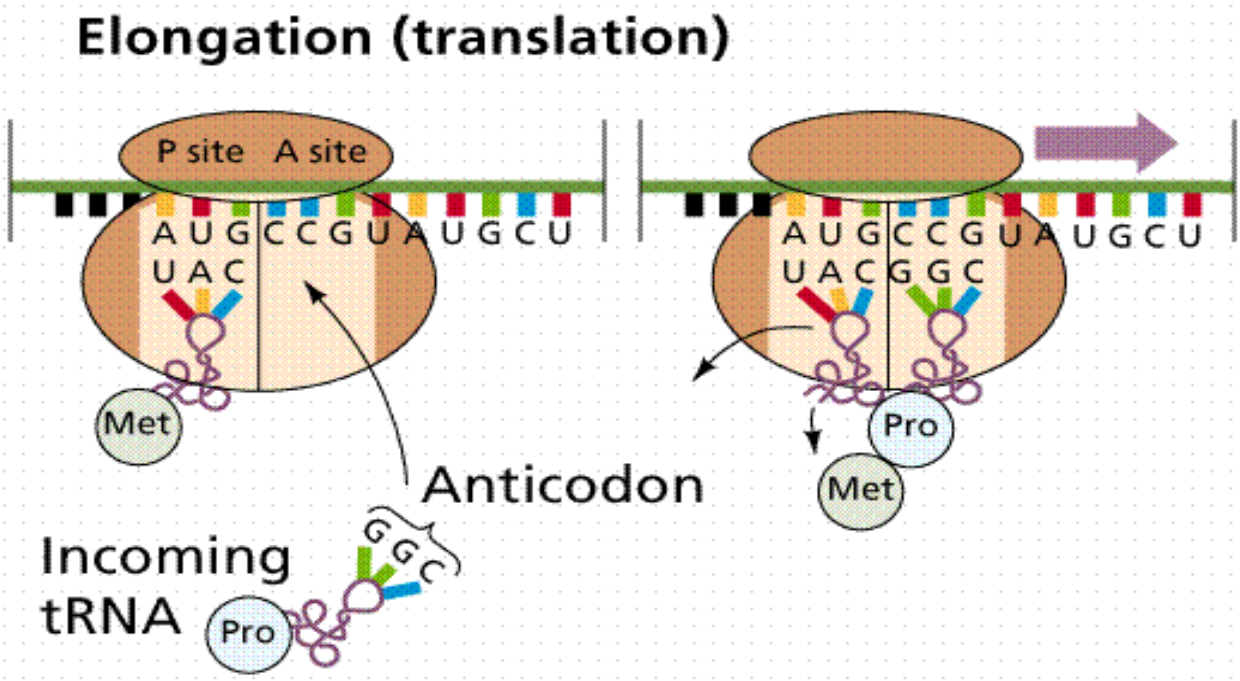
DNA Transcription – A Simulation using Corticon

