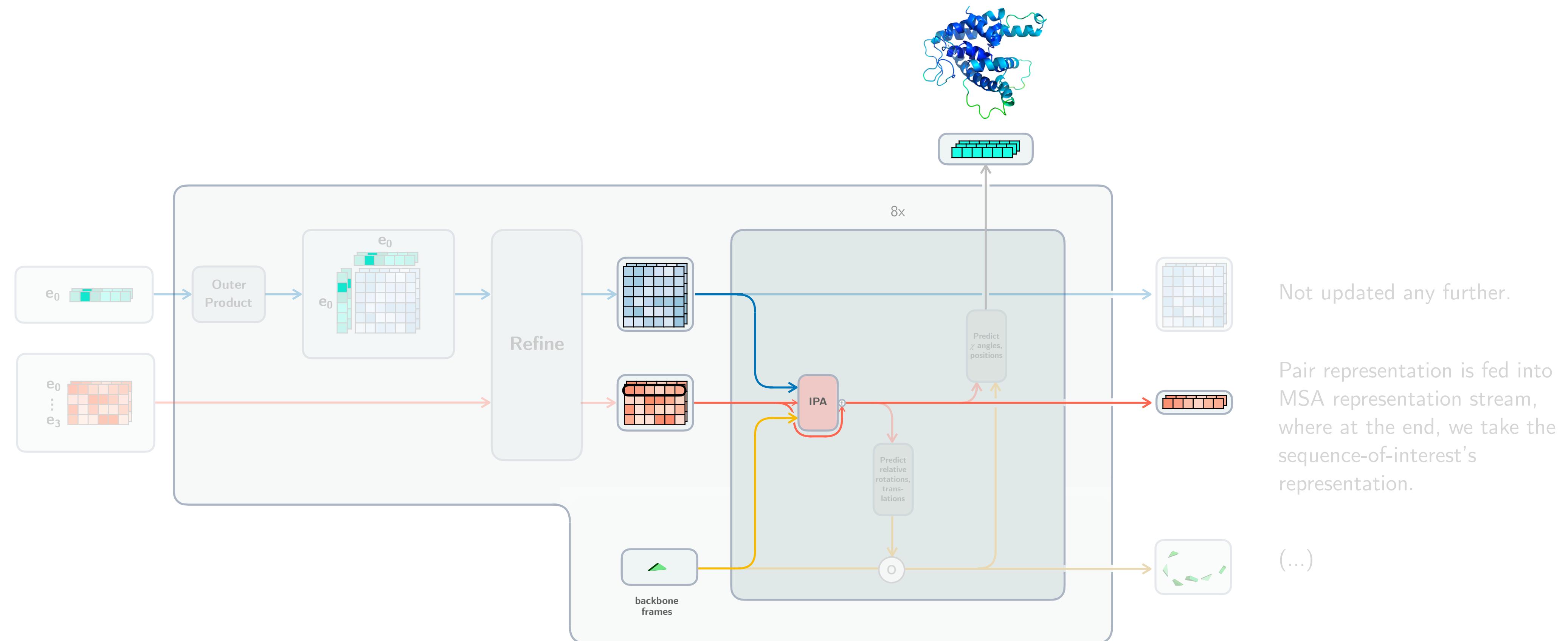
The Solution AlphaFold 2

Refining & Predicting



The Solution AlphaFold 2

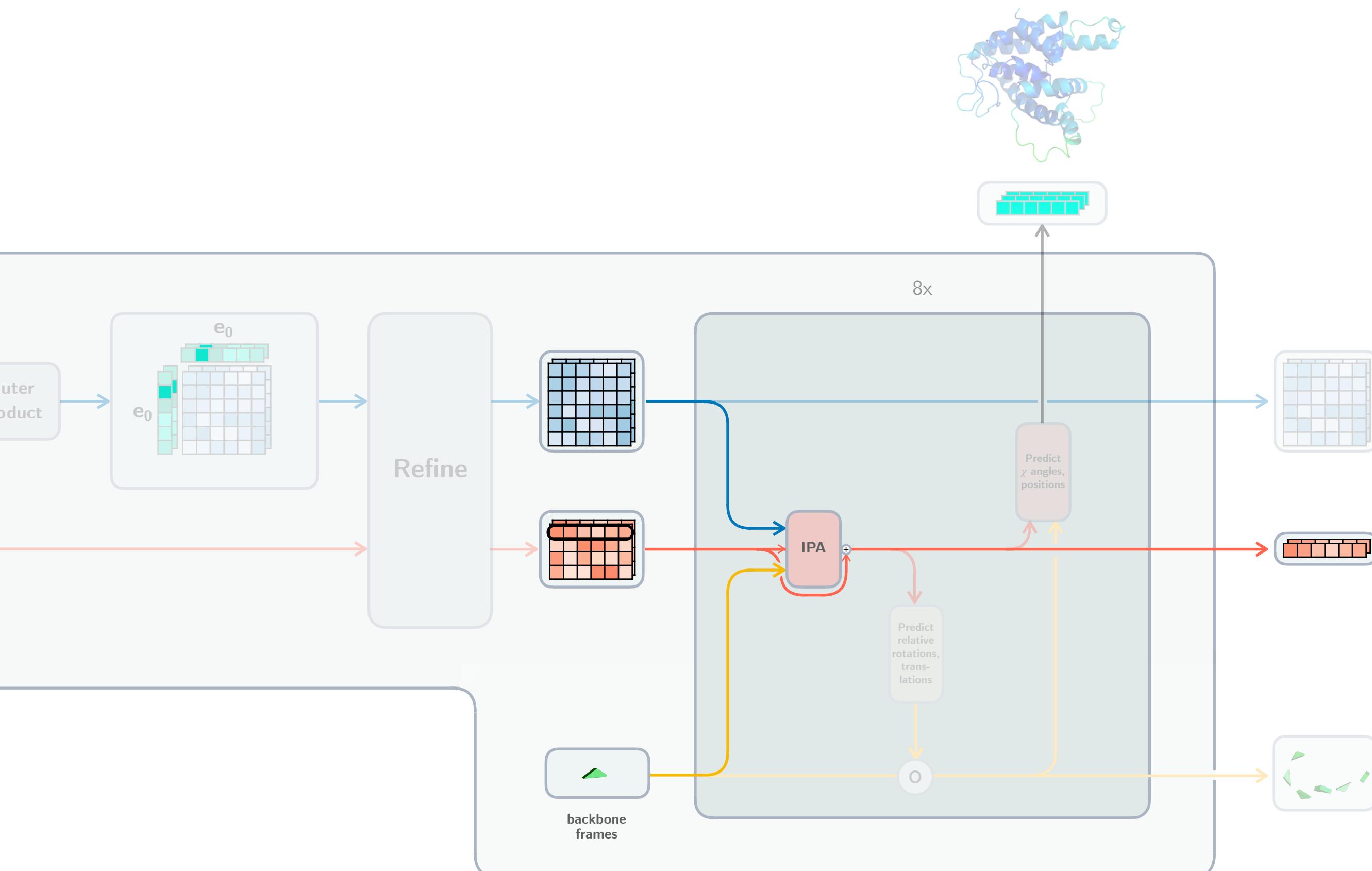
Refining & Predicting



AlphaFold and Protein Structure Prediction

