Science of 21 Century and the Computational Methods
H.Sugawara,2004

Computational Methods

1.realizing the natural data on the computer→discover the law
  this is basically the data handling method in,for example,

- experimental physics
- bio-informatics

2.simulate the data based on primary law(QCD)→secondary law
(nuclear force)

  I will discuss the second case in three examples.
 1.QCD→hadron physics,nuclear physics
  2.quantum gravity→early universe
  3.physical law→simple biological system

In all cases we have to be able to create the object(early universe or simple life form in cases 2 or 3 respectively)to claim the full understanding

Successes of QCD
- from point of view of physical principles:
  unified description of short to long scales within a single theory
  (asymptotic freedom and confinement)
- in terms of understanding hadron phenomena:
  1. Understanding the hadron spectrum
  2. Determination of the fundamental short distance parameters
     strong coupling constant, quark masses
     (unexpectedly small strange quark mass)
  3. physical properties of high-temperature quark-gluon plasma
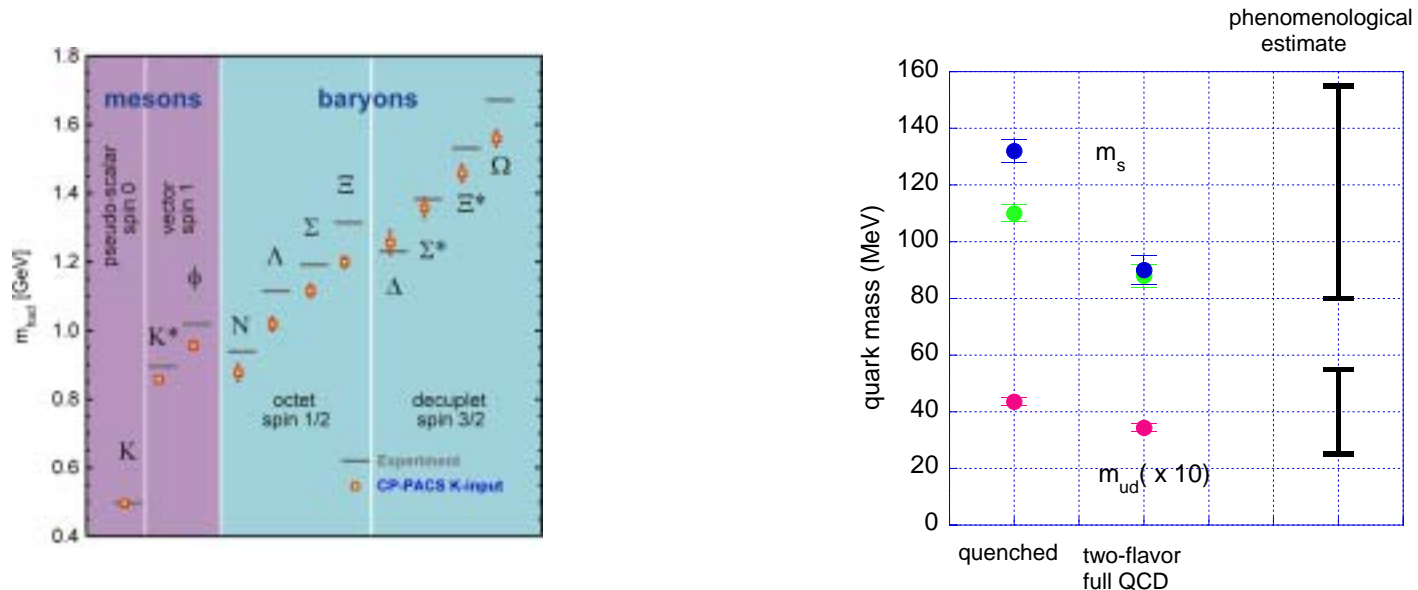
Remaining important tasks in QCD

1. Truly realistic QCD simulation (attempts now underway)
- dynamical up, down, strange quark
- Chiral symmetry(domain-wall/overlap fermion)

2. Are there still some surprises in hadron physics?
- 5-quark system
- heavy quark system
- quark gluon plasma at very high density(color superconductivity?)

3. Nuclear physics
- Can we justify the shell model,collective motions etc.etc.?
- How does nuclear force change with quark mass?? etc
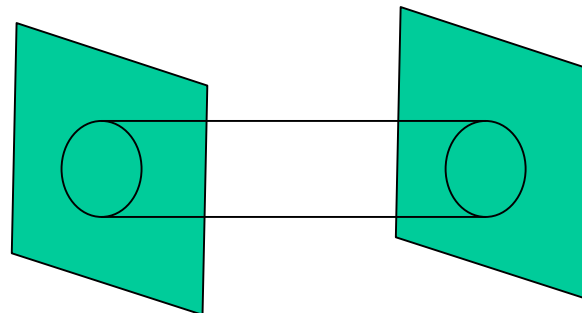
- We need >100Tflops machine

Quantum gravity
- 4-dimensional quantum gravity does not exist as a consistent
 theory!
- Many ideas ,such as the topology change in the early universe
 are at best dubious.

We must work within the framework of string
theory to understand the beginning of the
universe(10 dimension)

Most important property of string theory
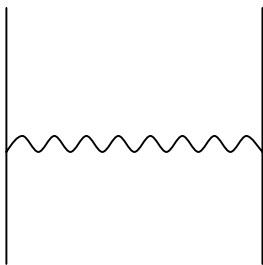
Particle exchange

(closed)string exchange

There are two ways to look at the string diagram
1. Exchange of closed string
2. Pair creation of open strings which have the end
    points on the branes

•Closed string theory is equivalent(dual) to
 open string theory with Dirichlet boundary
 conditions
•Gravity is universal➔Everything has the dual
 picture

Quantum gravity calculation is equivalent to
Open string calculation(gauge particle)

Gravitational force$\rightarrow$Casimir energy
of gauge theory(SU(N),N$\rightarrow\infty$)

Week gravity$\rightarrow$strong gauge coupling

Necessity of computer simulation

<u>4dimensional QCD</u>
renormalizable

<u>4dimensional gravity</u>
Non-renormalizable
(inconsistent as a quantum theory)

<u>10dimensional string</u>
Renormalizable(finite)

↓

2dimensional manifold

Given topology(genus)→
Geometry is unique up to
diffeomorphism

<u>11dimensional membrane</u>
__??

