Teaching computational physics without scrambling physics?

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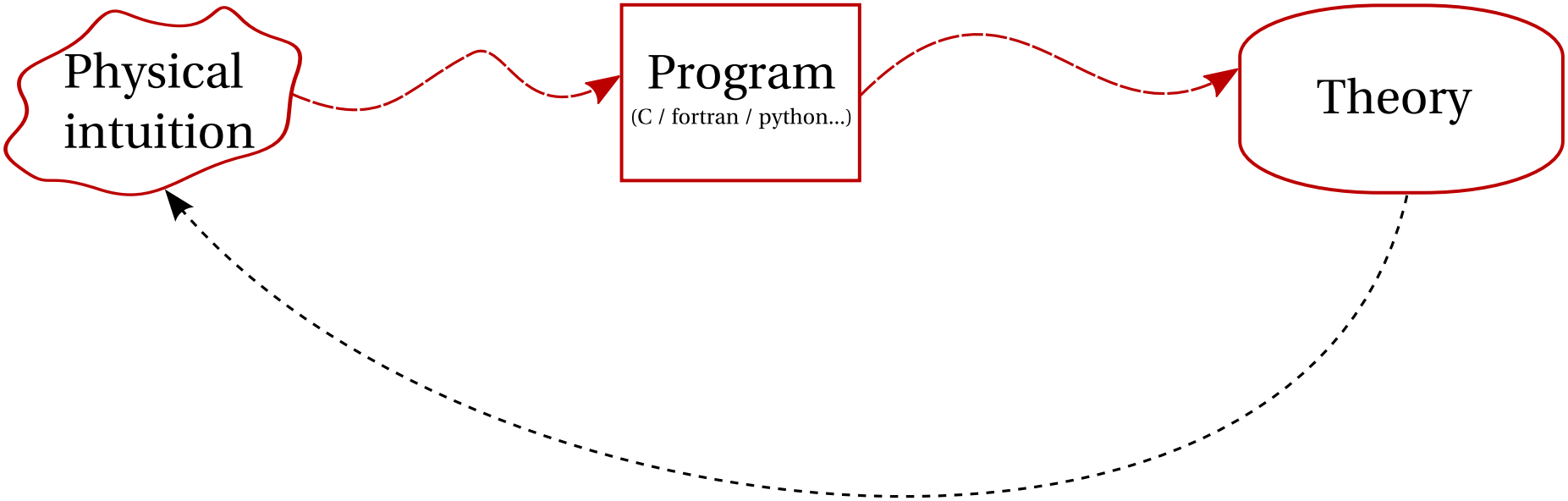
Computational Physics

From intuition to understanding



Computational Physics

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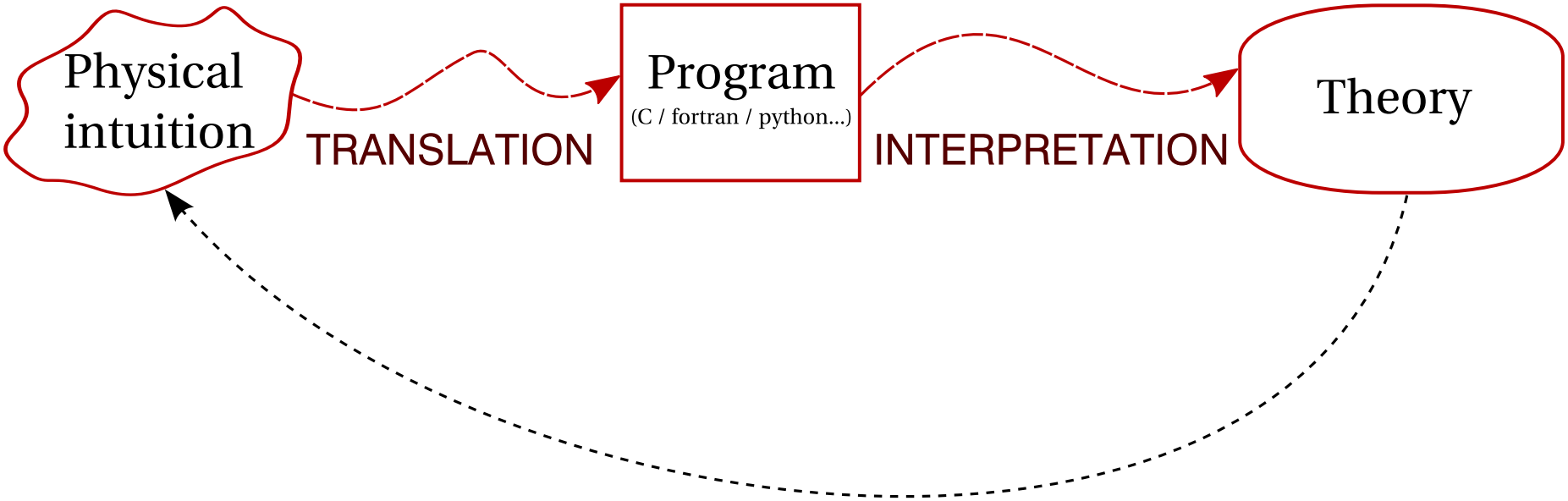

