Lezione 11

Bioinformatica

Mauro Ceccanti[‡] e Alberto Paoluzzi[†]

[†] Dip. Informatica e Automazione – Università “Roma Tre”
[‡] Dip. Medicina Clinica – Università “La Sapienza”

Lezione 10: Gene's 3D structure assembly

- Introduction to PyPlasm
- PyPlasm: some primitives
- New version: double DNA helix
- DNA base pairing
- 3D positioning of a base pair
- 3D structure of a generic DNA strand

Introduzione

in questa lezione calcoleremo la trasformazione di coordinate che deve essere applicata ad un componente di una struttura biologica per posizionarlo correttamente in una struttura più complessa

- L'argomento è di carattere generale, e si può adattare a molti contesti differenti. Lo introdurremo per posizionare una coppia di basi all'interno della doppia elica del DNA

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- Per essere certi della correttezza delle operazioni effettuate, posizioneremo sui "diametri" dell'elica delle stringhe di testo vettoriale che rappresentano i codici (a,t,g,c) delle basi coinvolte. La trasformazione così calcolata potrà essere applicata anche al modello molecolare relativo

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- Nella lezione si introduce anche il linguaggio di programmazione geometrica PLaSM, sviluppato alla Sapienza e a Roma Tre, che stiamo portando in Python, e che utilizzeremo per le operazioni geometrico-grafiche

Sommario

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$$F : Dom_1 \to Dom_2 \to Dom_3 \to Dom_4$$

where

- F returns a function $Dom_1 \to (Dom_2 \to Dom_3 \to Dom_4)$

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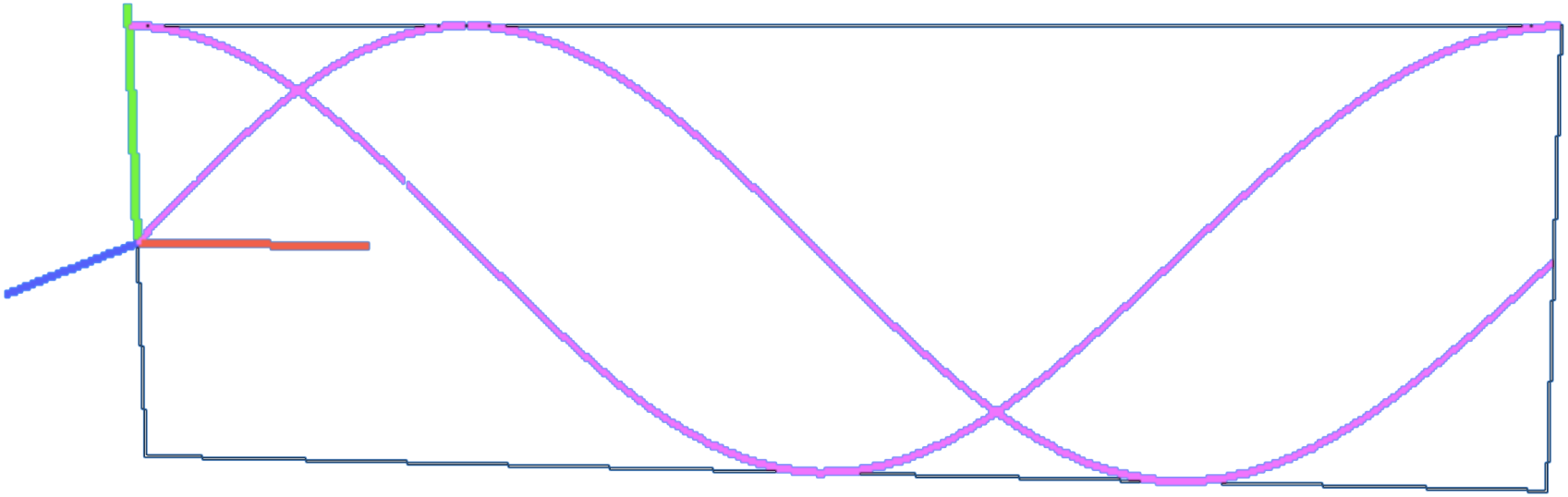
- $F(arg_1)(arg_2)(arg_3)$ returns an object in Dom_4

Introduction to PyPlasm



- f(x) is the application of function f to argument x

```
1  def drawgraph (f):
2      domain = INTERVALS(2*PI)(64)
3      return MAP([ S1, COMP([f,S1]) ])(domain)
4
5  VIEW(drawgraph(SIN))
6  VIEW(STRUCT([ drawgraph(SIN), drawgraph(COS) ]))
```

