



Lattice QCD @ Spain  
Palacio de la Magdalena  
Santander, June 9-10, 2011

## SAIL

*Study of SubAtomic Interactions through Lattice QCD  
simulations in Mare Nostrum*

*The overall goal of our project (and a central goal of nuclear physics) is to calculate  
important nuclear processes directly from quantum chromodynamics (QCD)*

Assumpta Parreño, U Barcelona  
Emmanuel Chang, U. Barcelona

(for the NPLQCD Collaboration)



# NPLQCD Collaboration



Silas R. Beane  
New Hampshire



Emmanuel Chang  
Barcelona



William Detmold  
William & Mary



Huey-Wen Lin  
U of Washington



Tom Luu  
Livermore



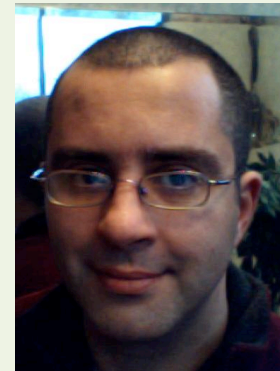
Kostas Orginos  
William & Mary



Assumpta Parreño  
Barcelona



Martin J. Savage  
U of Washington

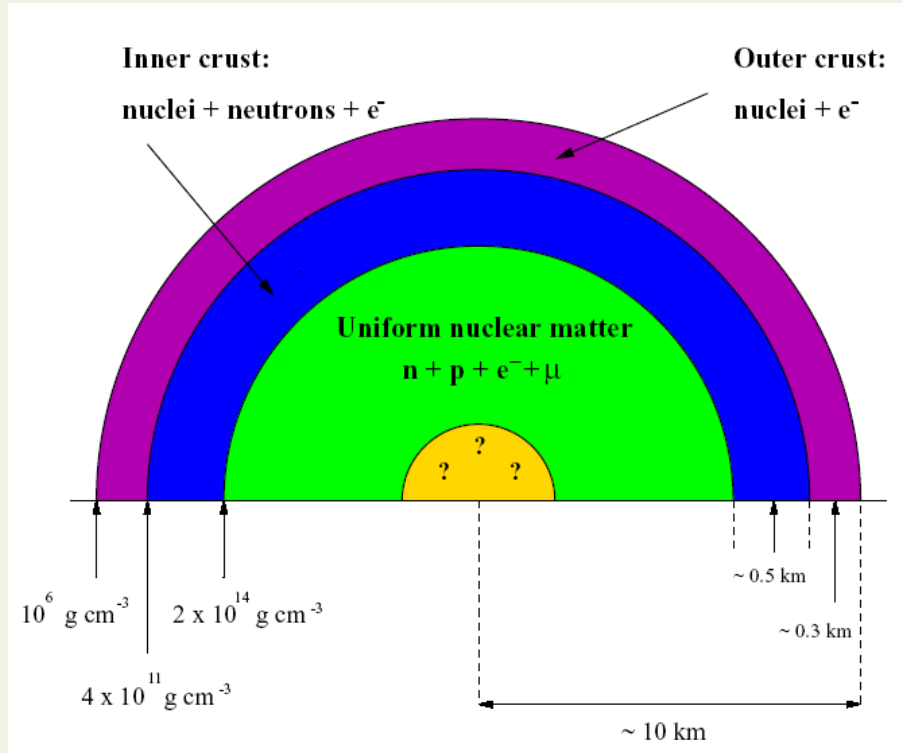
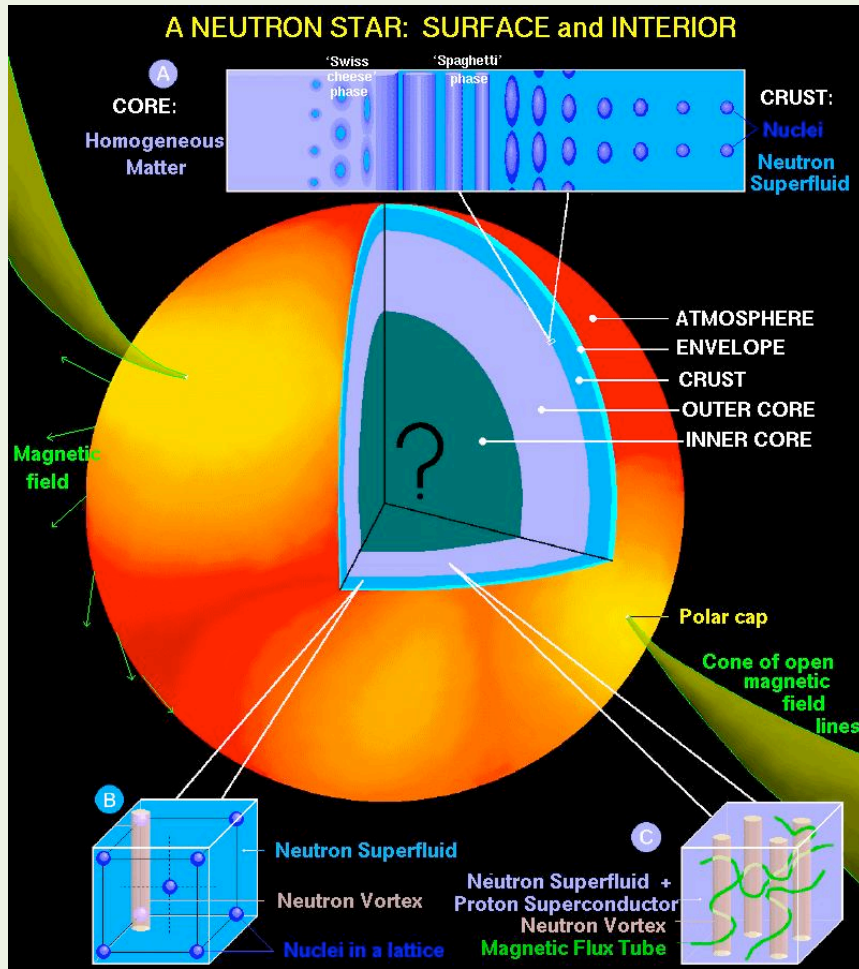