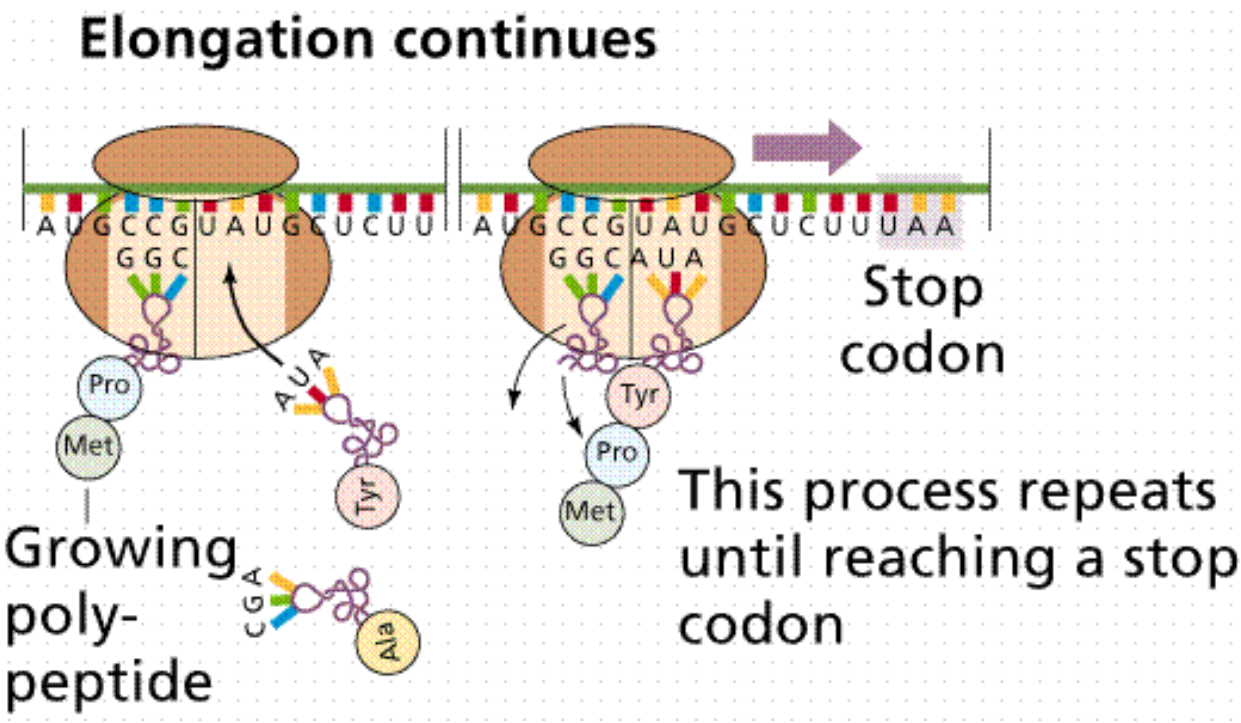
This Corticon rule model shows a simple simulation of the process of DNS transcription

The basic process:

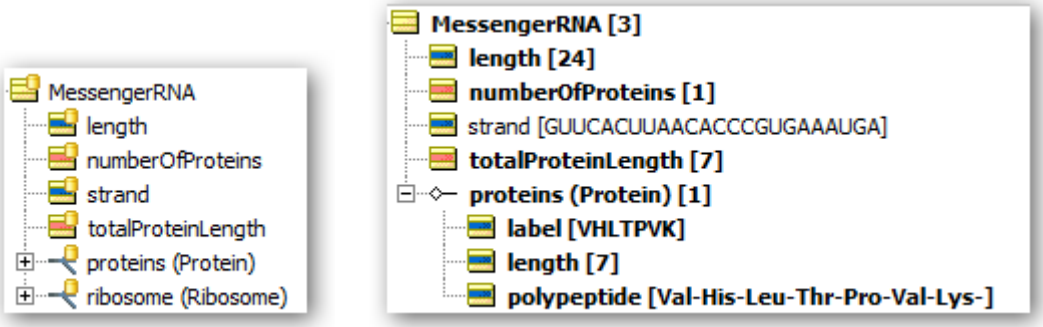
1. First the mRNA attaches itself to a ribosome.
2. Six bases of the mRNA are exposed.
3. A complementary tRNA molecule with its attached amino acid (EG methionine) base pairs via its anticodon UAC with the AUG on the mRNA in the first position P.
4. Another tRNA base pairs with the other three mRNA bases in the ribosome at position A.
5. The enzyme peptidyl transferase forms a peptide bond between the two amino acids.
6. The first tRNA (without its amino acid) leaves the ribosome.



The ribosome moves along the mRNA to the next codon (three bases).
The second tRNA molecule moves into position P.
Another tRNA molecule pairs with the mRNA in position A bringing its amino acid.
A growing polypeptide is formed in this way until a stop codon is reached.



