# *RAVEN interaction with External Applications*

RAVEN Workshop

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Idaho National Laboratory

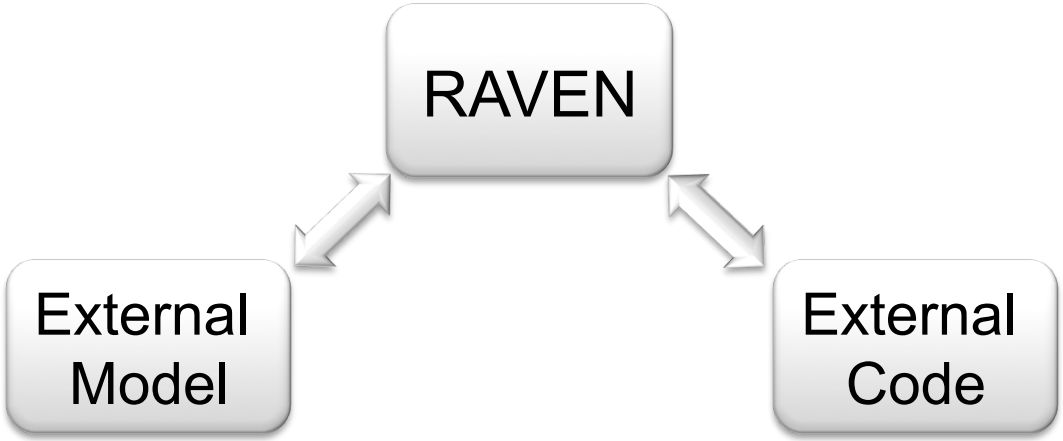
# Outline

- Overview of RAVEN interaction with external Applications
  - Available APIs: External Model and Code APIs
- Coupling a new Application through a Code Interface
  - Introduction
  - Code requirements
  - Interfaces that need to be implemented
  - Interaction with RAVEN
- Practical example of coupling a new code
  - Code overview
  - Creation of the input parser (coding)
  - Creation of the output parser (coding)
  - Execution of the interface (terminal)

# *Overview*

# *RAVEN Interaction with External Applications*

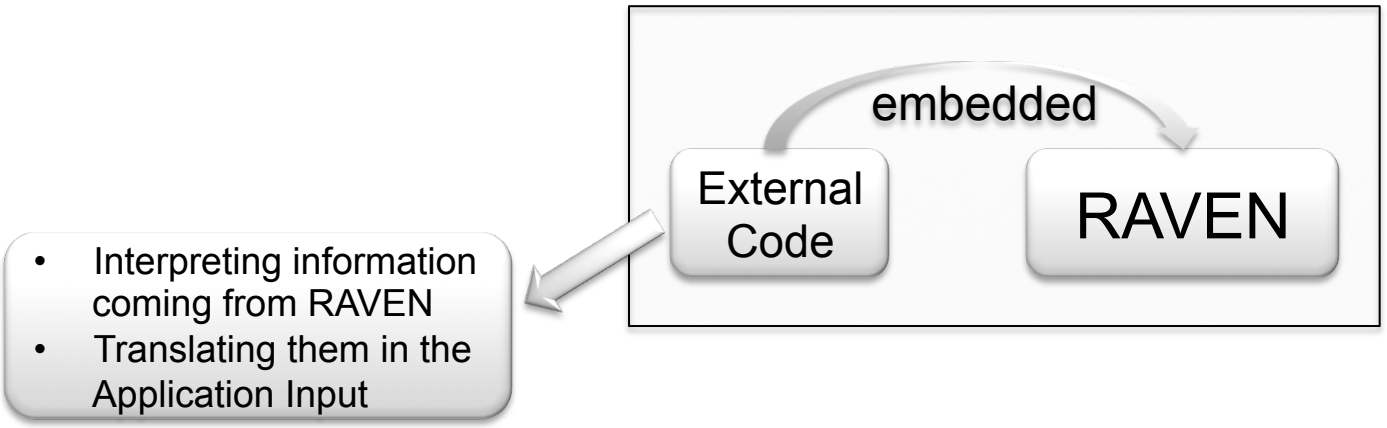
- RAVEN has two preferential APIs to interact with external Applications
  - *External Model*: An external Python "entity" that can act as a system model
  - *External Code*: API to drive external codes
- Both APIs are written in `PYTHON`