Aaron Torok  
Indiana



André Walker-Loud  
Berkeley

*attending this meeting*



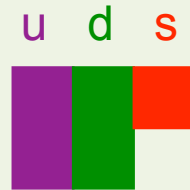
Dany P. Page, UNAM

¿Hyperon matter?

Strangeness

Confined

S, L, K



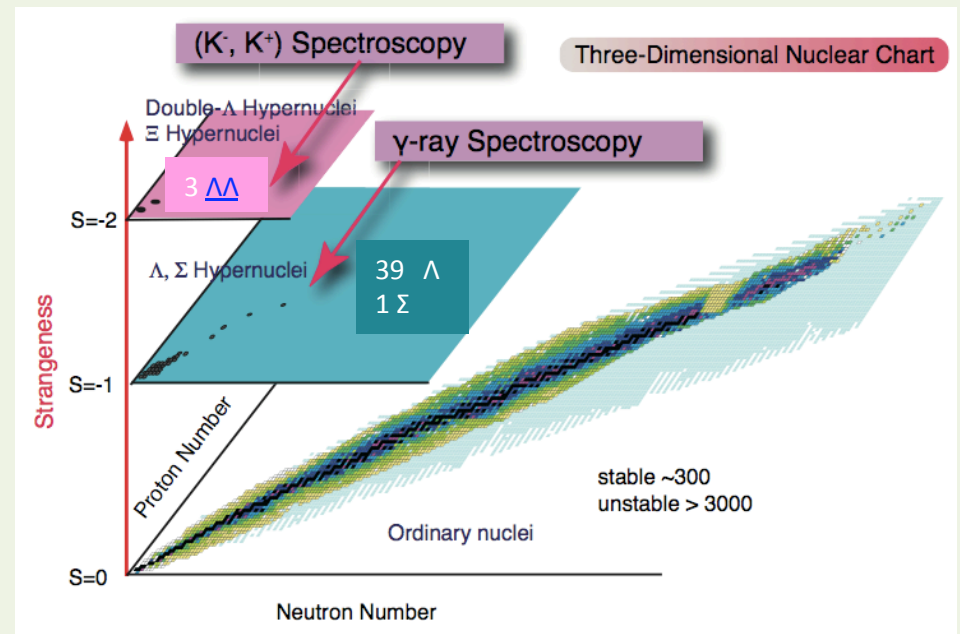
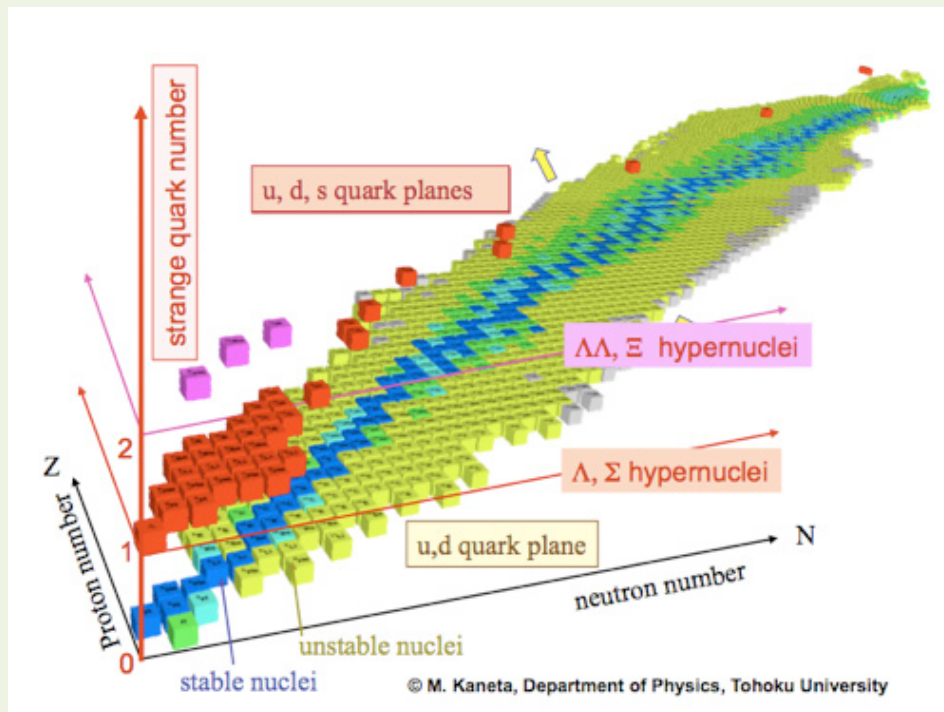