Computational Physics

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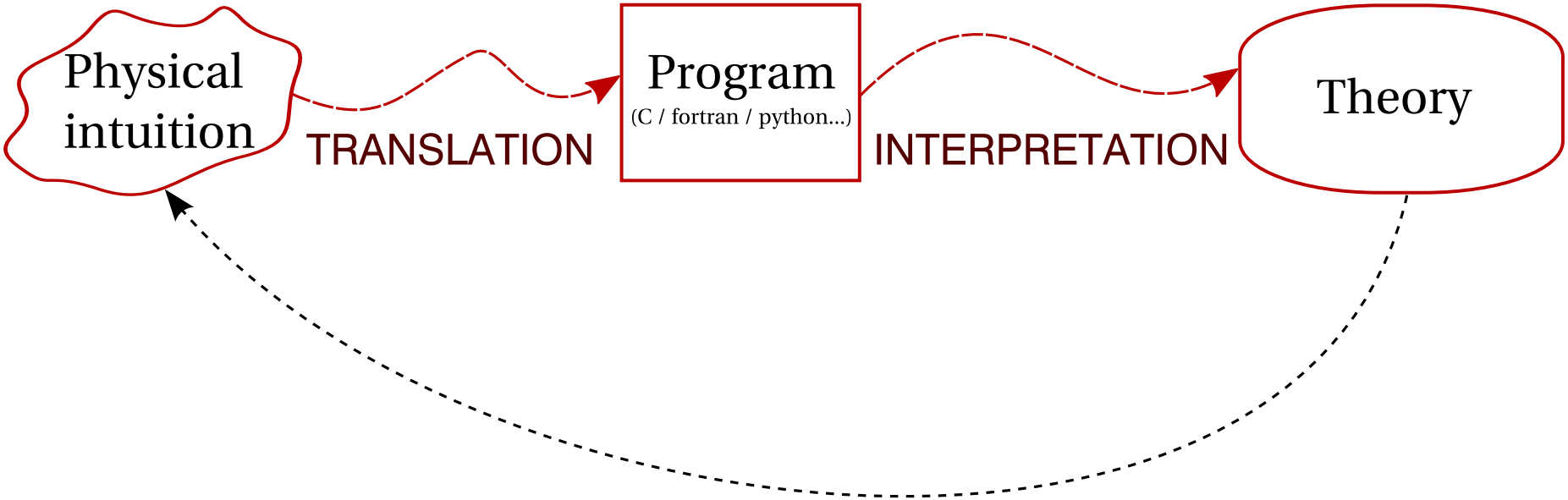

How can you teach this?

Automatic translation?

Automatic translation?

la vigilancia de la Isla.
El Faro de Isla Magdalena es visitado por los viajeros que se aventuran a estas latitudes. Continúa ayudando a la navegación, ofreciendo una luz cuyo rango alcanza las diez millas náuticas.

ISLA MAGDALENA

Situada a 25 millas al norte de Punta Arenas, en pleno Estrecho de Magallanes, Isla Magdalena es un reducto natural de pingüinos magallánicos, cormoranes y otras aves, que coexisten pacíficamente con lobos marinos. Allí encontraremos, en un espectáculo que impresiona, a más de 60 mil parejas de pingüinos, que vuelven a anidar año tras año a las mismas cuevas que ellos construyeron. Entre octubre y marzo, la mayoría de ellos se encuentran visibles, ocupando toda la isla, lo que la convierte en un paisaje único e incomparable. Es posible recorrer la isla a través de un sendero demarcado que conduce hasta un faro, el cual posee en su interior una exposición con fotografías y explicaciones sobre la fauna marina del Estrecho de Magallanes.

the personnel in charge of the alertness of the Island. Isla Magdalena's Faro is visited by the travelers who risk to these latitudes.