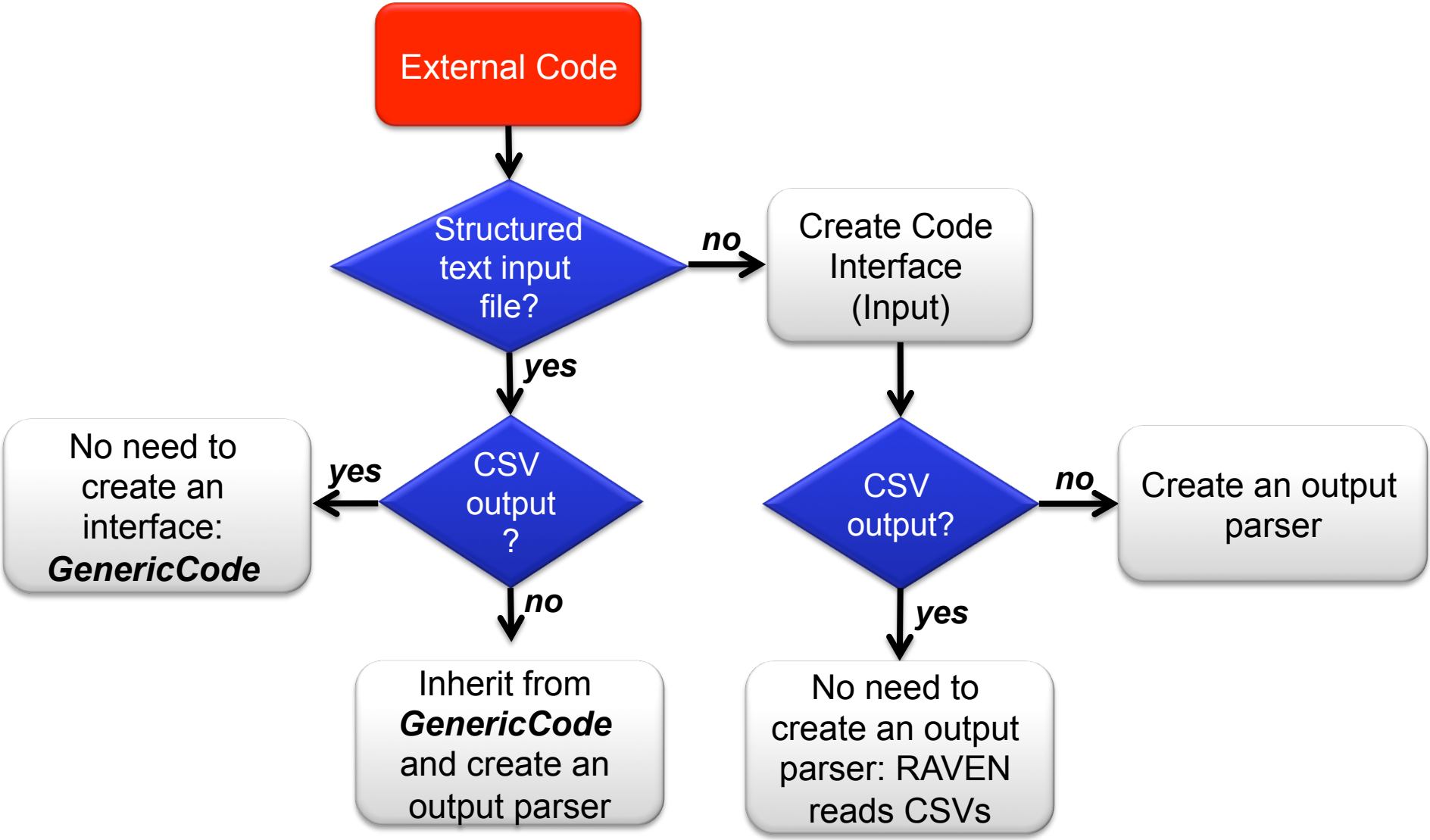
# *Coupling an Application through a code interface*