# interaction among hadrons: why lattice?

First principle QCD calculation

Quantifiable uncertainties

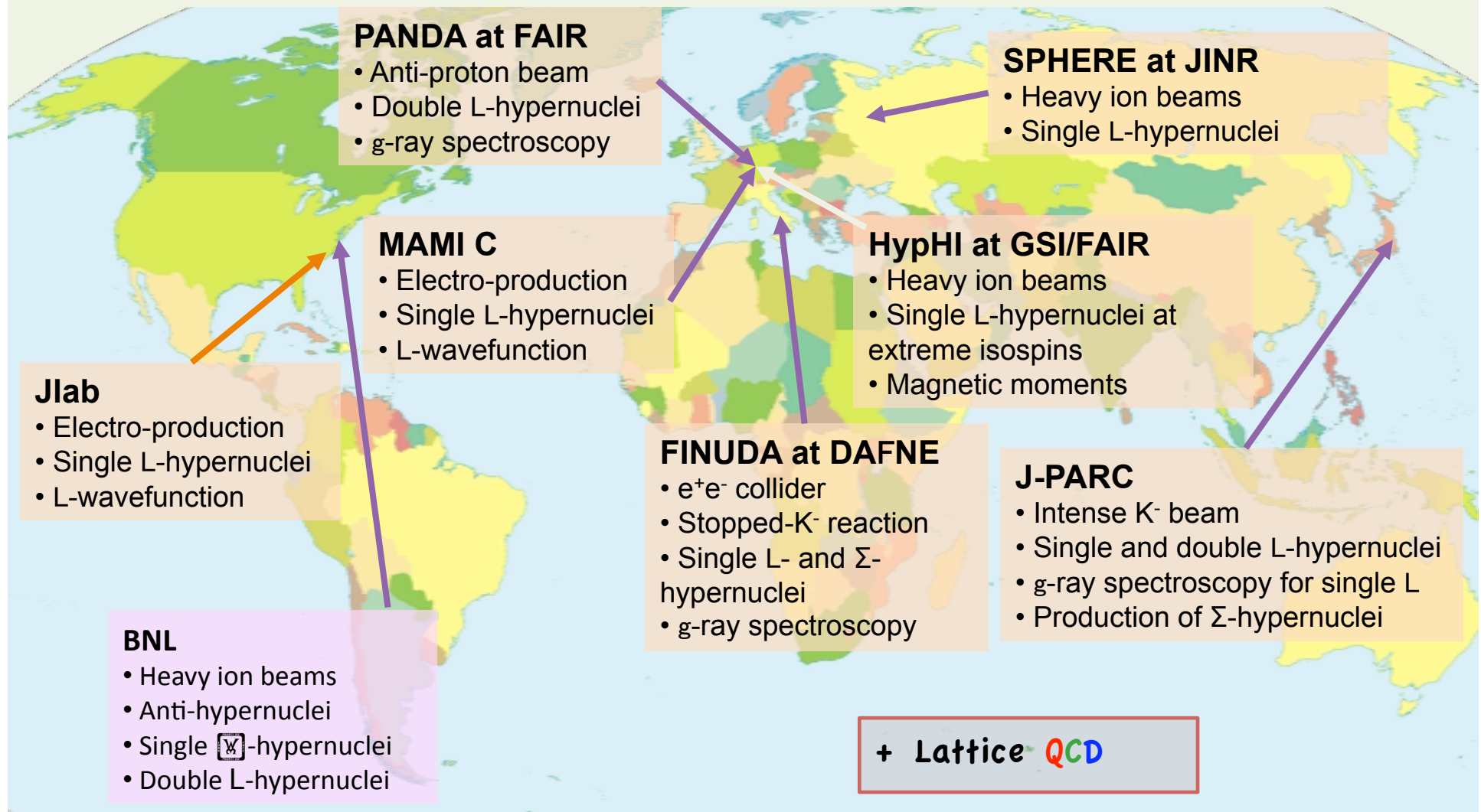
Possibility of study processes which are not accessible experimentally



LQCD

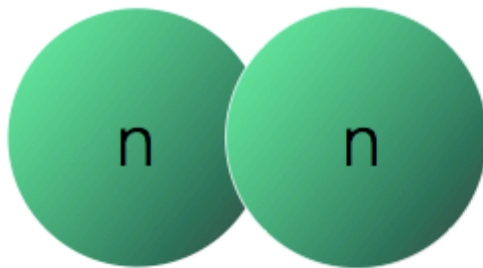
EFT, GFMC, NCSM, SRG ...  
many-body methods

# “strange” Experimental program

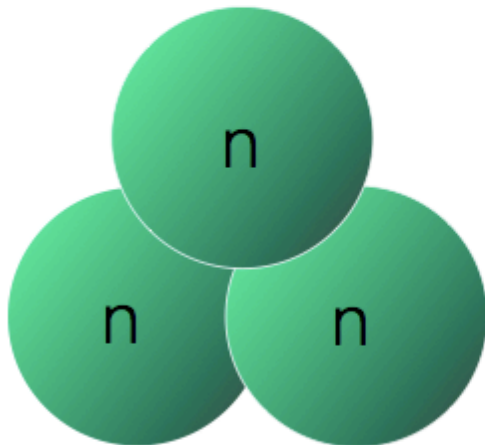
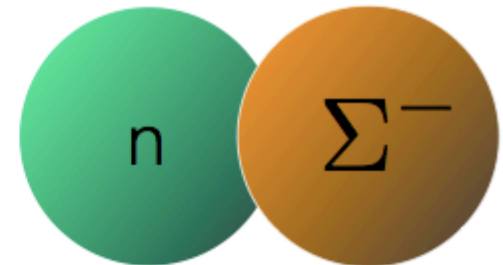