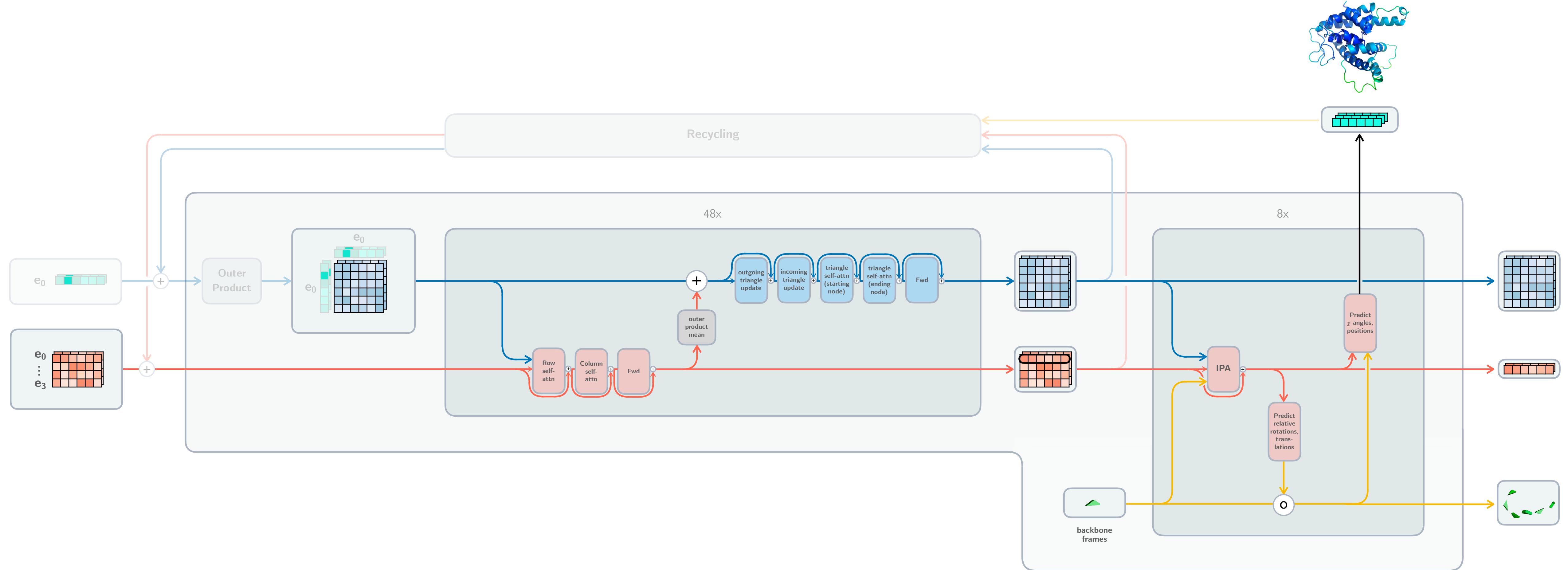
The Solution AlphaFold 2

Refining & Predicting



Invariant Point Attention

Refine single representation-of-interest





Thanks for your attention