# Coupling an Application with RAVEN: Introduction

- The procedure of coupling a new Application with RAVEN is a straightforward process
- The coupling is performed through a `Python` Interface
- The Interface has two functions:
  1. Interpret the information coming from RAVEN
  2. Translate such information in the input of the driven code
- The coupling procedure does not require any modification of RAVEN

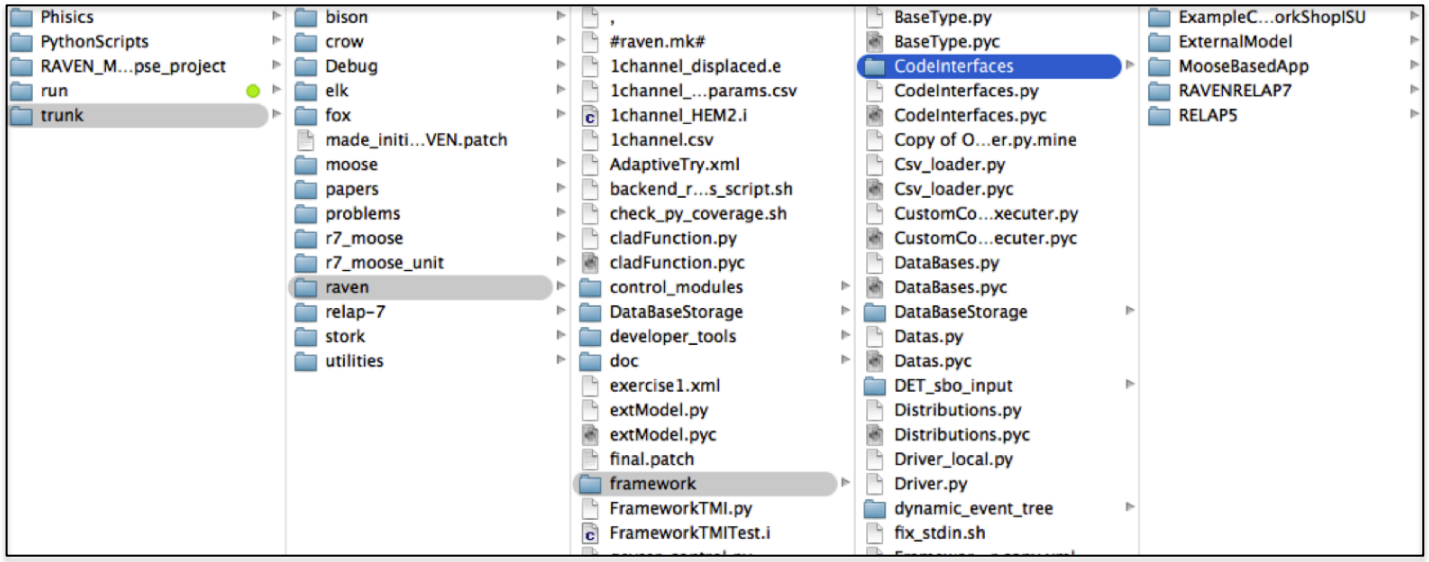


# Choose how to couple your Application to RAVEN



# Coupling an Application with RAVEN: Interfaces

- RAVEN becomes aware of the codes it can use as Models only at run-time
  - RAVEN looks for code interfaces and loads them automatically
- The code interface needs to be placed in a new folder under the directory "*./raven/framework/CodeInterfaces*"