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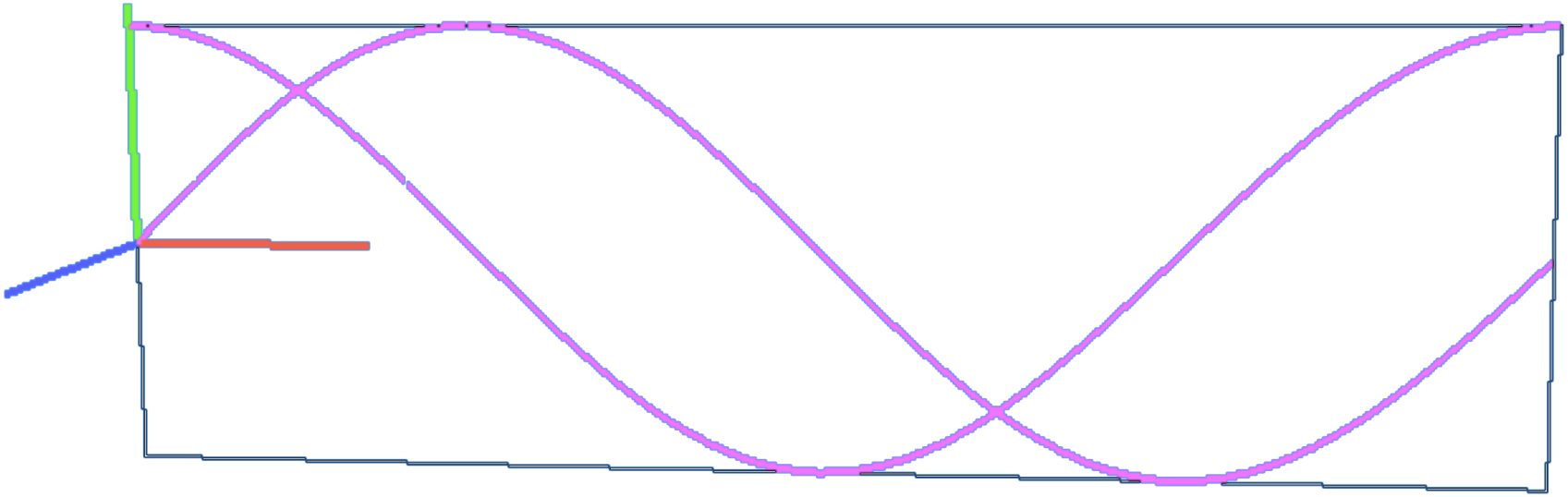

- f(x) is the application of function f to argument x
- STRUCT returns a single geometric value from its list of arguments

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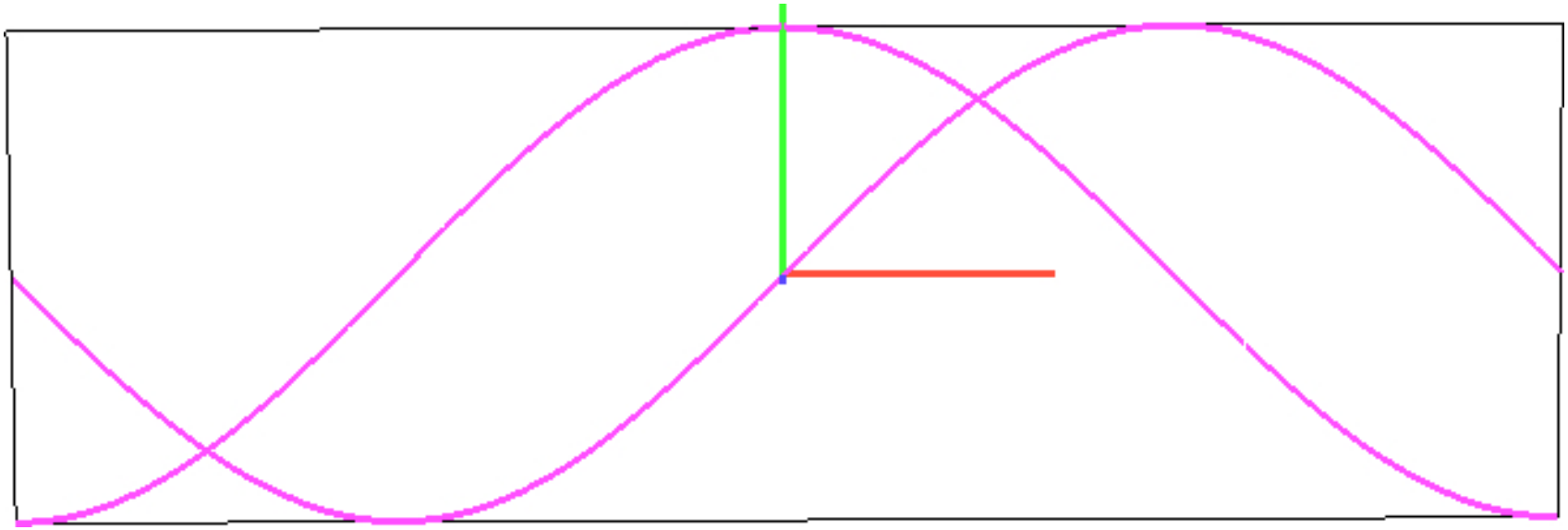