ISLAND SPONGE-CAKE

Placed to 25 miles to the north of Top Sands, in full Strait of Magellan, Isla Magdalena is a natural redoubt of penguins magallánicos, cormorants and other birds, which coexist pacifically with marine wolves. There we will find, in a spectacle that impresses, more than 60 thousand pairs(couples) of penguins, who return to nest year after year to the same caves that they constructed. Between October and March, the majority of they they are visible, occupying the whole island, which turns her into the only(unique) and incomparable landscape. It is possible to cross the island across a limited path that he(she) leads up to a beacon, which possesses in his(her,your) interior an exhibition with photographies and explanations on the marine fauna of the Strait of Magellan.

ıncia de Magallanes

Automatic translation? NOT YET AVAILABLE

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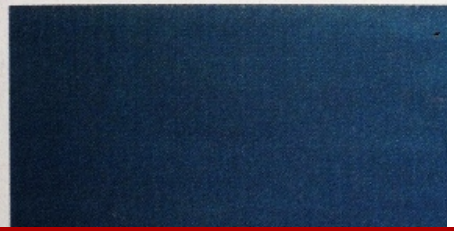


También podrá llegar por un hermoso sendero de excursión que visita restos de antiguas minas de carbón y atraviesa distintas etapas del bosque magallánico o por un circuito de bicicletas de montaña que se combina con la telesilla.

Also it(he,she) will be able to come for a beautiful path of excursion that visits remains of former mines of coal and crosses different stages of the forest magallánico or for a circuit of bicycles of mountain that is combined by the telesilla.

ESTANCIA RIO DE LOS CIERVOS

En el Km. 5,5 sur está la Estancia Río de los Ciervos. Su casa patronal, de la década de 1900, ha sido acondicionada como restaurante, con quincho para asados al palo, donde se prepara un rico salmón ahumado. Además, ofrece senderos de trekking, arriendo de caballos y cabalgatas guiadas a la laguna Lynch y al Cerro Mirador.

STAY I LAUGH AT THE DEER

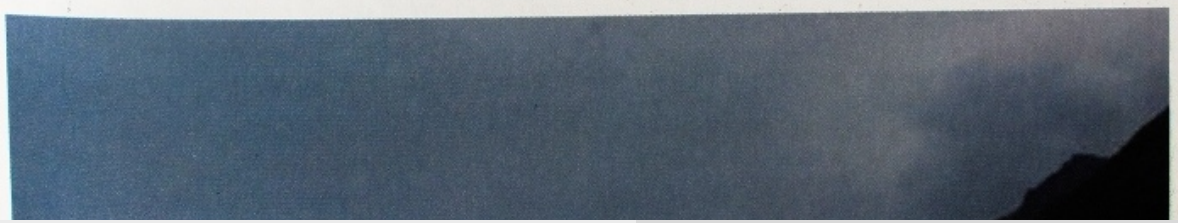
In the km 5,5 south the Stay is Rio of the Deer. His(her,your) employer(management) house, of the decade of 1900, has been conditioned as restaurant, with quincho for roasts to the stick(wood), where a rich smoked salmon is prepared. In addition, it(he,she) offers paths of trekking, I hire of horses and cavalcades guided to the lagoon Lynch and to the Hill Viewing-point.

AGUA FRESCA

Jineteadas y comidas típicas.