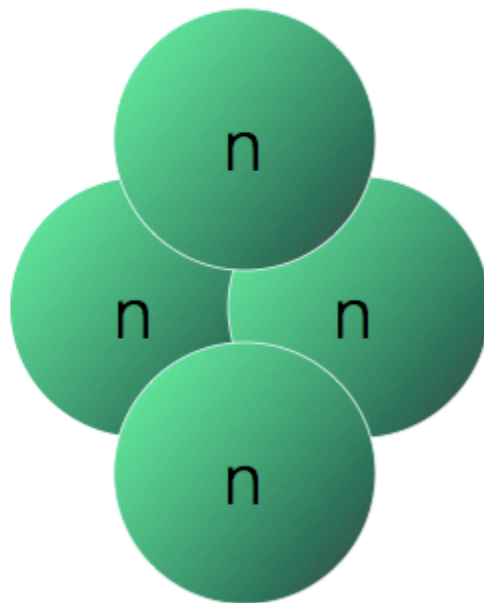
# hadronic interactions



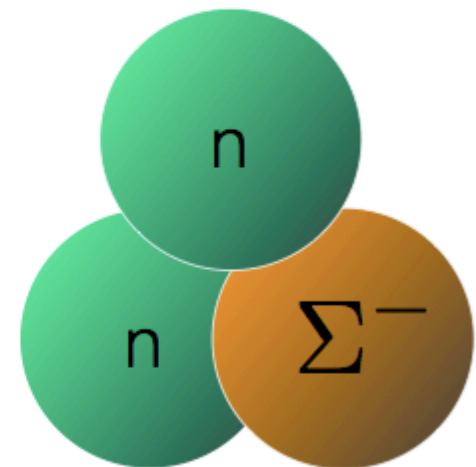
NN-interaction  
verification



NNN

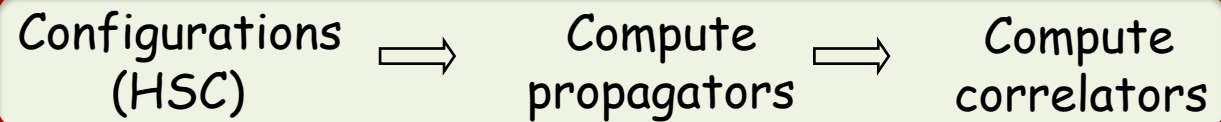


NNNN



YNN

The computation consists of generating quark propagators (up/down and strange) from gauge configurations and performing contractions to produce correlators with various meson and baryon (including non zero strangeness) states and study their interactions from first principles.



Code name: CHROMA, by Robert Edwards (edwards@jlab.org).

Our recent simulations (dynamical):

anisotropic lattices       $N_f=2+1$       clover-improved Wilson fermion actions

$L^3 \times T$	$16^3 \times 128$	$20^3 \times 128$	$24^3 \times 128$	$32^3 \times 256$
L (fm)	2.0	2.5	3.0	4.0
$m_\pi L$	3.86	4.82	5.79	7.71
$\exp(-m_\pi L)$	0.0205	0.0078	0.0030	0.00044
$m_\pi T$	8.82	8.82	8.82	17.64
$\exp(-m_\pi T)$	$1.48 \times 10^{-4}$	$1.48 \times 10^{-4}$	$1.48 \times 10^{-4}$	$2.18 \times 10^{-8}$

$m_\pi \sim 390$  MeV

## Nuclear physics: multi-hadron systems

To study the interaction of multi-meson/baryon states, a large number of contractions are required; in fact the number grows factorially with the number of particles involved.

# Wick contractions to form the correlation function is naively  $N_u! N_d! N_s!$   
 $((A + Z)!(2A - Z)!)$

→ cheapest 3-baryon system:  $X^0 X^0 n$ , with  $3! 2! 4! = 288$  Wick contractions

The triton (nnp) naively involves 2880 ( $N_u=4$  and  $N_d=5$ )

However some careful counting (or brute force numerical attack), can reduce this number to a smaller # of distinct contractions after anti-symmetrizing the proton block.

Recursive algorithms would be needed to study even the light nuclei.

This has been tested with multi-meson systems (*Detmold & Savage, Phys.Rev. D82 (2010) 014511* ). Work on multi-baryons is underway.



# Scattering

Beane, Bedaque, Parreño, Savage, Phys. Lett. B 585,1-2, 106-114 (2004)

M. Lüscher, Commun. Math. Phys. 105, 153-188 (1986)

$$i\mathcal{A} = \left[ \text{Cross} + \text{Cross} - \text{Bubble} + \dots \right] = \frac{1}{\frac{1}{\text{Cross}} - \text{Bubble}}$$

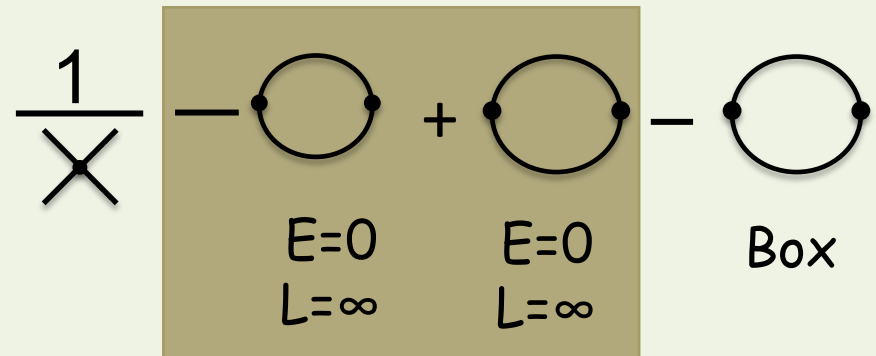
$$\mathcal{A} = \frac{\sum C_{2n} p^{2n}}{1 - I_0 \sum C_{2n} p^{2n}} \quad I_0 = \left(\frac{\mu}{2}\right)^{4-D} \int \frac{d^{D-1}\vec{q}}{(2\pi)^{D-1}} \frac{1}{E - \frac{|\vec{q}|^2}{M} + i\epsilon}$$