- domain is translated of $-$PI on the first coordinate

```
1  def drawgraph (f):
2      domain = T(1)(-PI)(INTERVALS(2*PI)(64))
3      return MAP([ S1, COMP([f,S1]) ])(domain)
4
5  VIEW(STRUCT([ drawgraph(SIN), drawgraph(COS) ]))
```

Sommario

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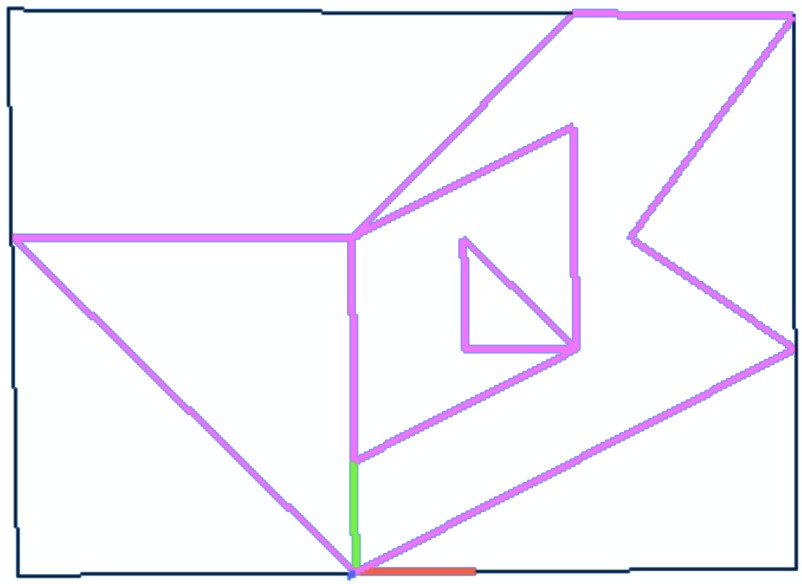
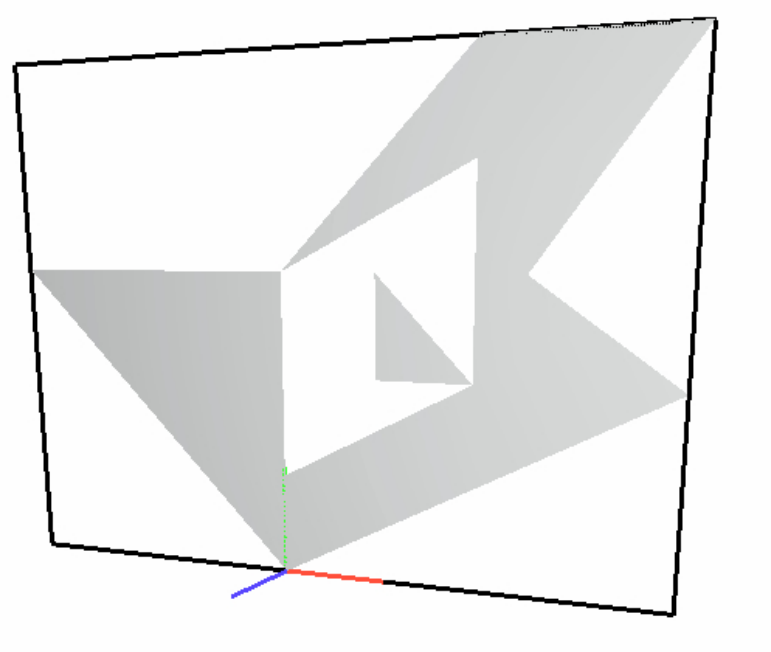
Example: VIEW(XOR([CIRCLE(1)([4,1]), CIRCLE(1)([3,1])]))

PyPlasm: some primitives

Some closed polylines (where $p_1 == p_m$), and the solid polygon they are boundary of