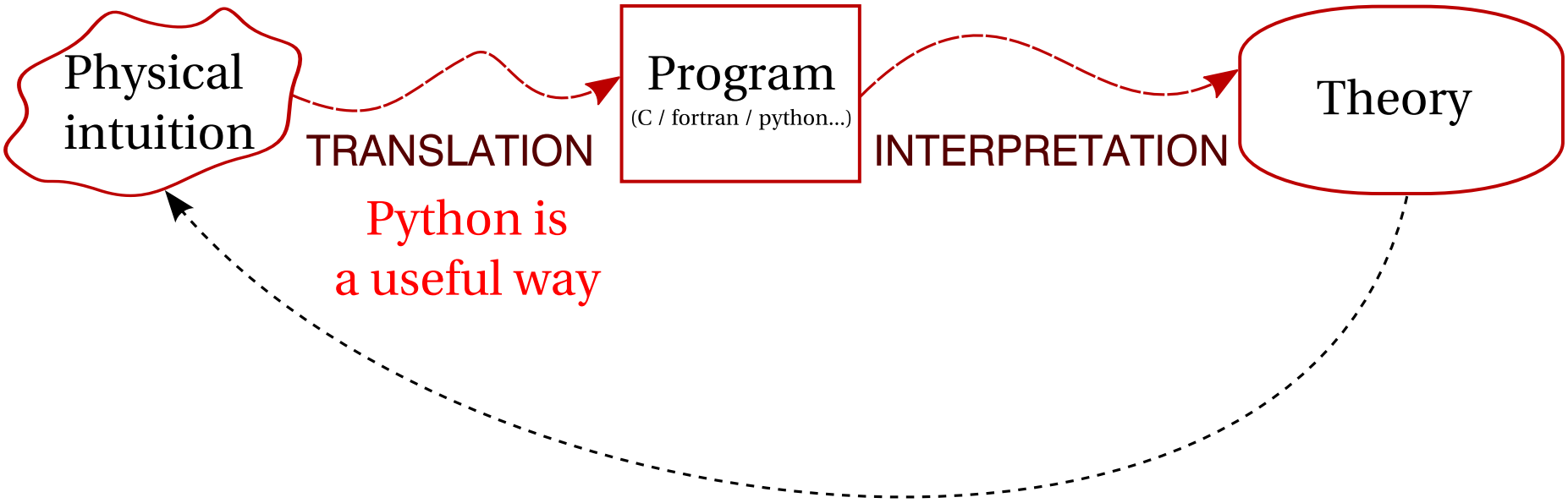
COLD WATER

Horse-breakings and show restraint typical.



Computational Physics

From intuition to results



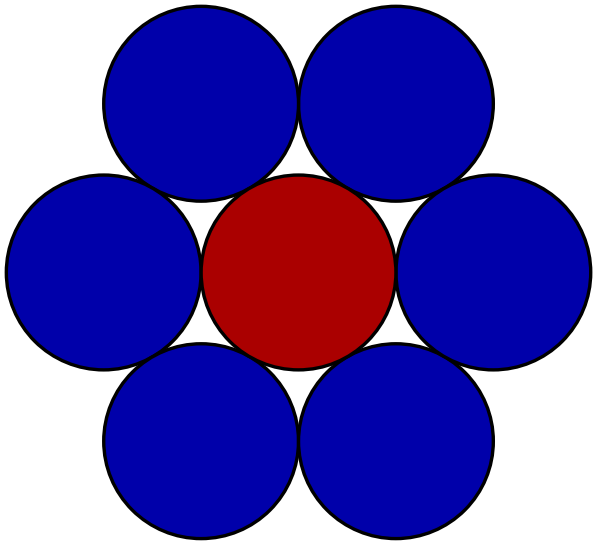
An example:

Computational Physics Lectures (W. Krauth) at 'Fundamental Concept of Physics' Master 2, ENS

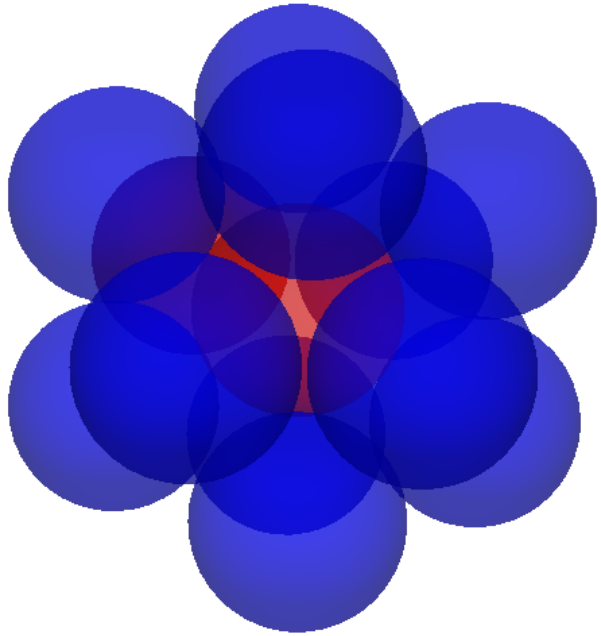
Web site: **`http://cours-physique.lps.ens.fr`**

(practical exercices by A. Rosso, VL)

A problem by Gregory and Newton



Six unit disks packed around a unit disk.
No space is left.