Energy eigenvalues:  
zeros of  $\text{Re}[1/\mathcal{A}]$

$$0 = \text{Re}[(i\mathcal{A})^{-1}] = \text{Re} \left[ \frac{1}{\text{Cross}} - \text{Bubble} \right] \quad \text{Box}$$

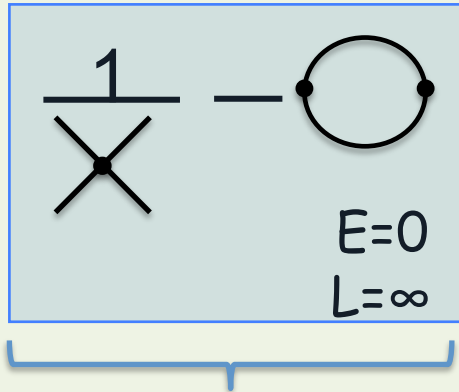
$$\frac{1}{\sum C_{2n} p^{2n}} - \text{Re}(I_0) = 0$$

$$I_0 \rightarrow \frac{1}{L^3} \sum_{\vec{k}} \frac{1}{E - \frac{|\vec{k}|^2}{M} + i\epsilon}$$

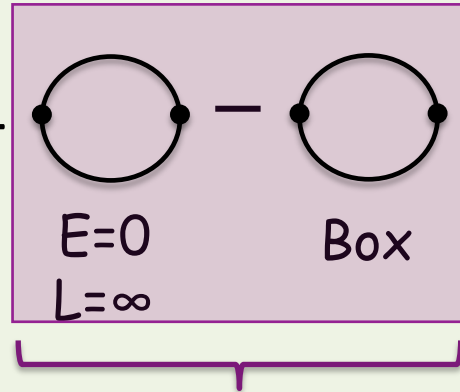


# Scattering

Beane, Bedaque, Parreño, Savage, Phys. Lett. B 585,1-2, 106-114 (2004)  
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$$p \cot \delta(p)$$



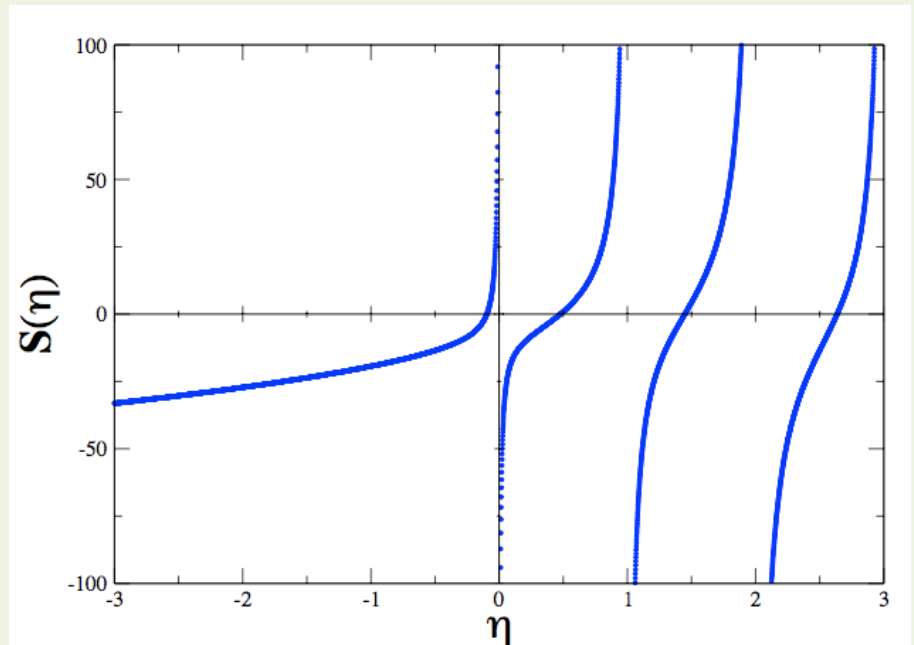
$$\frac{1}{\pi L} \sum_j \frac{1}{|\vec{j}|^2 - \left(\frac{Lp}{2\pi}\right)^2} - \frac{4\Lambda}{L}$$

$$p \cot \delta(p) = -\frac{1}{\pi L} S \left( \frac{p^2 L^2}{4\pi^2} \right)$$

$$\mathcal{A} = \frac{4\pi}{M} \frac{1}{p \cot \delta - ip}$$

$$p = \sqrt{ME}$$

$$p \cot \delta = -\frac{1}{a} + \frac{1}{2} r p^2 + \dots$$



# Lattice simulations $\boxtimes$ Evaluation of vacuum correlation functions:

$$C_{B_1 B_2, \Gamma}(\vec{p}_1, \vec{p}_2, t) = \sum_{\vec{x}_1 \vec{x}_2} e^{i\vec{p}_1 \vec{x}_1} e^{i\vec{p}_2 \vec{x}_2} \Gamma_{\alpha_1 \alpha_2}^{\beta_1 \beta_2} \left\langle B_{1, \alpha_1}(\vec{x}_1, t) B_{2, \alpha_2}(\vec{x}_2, t) \bar{B}_{1, \beta_1}(x_0, 0) \bar{B}_{2, \beta_2}(x_0, 0) \right\rangle$$