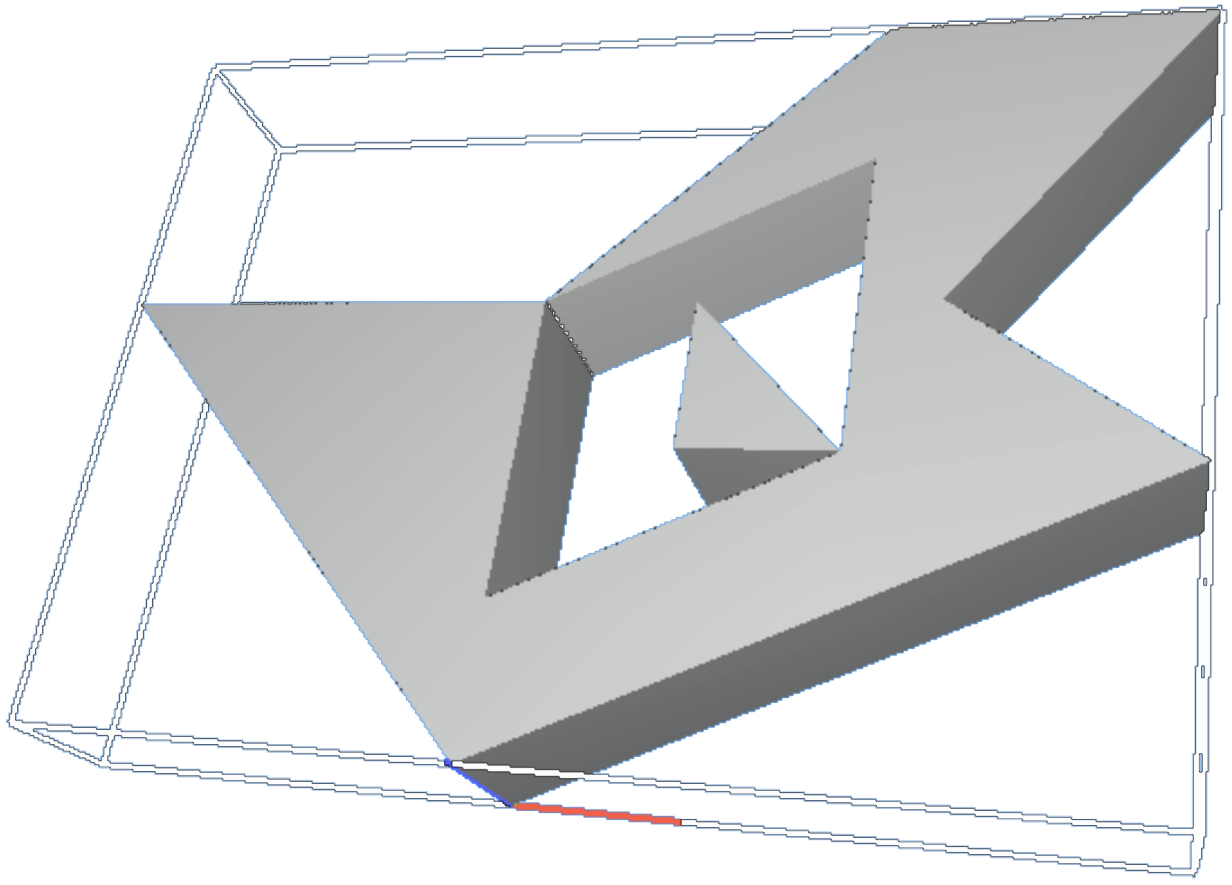




```
1  out = STRUCT( AA(POLYLINE)([
       [[0,0],[4,2],[2.5,3],[4,5],[2,5],[0,3],[-3,3],[0,0]],
        [[0,3],[0,1],[2,2],[2,4],[0,3]],
       [[2,2],[1,3],[1,2],[2,2]] ]))
2
3  VIEW(out)
4  VIEW(SOLIDIFY(out))
```

PyPlasm: some primitives

The Cartesian product of a 2D shape for a 1D interval—in this case Q(1)—produces a 3D shape



```
1 VIEW(PROD([ SOLIDIFY(out), Q(1) ]))
```

Sommario

New version: double DNA helix

- Riprendiamo il modello della doppia elica parametrizzata rispetto a raggio, passo e numero di giri, e lo modifichiamo leggermente per adattarlo all'uso delle primitive Plasm

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- l'attuale implementazione plasm tratta l'insieme dei vertici di un oggetto geometrico come una lista di liste (di coordinate), e non come un array a due indici di coordinate, come fatto in precedenza
- eviteremo dunque di effettuare continue trasformazioni di tipo, riferendoci ovunque possibile alla lista di liste di numeri (le coordinate dei vertici)