The Vocabulary



eg

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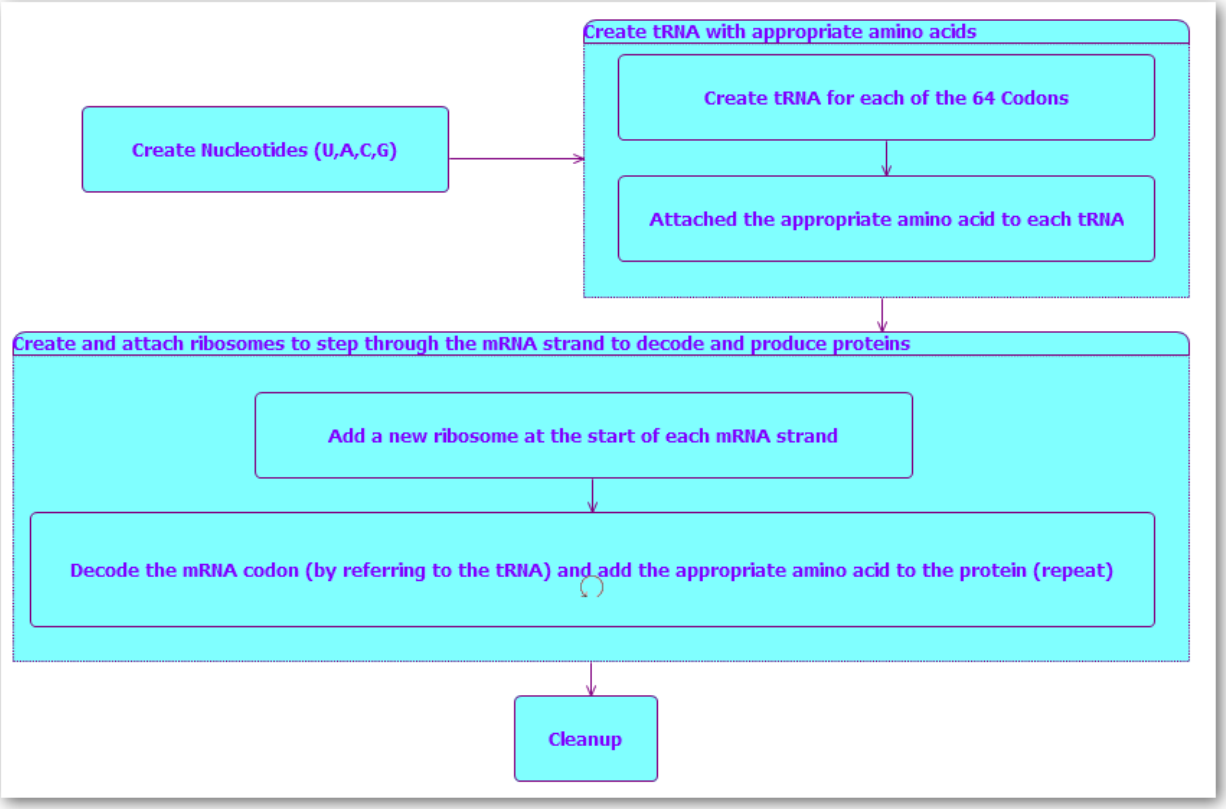
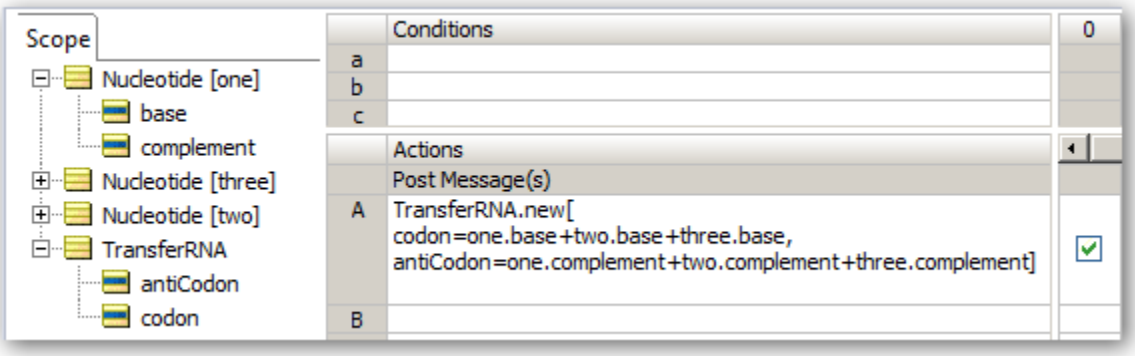


Create Nucleotides

Actions	
Post Message(s)	
Nucleotide.new[base='A',complement='U']	✓
Nucleotide.new[base='U',complement='A']	✓
Nucleotide.new[base='G',complement='C']	✓
Nucleotide.new[base='C',complement='G']	✓

Create tRNA

All possible 3 letter combinations of the base nucleotides will be created (64 in all)