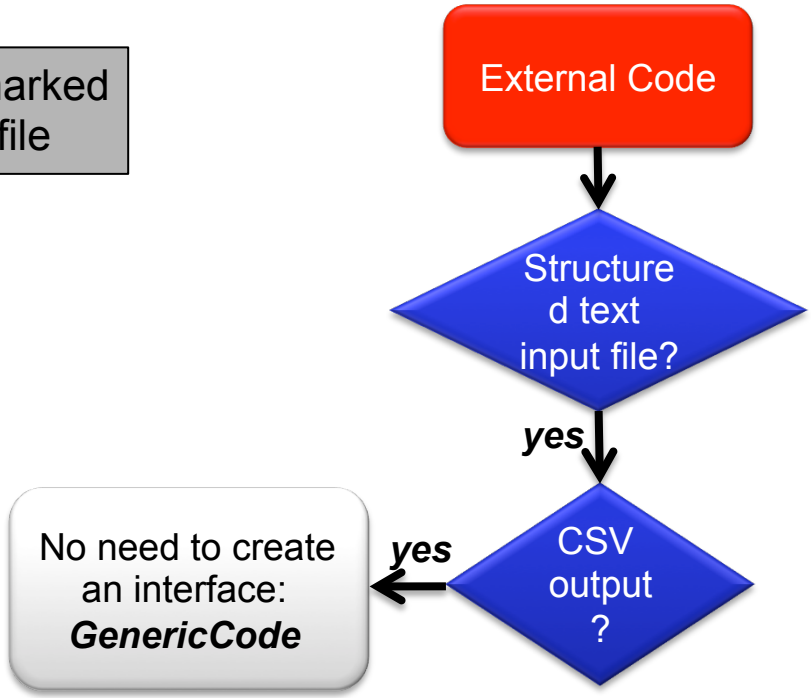
# Coupling strategy: GenericCode interface

- The *GenericCode* interface is meant to handle a wide variety of generic codes. The *GenericCode* interface can be used if the code:
  - Accepts a keyword-based input file with no cross dependent inputs
  - The outputs are stored in a CSV file

```
<variableToChange>
 $RAVEN-variableName$
</variableToChange>
```

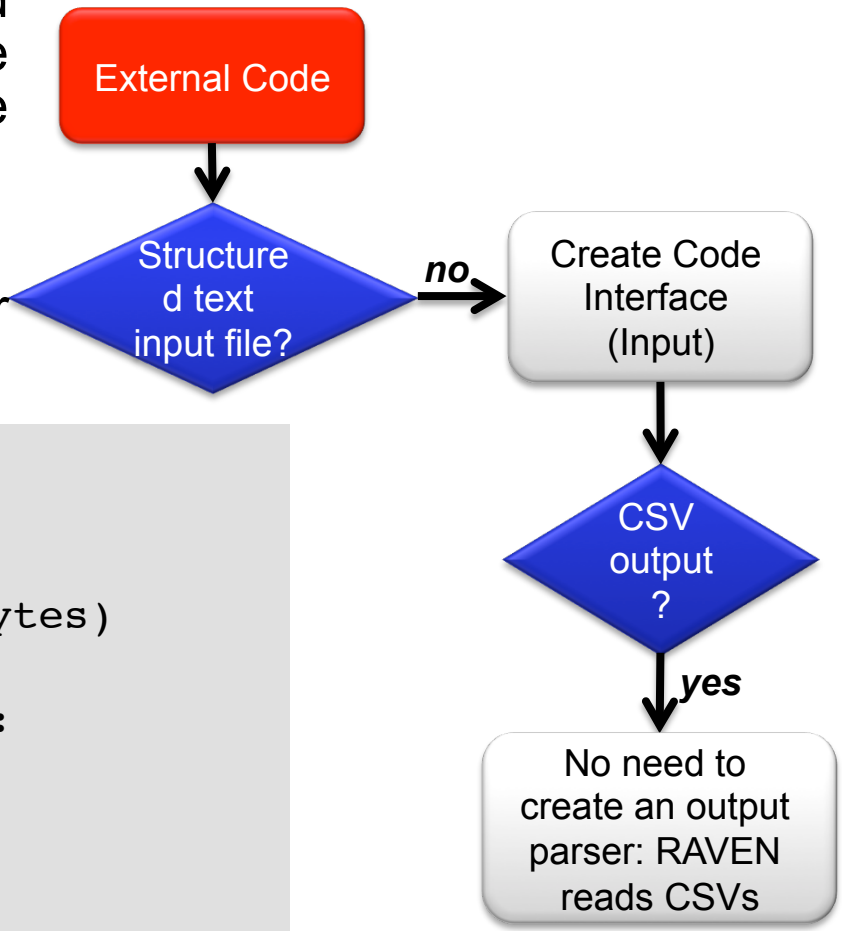
Variable needs to be marked in the original input file

```
<Code>
 <executable>path/to/exe</executable>
 <inputExtcensions>
  .xml,.aux
 </inputExtcensions>
 <clargs type='prepend' arg='python'/>
 <clargs type='input' arg='-i'
         extension='.xml'/>
 <clargs type='input' arg='-aux'
         extension='.aux'/>
 <clargs type='output' arg='-o'/>
</Code>
```