New version: double DNA helix

The code is adapted to fit the high-level geometric and graphics primitives of PyPlasm

```
1  from numpy import *
2  from trsxge import *
3
4  def helixPoints(radius,pitch,nturns):
5      c = linspace(0,2*pi*nturns,12*nturns)
6      return map(list, zip( cos(c),sin(c), c*(pitch/(2*pi)
           ) ))
7
8
9  def helix(radius,pitch,nturns):
10     return POLYLINE(helixPoints(radius,pitch,nturns))
11
12
13 VIEW(helix(1,1.5,6))
```

Note: (a) helixPoints returns a list of list ; (b) POLYLINE is UPPER-case

New version: double DNA helix

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doubleHelix returns a STRUCT of 2 p instances

```
1  def doubleHelix(radius,pitch,nturns):
2      p = POLYLINE(helixPoints(radius,pitch,nturns))
3      return STRUCT([p,R([1,2])(PI)(p)])
4
5
6  VIEW(doubleHelix(1,2,4))
```

- The second p instance is rotated of π around the z-axis

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```

- The second p instance is rotated of π around the z-axis
- The rotation tensor R([1,2])(PI) is a higher-level function (is appled more than one time to different arguments; every application returns a function)

New version: double DNA helix

The code is adapted to fit the high-level geometric and graphics primitives of PyPlasm

```
1  def dnaStructure(radius,pitch,nturns):
2      p = helixPoints(radius,pitch,nturns)
3      q = (matrix(p) * matrix([[-1,0,0], [0,-1,0],
           [0,0,1]])).tolist()
4      diameters = TRANS([p,q])
5      return STRUCT( AA(POLYLINE)(diameters) + [POLYLINE(p
           ), POLYLINE(q)] )
6
7  VIEW(dnaStructure(1,2,4))
```

AA (second-order function) stands for Apply−to−All:

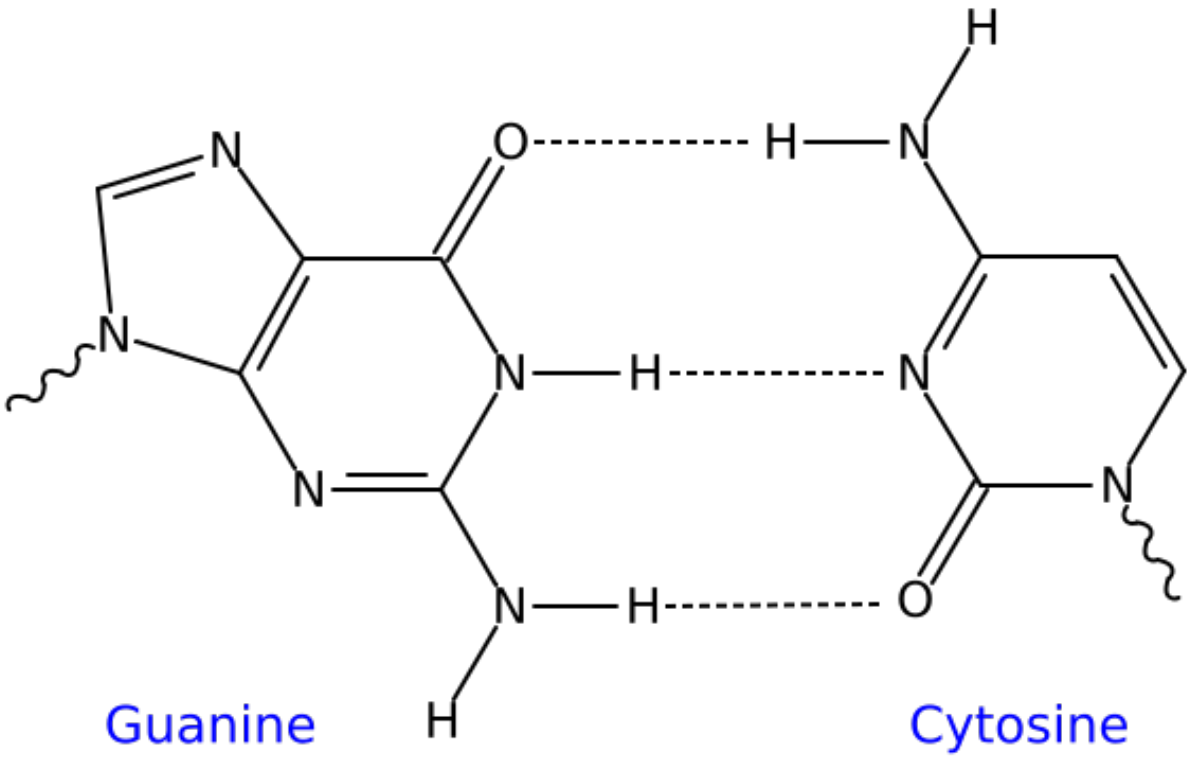
$AA(f)([x_1, x_2, ..., x_m]) \equiv [f(x_1), f(x_2), ..., f(x_m)]$