Attach Amino Acids

Conditions	1	2	3	4	5	6	7	8
TransferRNA.codon.substring(1,1)	'A'	'A'	'A'	'A'	'A'	'A'	'A'	'G'
TransferRNA.codon.substring(2,2)	'U'	'U'	'C'	'A'	'A'	'G'	'G'	'U'
TransferRNA.codon.substring(3,3)	{'A', 'C', 'U'}	'G'	-	{'C', 'U'}	{'A', 'G'}	{'C', 'U'}	{'A', 'G'}	-
Actions								
Post Message(s)								
TransferRNA.abbrev	'Ile'	'Met'	'Thr'	'Asn'	'Lys'	'Ser'	'Arg'	'Val'
TransferRNA.symbol	'I'	'M'	'T'	'N'	'K'	'S'	'R'	'V'
TransferRNA.aminoAcid	'Isoleucine'	'Methionine'	'Threonine'	'Asparagine'	'Lysine'	'Serine'	'Arginine'	'Valine'

Conditions	9	10	11	12	13	14	15	16
TransferRNA.codon.substring(1,1)	'G'	'G'	'G'	'G'	'U'	'U'	'U'	'U'
TransferRNA.codon.substring(2,2)	'C'	'A'	'A'	'G'	'U'	'U'	'C'	'A'
TransferRNA.codon.substring(3,3)	-	{'C', 'U'}	{'A', 'G'}	-	{'C', 'U'}	{'A', 'G'}	-	{'C', 'U'}
Actions								
Post Message(s)								
TransferRNA.abbrev	'Ala'	'Asp'	'Glu'	'Gly'	'Phe'	'Leu'	'Ser'	'Tyr'
TransferRNA.symbol	'A'	'D'	'E'	'G'	'F'	'L'	'S'	'Y'
TransferRNA.aminoAcid	'Alanine'	'Aspartate'	'Glutamate'	'Glycine'	'Phenylalanine'	'Leucine'	'Serine'	'Tyrosine'

Conditions	17	18	19	20	21	22	23	24	25
TransferRNA.codon.substring(1,1)	'U'	'U'	'U'	'U'	'C'	'C'	'C'	'C'	'C'
TransferRNA.codon.substring(2,2)	'A'	'G'	'G'	'G'	'U'	'C'	'A'	'A'	'G'
TransferRNA.codon.substring(3,3)	{'A', 'G'}	{'C', 'U'}	'A'	'G'	-	-	{'C', 'U'}	{'A', 'G'}	-
Actions									
Post Message(s)									
TransferRNA.abbrev	'STOP'	'Cys'	'STOP'	'Trp'	'Leu'	'Pro'	'His'	'Gln'	'Arg'
TransferRNA.symbol	'.'	'C'	'.'	'W'	'L'	'P'	'H'	'Q'	'R'
TransferRNA.aminoAcid	'STOP'	'Cysteine'	'STOP'	'Tryptophan'	'Leucine'	'Proline'	'Histidine'	'Glutamine'	'Arginine'

Attach Ribosome to mRNA Strand

Scope

- MessengerRNA [anyMRNA]
  - ribosome (Ribosome) [attachedRibosom
    - position
- Ribosome
  - position
  - protein
  - proteinLabel

	Conditions	0
	Actions	
	Post Message(s)	
A	attachedRibosome+= Ribosome.new[position=1, protein='', proteinLabel='']	✓
B		

Operate Ribosome

This is where all the work actually gets done.