spin tensor  $\nearrow$ 
 $\downarrow$  baryon interpolating operator

away from the source, i.e. at large t

source located at t=0

$$C_{H_A H_B}(\vec{p}, -\vec{p}, t) \sim \sum_n Z_{n; AB}^{(i)}(\vec{p}) Z_{n; AB}^{(f)}(\vec{p}) e^{-E_n^{AB}(\vec{0})t}$$

$$\frac{C_{H_A H_B}(\vec{p}, -\vec{p}, t)}{C_{H_A}(\vec{0}, t) C_{H_B}(\vec{0}, t)} \xrightarrow{t \rightarrow \infty} \sum_n \tilde{Z}_{0; AB}^{(i)}(\vec{p}) \tilde{Z}_{0; AB}^{(f)}(\vec{p}) e^{-\Delta E_0^{AB}(\vec{0})t} \sim G(t)$$

Effective Mass method

$$\log \frac{G(t)}{G(t+1)} \rightarrow \text{extract } \Delta E$$

$$\Delta E_n^{(AB)} \equiv \Delta E_n^{(AB)}(\vec{0}) \equiv E_n^{(AB)}(\vec{0}) - m_A - m_B$$



$$= \sqrt{q_n^2 + m_A^2} + \sqrt{q_n^2 + m_B^2} - m_A - m_B = \frac{q_n^2}{2\mu_{AB}} + \dots$$

obtained from the simulation

below inelastic thresholds

$$p \cot \delta = -\frac{1}{a} + \frac{1}{2} r p^2 + \dots \quad p \cot \delta(p) = \frac{1}{\pi L} S(\eta) = \frac{1}{\pi L} \sum_{\substack{|\vec{j}| < \Lambda \\ \vec{j}}} \frac{1}{|\vec{j}|^2 - \eta^2} - \frac{4\Lambda}{L} \quad \text{with} \quad \eta = \frac{L}{2\pi} p$$

If one retains only the scattering length in the  $\tan(\delta)$  expansion and performing a perturbative expansion on the momentum  $p^2$  (and playing a bit with the sums...)

$$E = \frac{p^2}{M} = \frac{4\pi a}{ML^3} \left[ 1 - c_1 \frac{a}{L} + \left( c_1^2 - \frac{1}{\pi^2} \sum_{\substack{\vec{j} \neq 0 \\ \vec{j} \in Z^3}} \frac{1}{|\vec{j}|^4} \right) \left( \frac{a}{L} \right)^2 + \dots \right] \quad \text{with} \quad c_1 = \frac{1}{\pi} \sum_{\substack{\vec{j} \in Z^3 \\ \vec{j} \neq 0}} \frac{1}{|\vec{j}|^2}$$

(recovering Lüscher's formula, [M. Lüscher, Commun. Math. Phys. 105, 153 \(1986\)](#))

For negatively energy shifted states (in the lattice volume):

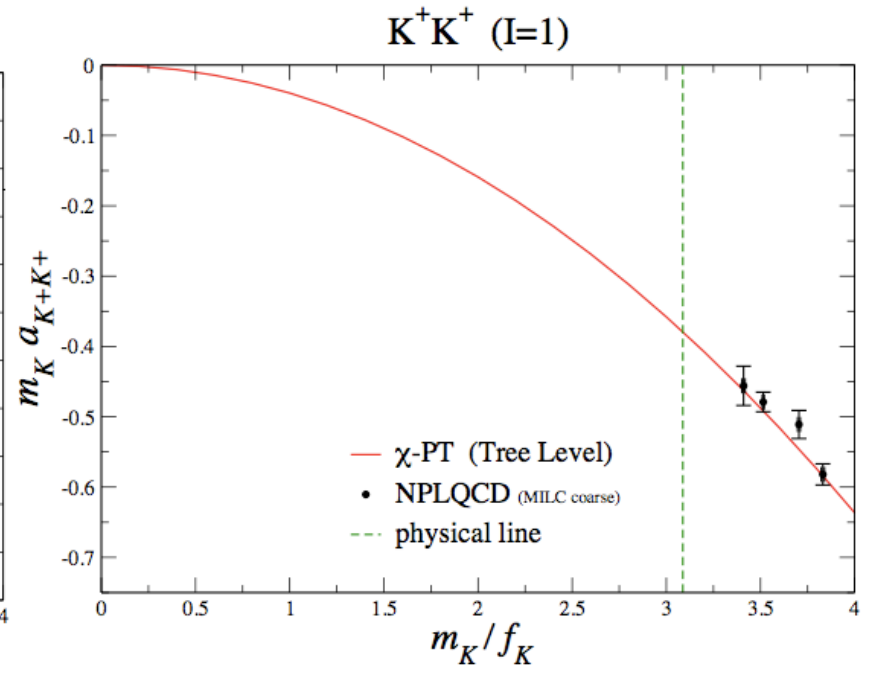
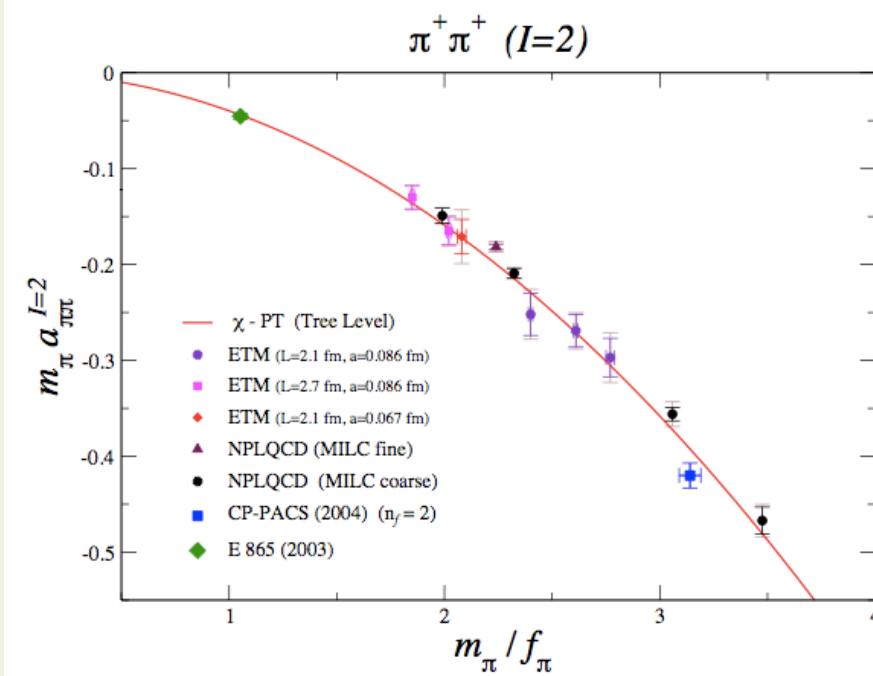
$$p = i \kappa, \quad \kappa = \gamma + \frac{g_1}{L} \left( e^{-\gamma L} + \sqrt{2} e^{-\sqrt{2} \gamma L} + \dots \right) \quad \text{with} \quad \gamma \ll m_\pi \quad B.E._\infty = \frac{\gamma^2}{M}$$