# Coupling strategy: No text-based input format

- If the code input file is not text-based (e.g. binary) or too complicated to handle with "wild-cards", the GenericCode interface can not be used:
  - An input-parser needs to be created
- If the output file is a CSV, no other parsers are needed



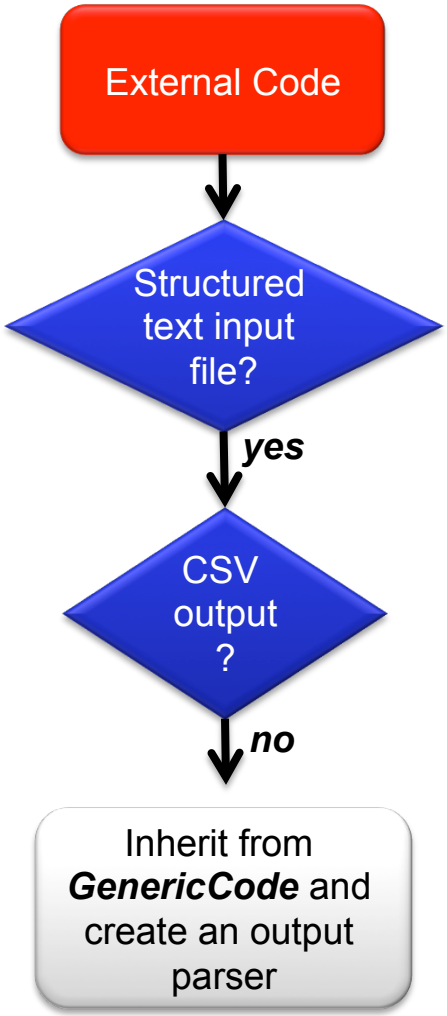

```
class parserBinaryInput():
  def __init__(self,filen):
    bytes=open(filen,"rb").read()
    self.unPack = struct.unpack("FMT", bytes)

  def perturbTheInput(self,inDictionary):
    # perturb the binary file

  def writeNewInput(self,filen):
    fileObj = open(filen, "wb")
    fileObj.write(struct.pack("FMT", self.unPack))
```