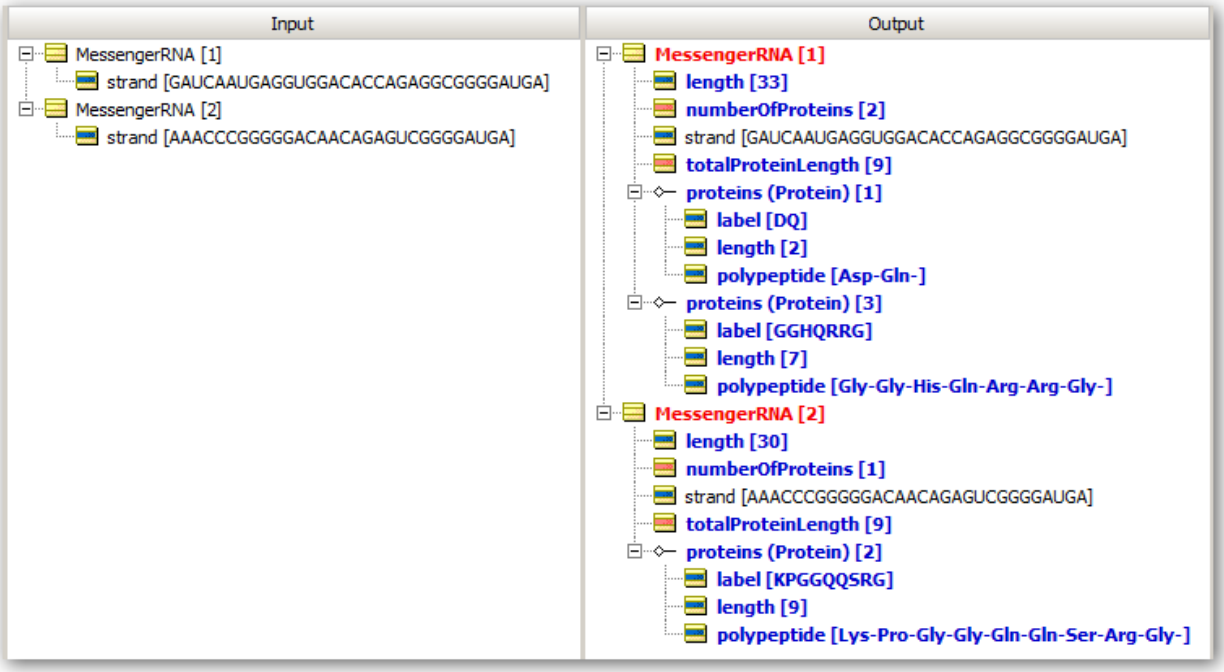
If the codon at the current position of the ribosome is other than a STOP then the amino acid attached to the corresponding tRNA will be attached to the growing protein).

This process continues with the ribosome moving up the mRNA strand (in units of three) until a STOP codon is encountered

Once a STOP codon is reached then the protein that has been assembled is detached (in this example we associate it with its parent mRNA strand using the new operator) and the protein and proteinLabels are reset.

Conditions	1	2
mRNA.strand.substring(ribosome.position,ribosome.position+2)=tRNA.codon	T	T
tRNA.codon	other	{'UAA', 'UAG', 'UGA'}
Actions		
Post Message(s)		
ribosome.protein+=tRNA.abbrev+'-'	✓	
ribosome.proteinLabel+=tRNA.symbol	✓	
ribosome.position+=3	✓	✓
protein+=Protein.new[polypeptide=ribosome.protein, label=ribosome.proteinLabel, length=ribosome.proteinLabel.size]		✓
ribosome.protein="		✓
ribosome.proteinLabel="		✓

Test Case



In the first strand two proteins are created (since there is a STOP codon UGA near the beginning)

The second strand creates just one protein.

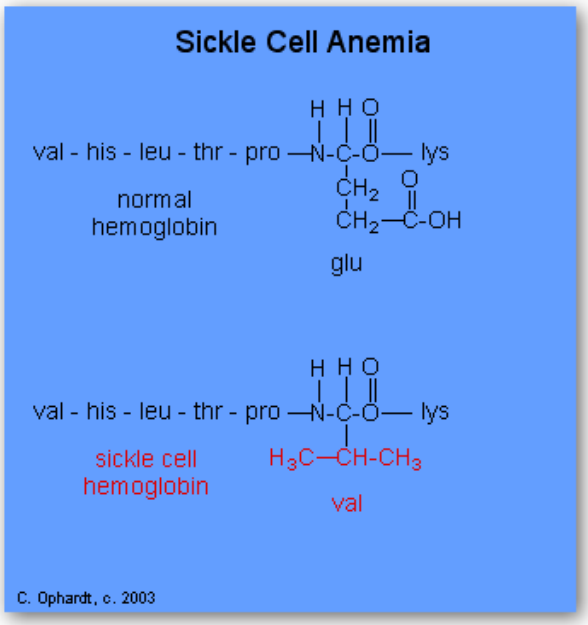
Next Steps

After the proteins are created they will fold. Modeling the rules for protein folding is left as an exercise for the reader. It's quite a hard problem.