(finite volume dependence suppressed exponentially by the binding momentum)

With simulations performed at two or more lattice volumes (with  $p^2 < 0$ ) it is possible to perform an extrapolation to determine the b.e. at infinite volume, and at this pion mass.

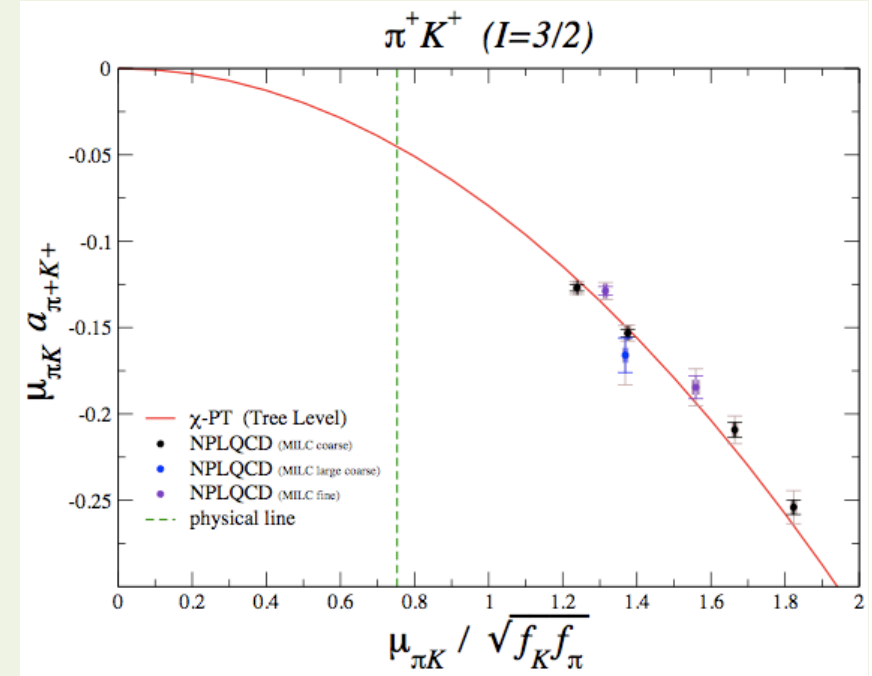


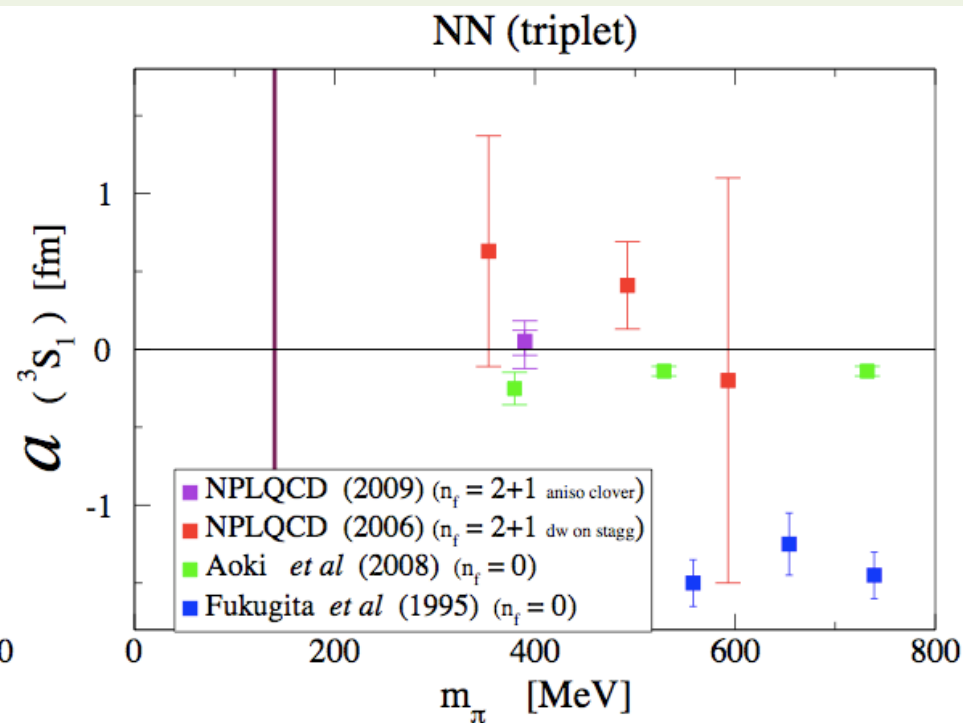
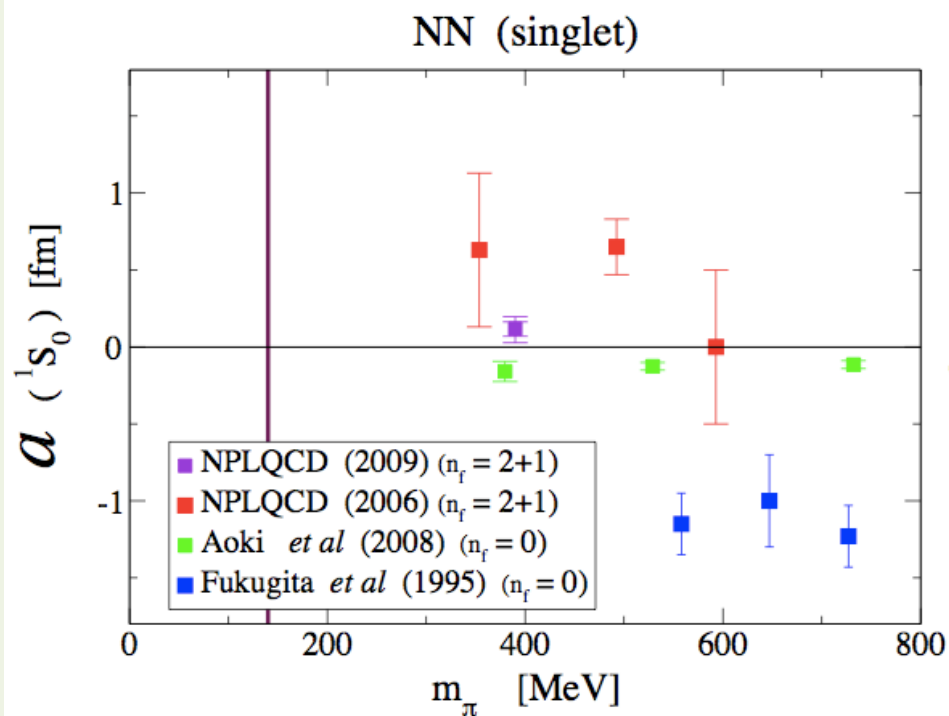
Simplest hadronic interactions  
(with mixed action: DWF on staggered)



$20^3 \times 64$  ( $L_5 = 16$ )  