# Coupling strategy: Text input but no CSV output

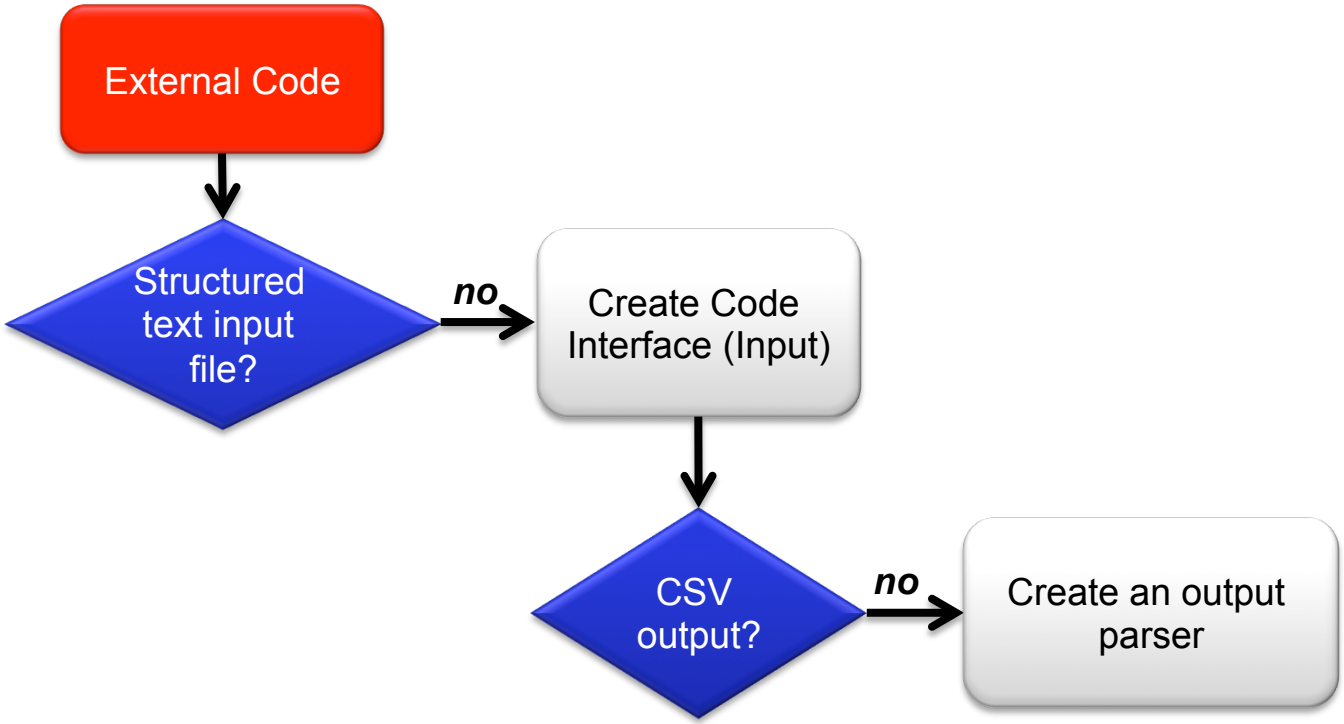
- If the code input file is text-based, the *GenericCode* interface can be used for the input perturbation
- If the output file is not a CSV, an output parser needs to be created




```
def convertOutputFileToCSV(outfile):
  keyDict = {}
  CSVfile = open(outputfile + '.csv')
  lines = open(outputfile).readlines()
  for line in lines:
    values = line.split("=")
    key,val = values[0], values[1]
    keyDict[key] = val
  CSVfile.write(','.join(keyDict.keys()))
  CSVfile.write(','.join(keyDict.values()))
```

# Coupling strategy: Brand-new interface

- If the input structure is too complicated or the interface developer prefers a more specific perturbation syntax and the output file is not a CSV, a new code interface needs to be created:
  - Input Parser, for the input reading and perturbation
  - Output Parser, for converting the output file(s) into a single CSV



# Coupling an App with RAVEN: Methods

- RAVEN imports all the “Code Interfaces” at run-time, without actually knowing the syntax of the driven codes
- In order to make RAVEN able to drive a new Application, a `Python` module containing few methods (strict syntax) needs to be implemented:

```
class newApplication(CodeInterfaceBase):
```

```
 def generateCommand(self,input,exe,clargs,fargs)
```
Required

```
 def createNewInput(self,inputs,oinputs,samplerType,**Kwargs)
```
Required

```
 def finalizeCodeOutput(self,command,output,workDir)
```
Optional

```
 def checkForOutputFailure(self,output,workDir)
```
Optional

```
 def getInputExtension(self)
```
Optional

```
 def setInputExtension(self, exts)
```
Optional

# Coupling an Application with RAVEN: generateCommand

- Used to:
  - retrieve the command needed to launch the driven Application
  - retrieve the root of the output file
- The return data type must be a TUPLE

```
def generateCommand(self,inputs,exe,clargs,fargs):
  (…)
  return (executeCommand,outfile)
```

Required

- Arguments:
  - *inputs:* *list of current input files*
  - *exe:* *executable absolute path*
  - *clargs:* *dictionary of command line flags the user can specify under the <Code> block*
  - *fargs:* *dictionary of command line flags for identifying auxiliary input files that the user can specify under the <Code> block*