Twelve unit outer spheres packed around a unit inner sphere.

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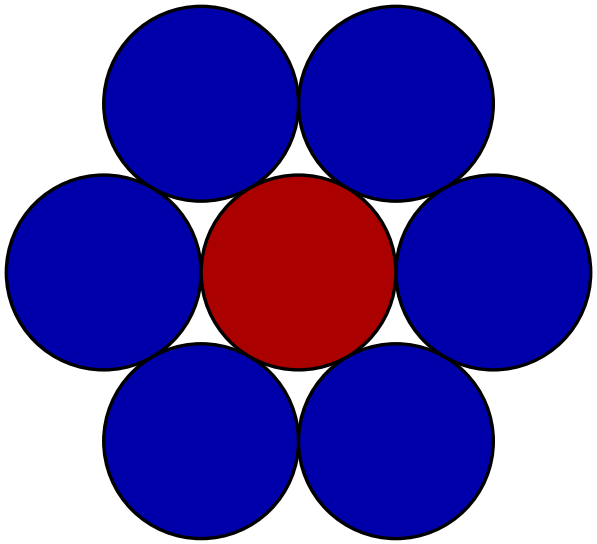

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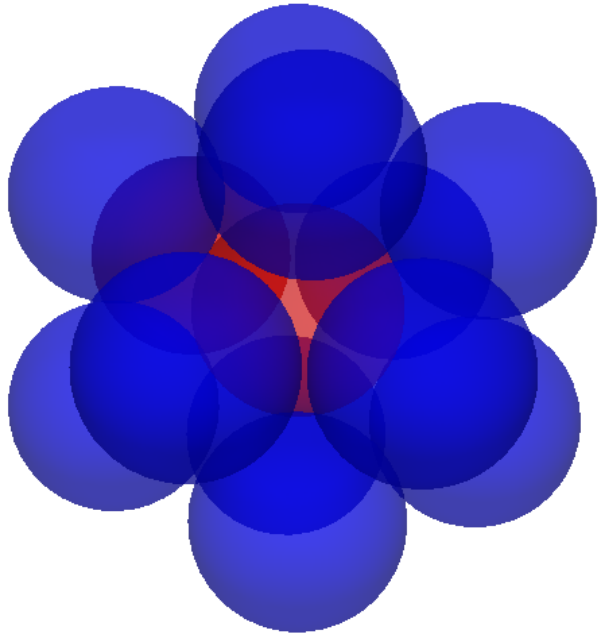

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Is that enough for a 13th sphere?

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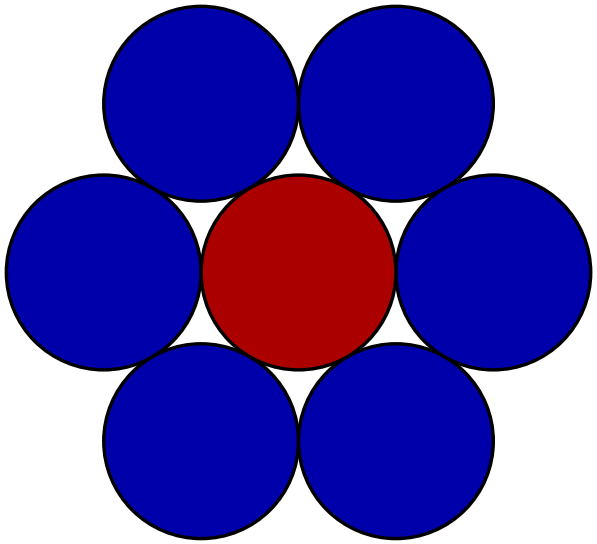

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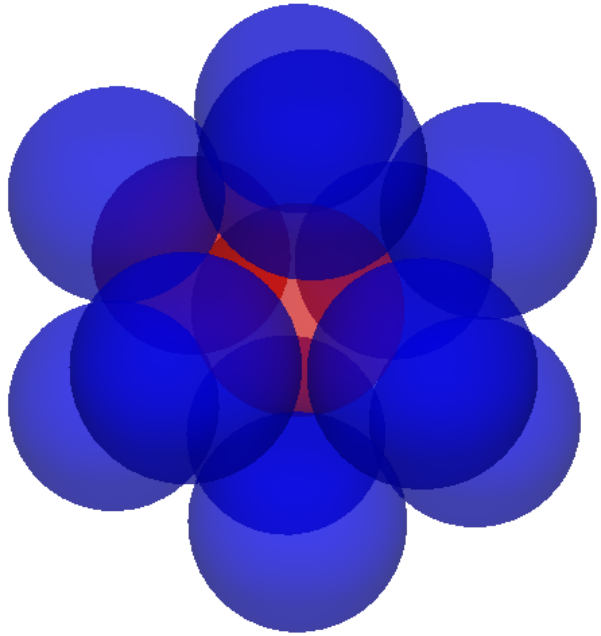

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Space is left.
Is that enough for a 13th sphere?