Sickle Cell Anemia:

An incorrect amino acid sequence in a protein may lead to fatal consequences. For example, the inherited disease, sickle cell anemia, results from a single incorrect amino acid at the 6th position of the beta - protein chain out of 146. Hemoglobin consists of four protein chains - two beta and two alpha.

See the graphic on the right for the sequences. This one alteration of the sequence of amino acids in hemoglobin changes its molecular geometry and hence its ability to carry oxygen and its solubility characteristics. The red blood cells change into a sickled shape instead of the normal round shape, become trapped in the small blood capillaries, and cause a great deal of pain.



Test Case for Sickle Cell Anemia

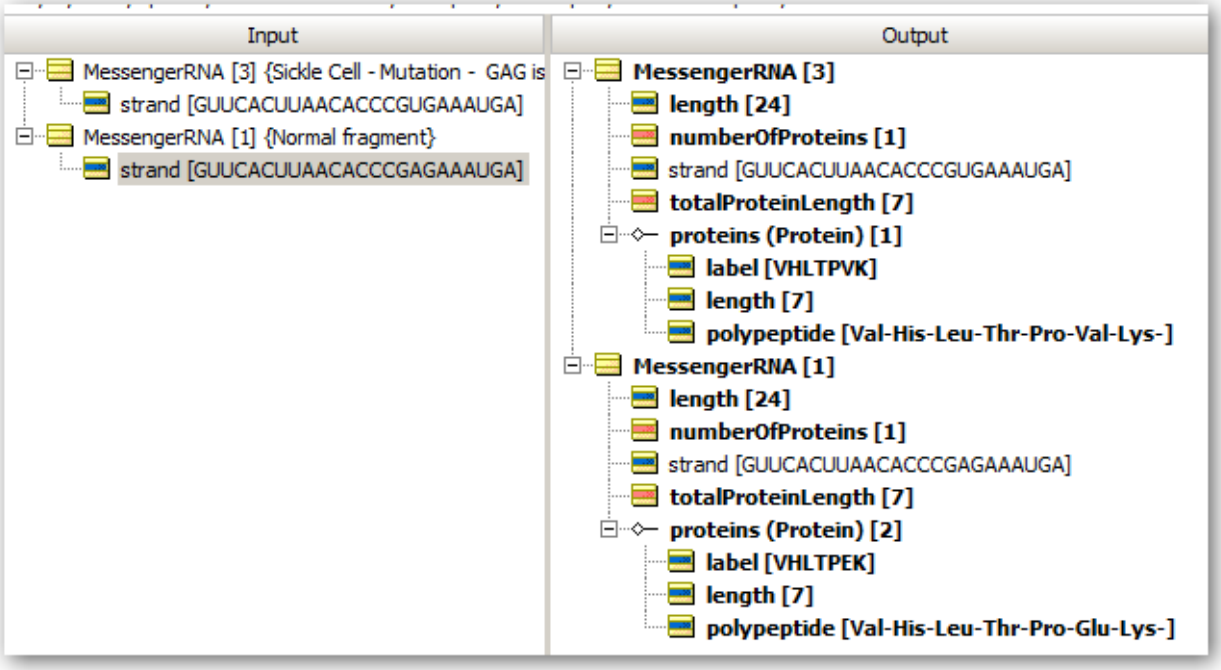


Table of codon-amino acid assignments

Amino Acid	Codons					
Isoleucine			AUU	AUC	AUA	
Phenylalanine			UUU	UUC		
Valine			GUU	GUC	GUA	GUG
Leucine	UUA	UUG	CUU	CUC	CUA	CUG
Methionine						AUG
Tryptophan						UGG
Alanine			GCU	GCC	GCA	GCG
Glycine			GGU	GGC	GGA	GGG
Cysteine			UGU	UGC		
Tyrosine			UAU	UAC		
Proline			CCU	CCC	CCA	CCG
Threonine			ACU	ACC	ACA	ACG
Serine	AGU	AGC	UCU	UCC	UCA	UCG
Histidine			CAU	CAC		
Glutamate					GAA	GAG
Asparagine			AAU	AAC		
Glutamine					CAA	CAG
Aspartate			GAU	GAC		
Lysine					AAA	AAG
Arginine	AGA	AGG	CGU	CGC	CGA	CGG
STOP	UGA				UAA	UAG