It has the same semantics of the Python's map(f, $[x_1, x_2, ..., x_m]$)

Sommario

DNA base pairing

We know that two nucleotides on opposite complementary DNA or RNA strands that are connected via hydrogen bonds are called a base pair



So, let define a set of allowed pairs

basepairs =[[’a’,’t’],[’t’,’a’],[’g’,’c’],[’c’,’g’]]

DNA base pairing

We write a simple filtre to produce the sequence of base pairs associated to a DNA strand

```
1  strand = 'atgaaaatgaataaaagtctcatcgtcc'
2
3  def doublestrand (strand):
4      bases = ['t','a','g','c']
5      basepairs =[['a','t'],['t','a'],['g','c'],['c','g']]
6      return [[a,b] for a in strand for b in bases if [a,b
           ] in basepairs]
7
8  doublestrand(strand) ≡
9  [['a','t'],['t','a'],['g','c'],['a','t'],['a','t'],['a',
       't'],['a','t'],['t','a'],['g','c'],['a','t'],['a','t'
       ],['t','a'],['a','t'],['a','t'],['a','t'],['a','t'],[
       'g','c'],['t','a'],['c','g'],['t','a'],['c','g'],['a'
       ,'t'],['t','a'],['c','g'],['g','c'],['t','a'],['c','g
       '],['c','g']]
```

REMARK: We use a List Comprehension construct, with a doubly-nested cycle to select the only allowed base pairs

Sommario

3D positioning of a base pair

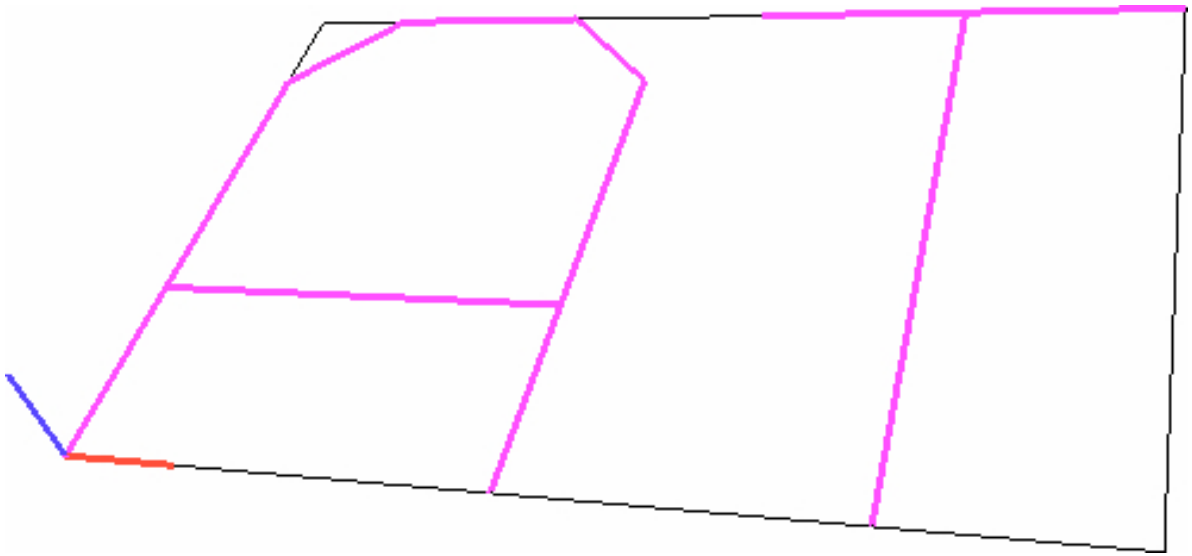
A vector text string is generated in the $z = 0$ plane

```
1  def TEXT:  ... return hpc
2  VIEW(TEXT('AT'))
3
4  def TEXTWITHATTRIBUTES (TEXTALIGNMENT, TEXTANGLE,
       TEXTWIDTH, TEXTHEIGHT, TEXTSPACING):
5  ... return hpc
6
7  VIEW(TEXTWITHATTRIBUTES('centre',0,0.5,1.0,0.125)('AT'))
8  VIEW(R([2,3])(PI/2)(TEXTWITHATTRIBUTES('centre',0,0.5,
       1.0,0.125)('AT')))
```