Newton guessed that this was not possible.
The proof came only in 1953 (Schütte and van der Waerden).

A related problem: packing spheres on a sphere

Exercice:

- Determine the maximal radius R of N spheres that we would like to pack around a sphere of unit radius.
- It happens that for $N = 13$ this maximal radius R is < 1.
- Its determination and the determination of a/the optimal configuration is a complex *optimization problem*.
- We examine some solutions inspired by statistical mechanics.

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Naive answers:

- Direct sampling: sample N points on the surface of the unit sphere. The sample is rejected until the spheres do not overlap.
- Monte-Carlo: move N points, preserving detailed balance wrt the uniform measure on the sphere, until the spheres do not overlap.

Both work. Very slowly.

Simulated annealing

In words:

- “Shake the system while decreasing temperature until it reaches a minimum.”
- Start from N non-overlaping spheres of low radius.
- Shake: apply Monte-Carlo steps.
- Increase the radius.

Simulated annealing – Python code (i)

```
import random, math, numpy
N=13;r=.25;R=1./(1./r-1.);tmax=200000;sig=.25;gamma=0.05;random.seed(137)
#Initialisation
test=True
while test:
    positions=[unif_sphere() for j in range(N)]
    if allowed(positions): test=False
#Moves
count=0
for t in range(tmax):
    k=random.randint(0,N-1)
    newpos=[positions[k][0]+random.gauss(0,sig),positions[k][1]+random.ga
    norm= math.sqrt(sum(xk**2. for xk in newpos))
    newpos=[xk/norm for xk in newpos]
    if allowed_move(positions,k,newpos):
        positions=positions[:k]+[newpos]+positions[k+1:]
        count+=1
    if t%100==0:
        dists=[]
        for l in range(N):
            dists.extend([dist(positions[k],positions[l]) for k in range(l)
        Upsilon=min(dists)/2.
        r=r+gamma*(Upsilon-r)
```

Simulated annealing – Python code (ii)

```
def dist(a,b): return math.sqrt((b[0]-a[0])**2+(b[1]-a[1])**2+(b[2]-a[2])
def allowed(positions):
    dists=[]
    for l in range(N):
        dists.extend([dist(positions[k],positions[l]) for k in range(l)])
    return min(dists)>2*r
def allowed_move(positions,k,newpos):
    dists=[dist(positions[l], newpos) for l in range(k)+range(k+1,N)]
    return min(dists)>2*r
def unif_sphere():
    sigma=1./math.sqrt(3.)
    x=[random.gauss(0,sigma) for i in range(3)]
    norm= math.sqrt(sum(xk**2. for xk in x))
    return [xk/norm for xk in x]
```

Simulated annealing – A refinement

Adapt the variance σ of the Gaussian distribution in Monte Carlo tentative moves:

Divide σ by 2 any time the acceptance rate becomes lower than a threshold.