↓

3dimensional manifold
• Topology
• Geometry
Given topology→geometry may
be Unique(S3,E3,H3,sol,nil,
SL(2,R),S2xS1,H2xS1)
----Thurston conjecture----

Physical law→simple biological system

1. Complete 3dimensional structure of
* RNA---------4**N
* DNA---------4**N
* Protein-------20**N

N is over 10**5

 almost impossible and maybe not needed

2.Understanding of Central Dogma
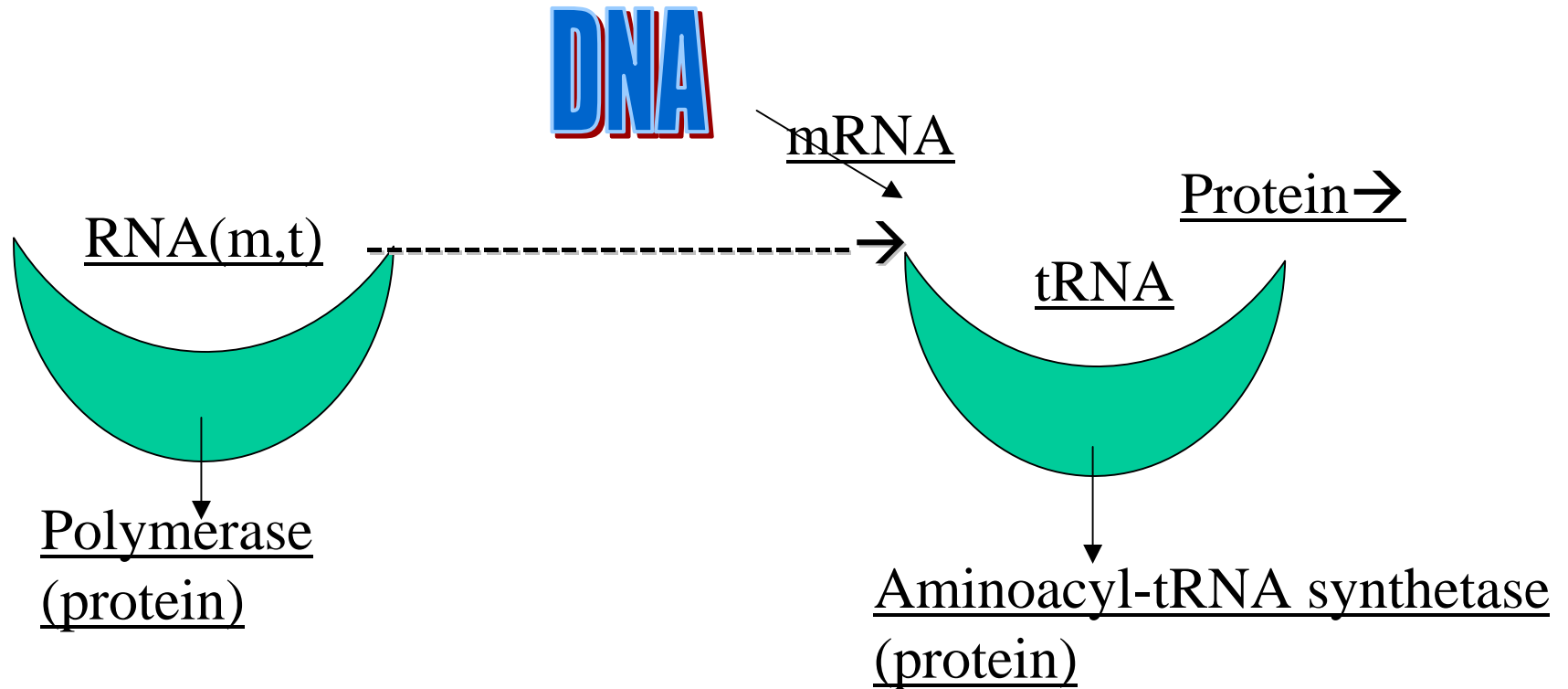
Question: is central dogma necessary
for life?

•Simple life forms are supposed to evade
the central dogma

RNA world

Protein world

RNA-Protein world

Central dogma

1. RNA world

Polymerase→Ribozyme(RNA)

Synthetase→Ribozyme

DNA→RNA(as a coding device)

2. RNA-Protein world

DNA→RNA

In principle the others can stay as protein but may be natural to replace them by an appropriate ribozyme

The role of computational science here is to create on the computer a rybozime which has the similar 3dimensional structure to a polymerase or a synthetase to help creating it Experimentally.

3.protein world

This is to create "a house without a design book".

The idea is to create a self catalyzing protein →polymerase and synthetase→RNA-Protein world

• Is it possible to create(fabricate) not too unstable but not completely stable self catalyzing substance(RNA or Protein) and the coding structure?

• How can the system distinguish which element belongs to the descendant?→ beginning of the cell division

• Death is inevitable?

conclusion

Computer simulation method will be increasingly important both in physical science and in life science.

In particular,the issue of the earliest universe and that of the simplest life form will be crucial in testing the limit of the physical laws among which the superstring theory seems to be the most fundamental.