In (8) the resulting geometric object is rotated in the $y = 0$ plane via the rotation tensor R([2,3])(PI/2)

3D positioning of a base pair

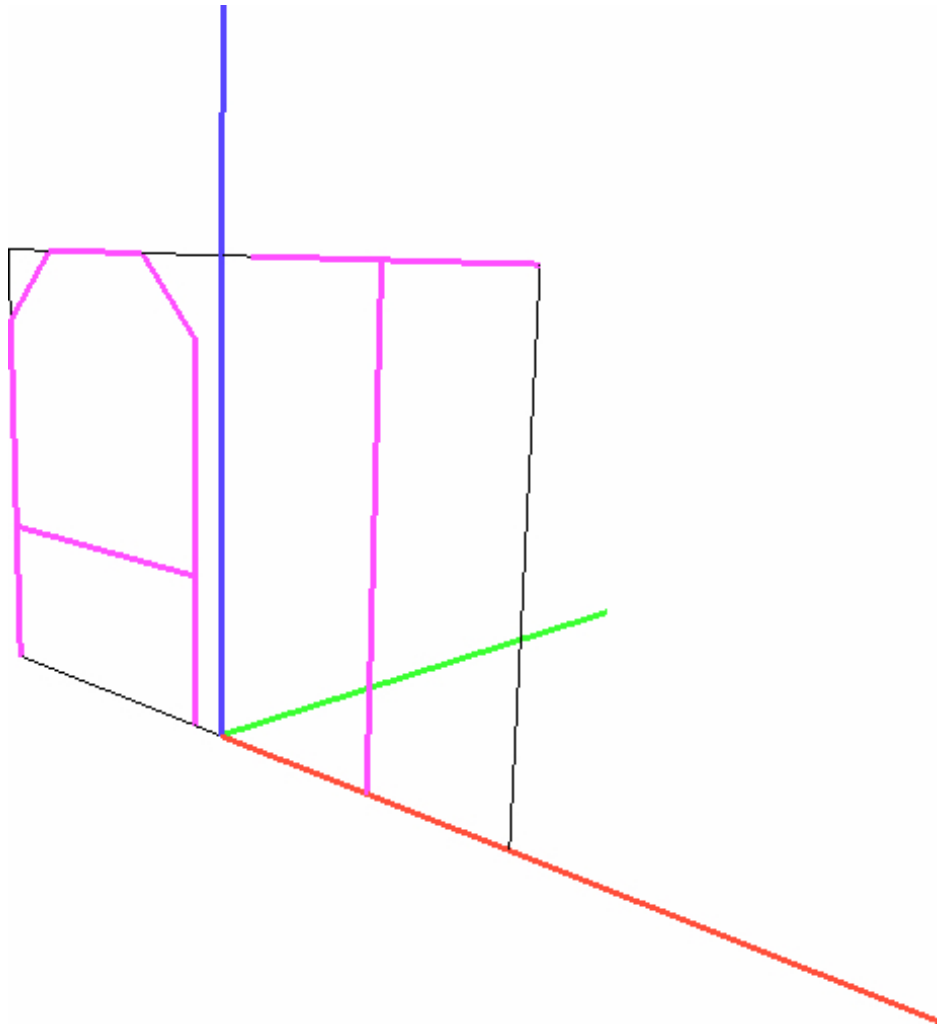
A vector-text string is generated in the $z = 0$ plane. The native dimensions of caracters of the vector font are pretty big



VIEW(TEXT('AT'))

3D positioning of a base pair

A vector-text string is generated in the $z = 0$ plane and rotated in the $y = 0$ plane



R([2,3]) (PI/2) (TEXTWITHATTRIBUTES('centre',0.0,0.5,1.0,0.125)('AT'))

3D positioning of a base pair

The function `return` the text string transformed and translated in its proper 3D space position

In particular, we compute the affine transformation from the standard position seen above, to the proper space position of each base pair

- input data: $p_1, q_1 \in strand_1$, $p_2 \in strand_2$

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TRANSF to bring $\mathbf{e}_1$ to $\mathbf{r}_1$, $\mathbf{e}_2$ to $\mathbf{r}_2$, and $\mathbf{e}_3$ to $\mathbf{r}_3$,
where $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are the standard basis of $\mathbb{E}^3$, and

$$\mathbf{r}_1 = \mathbf{p}_2 - \mathbf{p}_1, \quad \mathbf{r}_2 = \mathbf{q}_1 - \mathbf{p}_1, \quad \mathbf{r}_3 = \mathbf{r}_1 \times \mathbf{r}_2$$