# Coupling an Application with RAVEN: createNewInput

- Used to generate an input based on the information that RAVEN s
- This method needs to return a list containing the path and filenames of the modified input files

```
def createNewInput(self,inputs,oinputs,samplerType,**Kwargs):
  (…)
  return newInputFiles
```

Required

- Arguments:
  - *inputs : list of current input files (the one that should be modified)*
  - *oinputs : list of original input files (unperturbed ones)*
  - *samplerTyp: sampler type (e.g. None, MonteCarlo, Grid, etc.)*
  - *Kwargs : dictionary of all the information needed to create an input. Eg:*
    - *executable: executable absolute path*
    - *SampledVars: dictionary of the sampled variables ({'var1":newValue}*
    - *ProbabilityWeight*: float representing the Pb weight of this realization
    - *crowDist*: dictionary containing the info regarding the distributions associated to the variables
    - etc.

# Coupling an Application with RAVEN: finalizeCodeOutput

- This method is called, if present, by RAVEN at the end of each run. It can be used, for example, to convert the whatever Application output format into a CSV
- RAVEN checks if a string is returned
  - RAVEN interprets that string as the new output file root

```
def finalizeCodeOutput(self,command,output,workDir):
  (…)
  return newOutputRoot
```

Optional

- Arguments:
  - *command* : *the command that has been generated by **generateCommand** method*
  - *output* : *the current output root (from **generateCommand** method)*
  - *workDir* : *the current working directory (where the code is currently outputting)*

# Coupling an App with RAVEN: checkForOutputFailure

- Used to check if a run failed even if the *returncode = 0*
- This method is called, if present, by RAVEN at the end of each run.
- It must return a Boolean value. True if failure, False otherwise

```
def checkForOutputFailure(self,output,workDir):
  (…)
  return failure
```

Optional

- Arguments:
  - *output* : *the current output root (from **generateCommand** method)*
  - *workDir* : *the current working directory (where the code is currently outputting)*

# *Practical example*

# Practical example: Simple code I/O overview

- Simple Python code that simulates 4 isotope chain evolutions

**Input File**

```
<AnalyticalBateman>
  <totalTime>10</totalTime>
  <powerHistory>1 1 1</powerHistory>
  <flux>10000 10000 10000</flux>
  <stepDays>0 100 200 300</stepDays>
  <timeSteps>10 10 10</timeSteps>
  <nuclides>
    <A>
        <equationType>N1</equationType>
        <initialMass>1.0</initialMass>
        <decayConstant>1e-08</decayConstant>
        <sigma>6.16193701021</sigma>
        <ANumber>230</ANumber>
    </A>
    <B>
        <equationType>N2</equationType>
        <initialMass>1.0</initialMass>
        <decayConstant>1e-08</decayConstant>
        <sigma>6.16193701021</sigma>
        <ANumber>200</ANumber>
    </B>
    <C>
        <equationType>N3</equationType>
        <initialMass>1.0</initialMass>
        <decayConstant>0.000000005</decayConstant>
        <sigma>45</sigma>
        <ANumber>150</ANumber>
    </C>
    <D>
        <equationType>N4</equationType>
        <initialMass>1.0</initialMass>
        <decayConstant>0.00000008</decayConstant>
        <sigma>3</sigma>
        <ANumber>100</ANumber>
    </D>
  </nuclides>
</AnalyticalBateman>
```