Simulated annealing – A refinement

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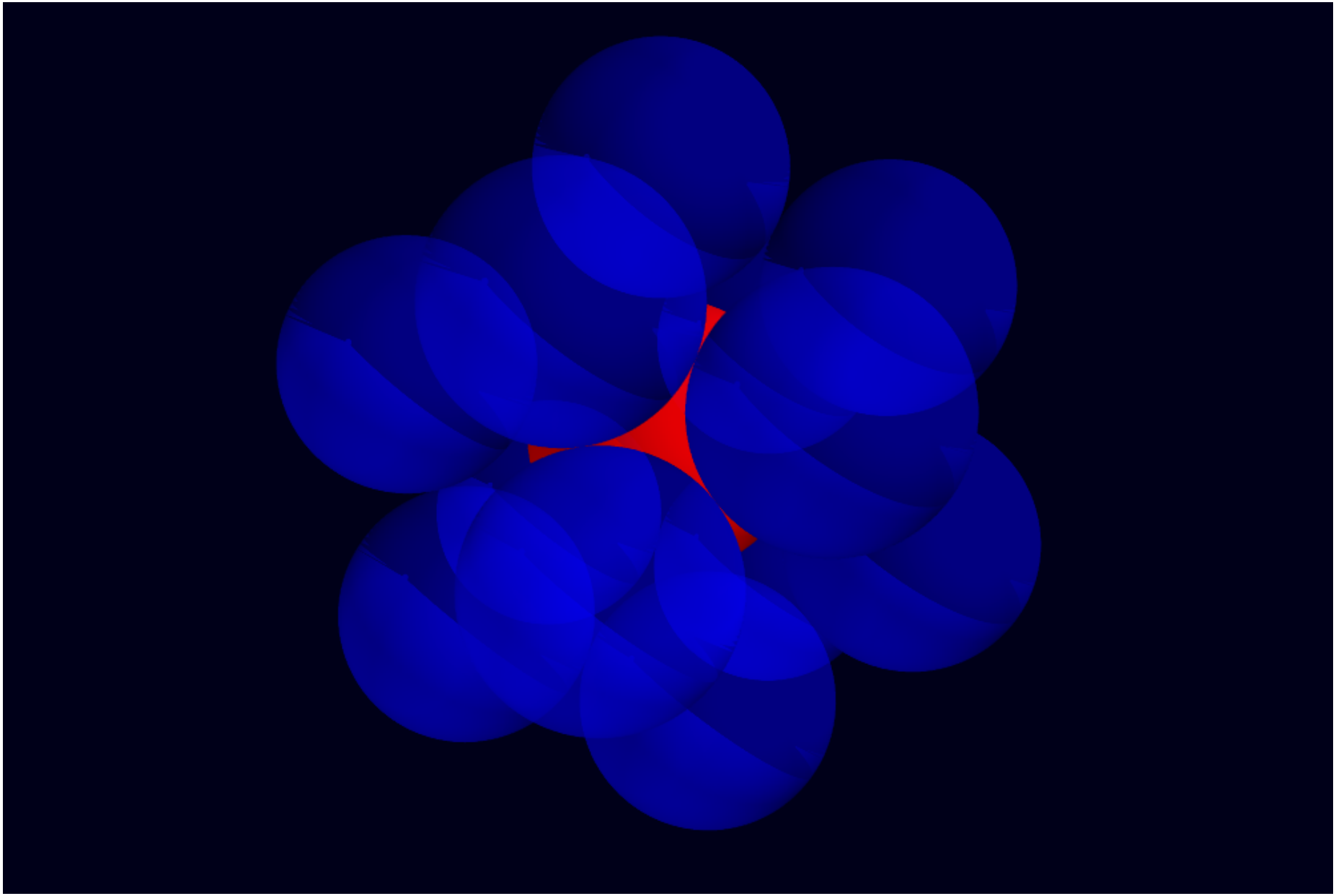
    norm= math.sqrt(sum(xk**2. for xk in newpos))
    newpos=[xk/norm for xk in newpos]
    if allowed_move(positions,k,newpos):
        positions=positions[:k]+[newpos]+positions[k+1:]
        count+=1
    if t%100==0:
        accept=count2/100.
        if accept<.2: sig=sig/2
        count=0
        dists=[]
        for l in range(N): dists.extend([dist(positions[k],positions[l])
        Upsilon=min(dists)/2.
        r=r+gamma*(Upsilon-r)
```

We reach a configuration with R=0.9164678249 in a few seconds



References:

- Schütte K. und van der Waerden B. L., *Das Problem der dreizehn Kugeln*, Mathematische Annalen 125, 325 (1953)
- Krauth W., *Statistical Mechanics Algorithms and Computations*, Cambridge University Press (2006)
- Web site of the Master 2 course *Computational Physics*: **`http://cours-physique.lps.ens.fr`**

Thank you for your attention!

3d visualisation: mayavi

```
from mayavi.mlab import points3d,show,figure
figure(bgcolor=(0,0,.1),size=(1000, 700))
m=1.+R
x,y,z=[m*pos[0] for pos in positions],[m*pos[1] for pos in positions],[m*
rad=[2*R for pos in positions]
x.append(0);y.append(0);z.append(0);rad.append(2)
points3d(x,y,z, rad, scale_factor=1, resolution=100,transparent=True)
show()
```