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TRANSL to bring the origin to point $\mathbf{p}_m = (\mathbf{p}_1 + \mathbf{p}_2)/2$ of diameter

3D positioning of a base pair

The function **return** the text string transformed and translated in its proper 3D space position

clearly we must have

$$\mathbf{Q}\begin{bmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{r}_1 & \mathbf{r}_2 & \mathbf{r}_3 \end{bmatrix}$$

so that, in homogeneous coordinates, we have:

$$\mathbf{Q} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \mathbf{0} & \mathbf{r}_1 & \mathbf{r}_2 & \mathbf{r}_3 \end{bmatrix}.$$

If we include the translation, the desired transformation becomes:

$$\bar{\mathbf{Q}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \mathbf{p}_m & \mathbf{r}_1 & \mathbf{r}_2 & \mathbf{r}_3 \end{bmatrix},$$

where $\mathbf{p}_m = (\mathbf{p}_1 + \mathbf{p}_2)/2$.

3D positioning of a base pair

The function **return** the text string scaled, rotated and translated in its proper 3D space position

```
1  def basepair (args):
2      """ p1,p2,q1 are 3D points, pair a two-letter string
3      returns a geometric value """
4      p1,p2,q1,pair = args
5      pm = SCALARVECTPROD([ SUM([p1,p2]), 0.5 ])
6      t = T([1,2,3])(pm)
7      q2 = UNITVECT(DIFF([p1,pm]))
8      q3 = [q2[1], -q2[0], 0]
9      w = [0,0,1]
10     sizex, sizez = VECTNORM(q2)/4, VECTNORM(q3)/2,
11     obj = TEXTWITHATTRIBUTES('centre',0.0,sizex,
12           sizez,sizex/16)(''.join(['__',pair[0],'__',
                 pair[1],'__']))
13     return (t(MAT(INV(MATHOM([q2,w,q3])))(obj)))
```

Sommario

3D structure of a generic DNA strand

Here we give yet another version of the dnaStruct function, where the number of turns of each helix is determined by the length of the DNA strand, and where each basepair symbol is properly located in 3D space

In the following dnaStruct(radius,pitch)(strand) implementation, we introduce some variations w.r.t. the previous version:

- n = len(strand) is the number of basepairs in the input strand

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- n = len(strand) is the number of basepairs in the input strand
- basepairs is the list of pairs of strings to be transformed into vector text
- map(basepair, zip(p[:−1],q[:−1],p [1:], basepairs)) apply the proper *string* $\rightarrow$ *text* transformation to each tuple of properly aligned points (and symbols) from the two helices p and q (and from the basepairs list of symbols)

3D structure of a generic DNA strand

We give here a function of second order, that must by first applied to the 2 intrinsic scaling factors of the structure (radius, pitch), and then to the DNA strand to be modeled, given as a string. From the programming viewpoint, notice how a higher-level function is structured: is returns either partial functions or the final value

```
1  def dnaStruct(radius,pitch):
2
3      def dna (strand):
4          n = len(strand)
5          p = helixPoints(radius,pitch,n/12)
6          q = (matrix(p) * matrix([[-1,0,0], [0,-1,0],
               [0,0,1]])).tolist()
7          basepairs = doublestrand(strand)
8          basepairs3D = map(basepair, zip(p[:-1],q[:-1],p
               [1:],basepairs))
9          return STRUCT(basepairs3D + [POLYLINE(p),
               POLYLINE(q)])
10
11     return dna
12
13 VIEW(dnaStruct(1,4)(strand))
```

3D structure of a generic DNA strand

```
1 strand = 'acagtaacacactctgttaacctt'
2
3 doublestrand(strand) = [['a', 't'],
      ['c', 'g'], ['a', 't'], ['g', 'c
      '], ['t', 'a'], ['a', 't'], ['a'
      , 't'], ['c', 'g'], ['a', 't'],
      ['c', 'g'], ['a', 't'], ['c', 'g
      '], ['t', 'a'], ['c', 'g'], ['t'
      , 'a'], ['g', 'c'], ['t', 'a'],
      ['t', 'a'], ['a', 't'], ['a', 't
      '], ['c', 'g'], ['c', 'g'], ['t'
      , 'a'], ['t', 'a']]
4
5 VIEW(dnaStruct(1,4)(strand))
```