**Text output**

```
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------------------------------------------------------------------------

Input is   : batemanWorkshopInput.xml
Outputs are: results.csv | results.out

------------------------------------------------------------------------
RESULTS:
time         A            C            B            D
0.000000E+00 1.000000E+00 1.000000E+00 1.000000E+00 1.000000E+00
8.640000E+06 9.172273E-01 9.577198E-01 9.711734E-01 1.042627E+00
1.296000E+07 8.784467E-01 9.372549E-01 9.568156E-01 1.063448E+00
1.728000E+07 8.413059E-01 9.172273E-01 9.424941E-01 1.083870E+00
2.592000E+07 7.716687E-01 8.784467E-01 9.140025E-01 1.123975E+00
CPU TIME: 0.00283598899841 s----------------------------------------
SUCCESS
```
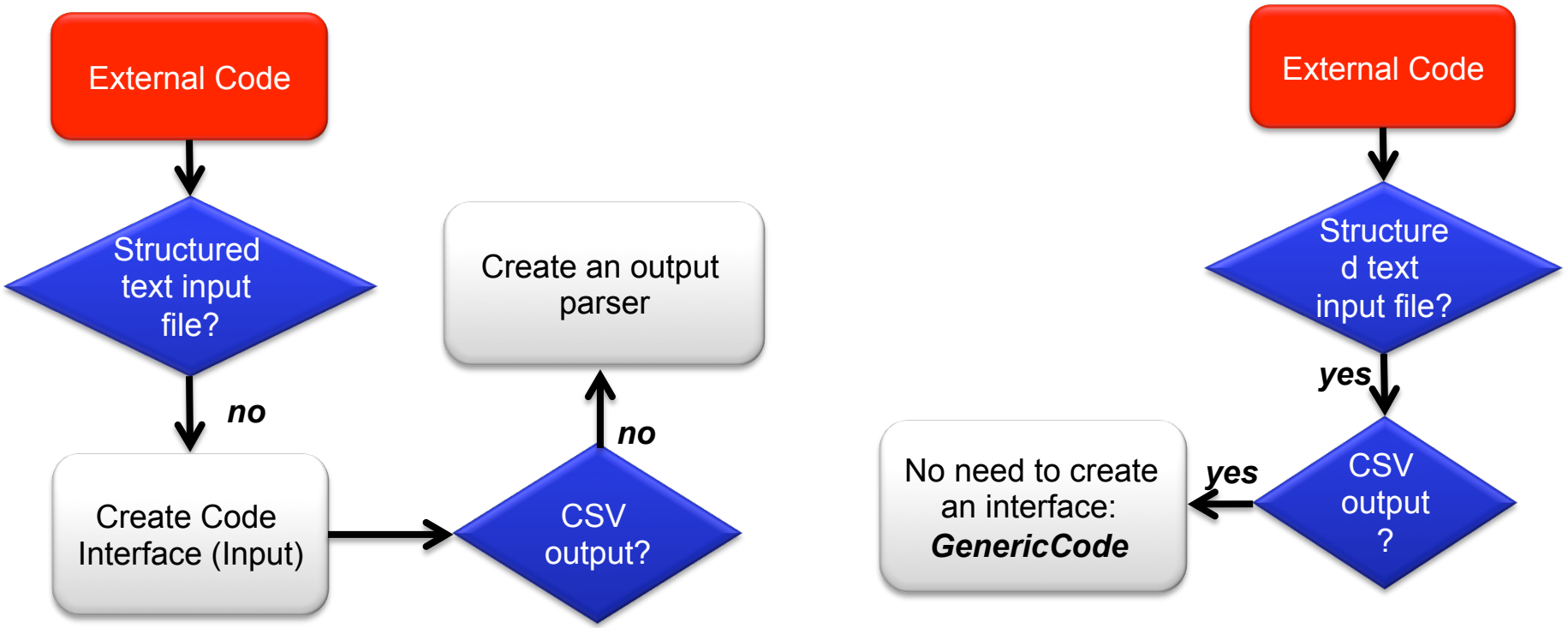

**CSV output**

| time | A | C | B | D |
|---|---|---|---|---|
| 0.00E+00 | 1.00E+00 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| 8.64E+06 | 9.17E-01 | 9.58E-01 | 9.71E-01 | 1.04E+00 |
| 1.30E+07 | 8.78E-01 | 9.37E-01 | 9.57E-01 | 1.06E+00 |
| 1.73E+07 | 8.41E-01 | 9.17E-01 | 9.42E-01 | 1.08E+00 |
| 2.59E+07 | 7.72E-01 | 8.78E-01 | 9.14E-01 | 1.12E+00 |

# Practical example: 2 Examples

- This simple code allows to test two distinct examples:
  1. Creation of a brand new interface (parsing the XML input and the Text Output)
  2. Usage of the *GenericCode* interface since the XML input can be perturbed with “wild-cards” and the code generates already a CSV



*Thank you*

*Questions?*