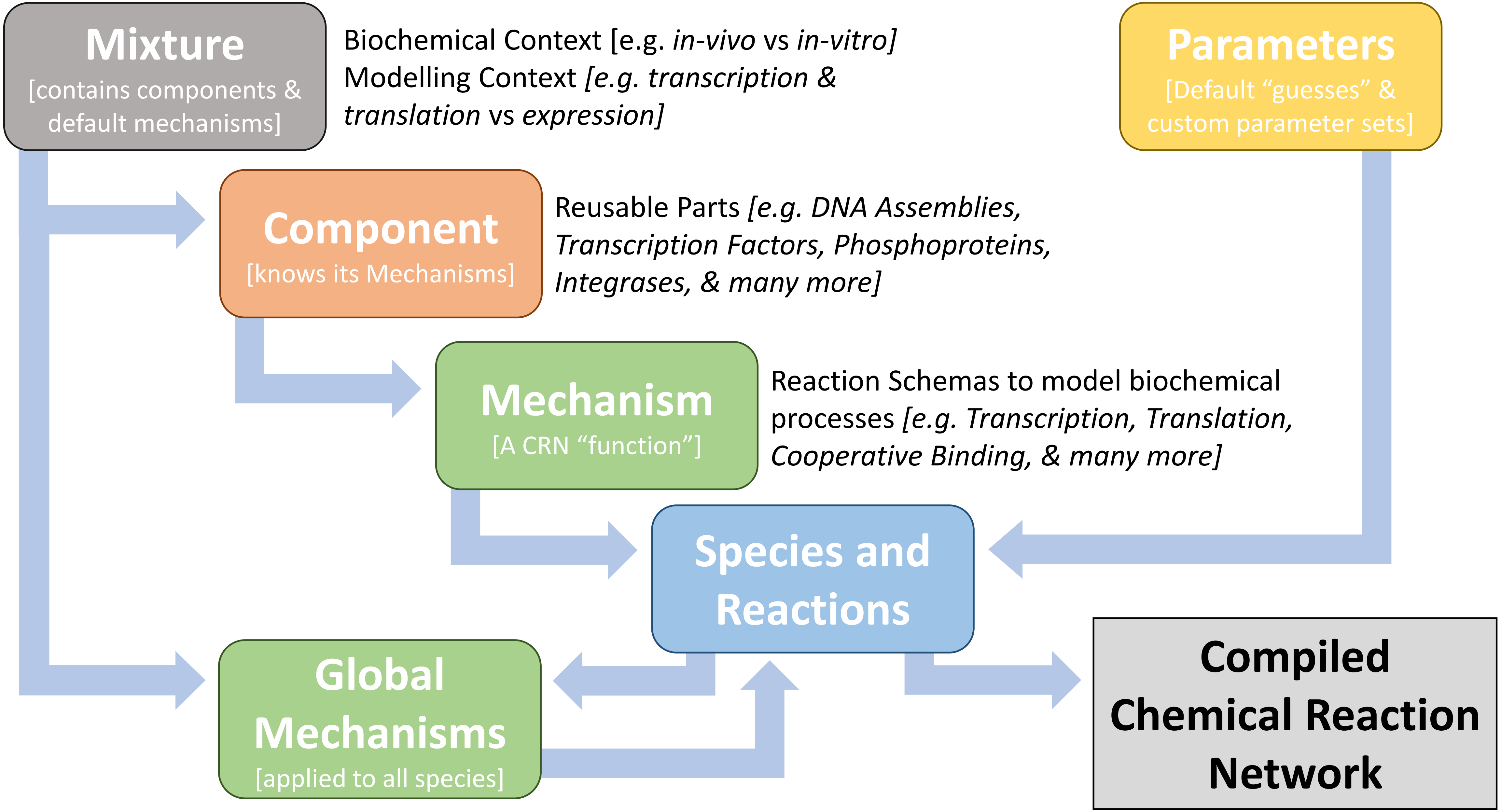

Mixture
[contains components & default mechanisms]

Biochemical Context [e.g. *in-vivo* vs *in-vitro]*
Modelling Context *[e.g. transcription & translation* vs *expression]*

Parameters
[Default "guesses" & custom parameter sets]

Component
[knows its Mechanisms]

Reusable Parts *[e.g. DNA Assemblies, Transcription Factors, Phosphoproteins, Integrases, & many more]*

Mechanism
[A CRN "function"]

Reaction Schemas to model biochemical processes *[e.g. Transcription, Translation, Cooperative Binding, & many more]*

Species and Reactions

Global Mechanisms
[applied to all species]

Compiled Chemical Reaction Network

```
#Parameters can be loaded from a default or custom parameter file
parameter_file = "default_parameters.txt"
#Parameters can also be overwritten programmatically
#Parameter keys allow for sharing of parameters and automatic defaulting.
expression_params = {("negativehill_transcription", "k"):2.8}
```

```
#Create CRN Species for Protein Repressors
lacI = Species(name= "lacI", material_type = "protein")
tetR = Species(name = "tetR", material_type = "protein")
cl = Species(name = "cl", material_type = "protein")

#Create Promoter Components Modelled with Hill Functions
pLac = RepressablePromotor(name = "pLac", transcript = "tetR", repressor = lacI)
pTet = RepressablePromotor(name = "pTet", transcript = "cl", repressor = tetR)
pCl = RepressablePromotor(name = "pCl", transcript = "lacI", repressor = cl)

#Create DNAAssembly Components with each Promoter
placI_tetR = DNAassembly(name = "lacI_tetR", promoter = pLac, rbs = "BCD8", protein = tetR)
ptetR_cl = DNAassembly(name = "tetR_cl", promoter = pTet, rbs = "BCD8", protein = cl)
pcl_lacI = DNAassembly(name = "cl_lacI", promoter = pCl, rbs = "BCD8", protein = lacI)
```

```
#Produce an idealized model with just gene expression
RepressilatorExp = ExpressionDilutionMixture(name = "expression",
              components = [placI_tetR, ptetR_cl, pcl_lacI],
              parameter_file = parameter_file, #can use multiple parameter sources
              parameters = expression_params)  #custom parameters take precedent
RepressilatorExpCRN = RepressilatorTxTl.compile_crn()
```

```
#Produce a more complex model with transcription and translation
RepressilatorTxTl = SimpleTxTlDilutionMixture(name = "txtl",
              components = [placI_tetR, ptetR_cl, pcl_lacI],
              parameter_file = parameter_file)
RepressilatorTxTlCRN = RepressilatorTxTl.compile_crn()
```

```
#Produce a cell-like model with limited resources and loading effects
RepressilatorColi = TxTlDilutionMixture(name = "e coli",
              components = [placI_tetR, ptetR_cl, pcl_lacI],
              parameter_file = parameter_file)
RepressilatorColiCRN = RepressilatorTxTl.compile_crn()
```

Flexible Parameter System: includes default parameters for rapid model building, allows programmatic access via dictionaries or custom parameter files. All parameters can be customized at the Mixture or Component level.

Modular Components: can be combined together and compiled in many contexts represented by different **Mixtures**. Compiled CRNs are saved as SBML files for simulation.

Expression Mixture: CRN contains 6 Species and 9 Reactions modelling gene expression (with leak) and dilution.

TxTl Mixture: CRN contains 9 Species and 18 Reactions modelling transcription (with leak), translation, and dilution.

E Coli Mixture: produces a CRN with 24 Species and 41 Reactions including transcription via RNA-Polymerase, translation via ribosomes, mRNA-degradation via endo-nucleases, background cellular loading, and dilution.