 $b = 0.125$  fm  $L = 2.5$  fm

	$m_p$ (MeV)	$m_K$ (MeV)	no. conf x no. src
$m_l=030$ $m_s=050$	591	675	564 x 8
$m_l=020$ $m_s=050$	491	640	486 x 8
$m_l=010$ $m_s=050$	352	595	769 x 8
$m_l=007$ $m_s=050$	291	580	1039 x 8





physical values

$$a_s^{{}^1S_0} = -23.714 \text{ fm}$$

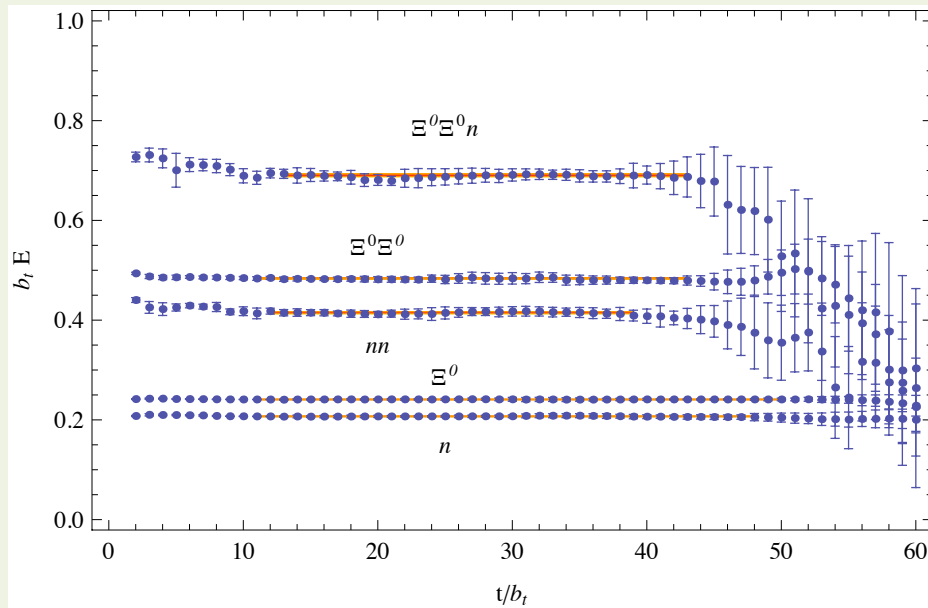
$$a_s^{{}^3S_1} = 5.425 \text{ fm}$$

$$\frac{\text{noise}}{\text{signal}} \xrightarrow{t \rightarrow \infty} \frac{1}{\sqrt{N}} e^{A(m_p - \frac{3}{2}m_\pi)t}$$

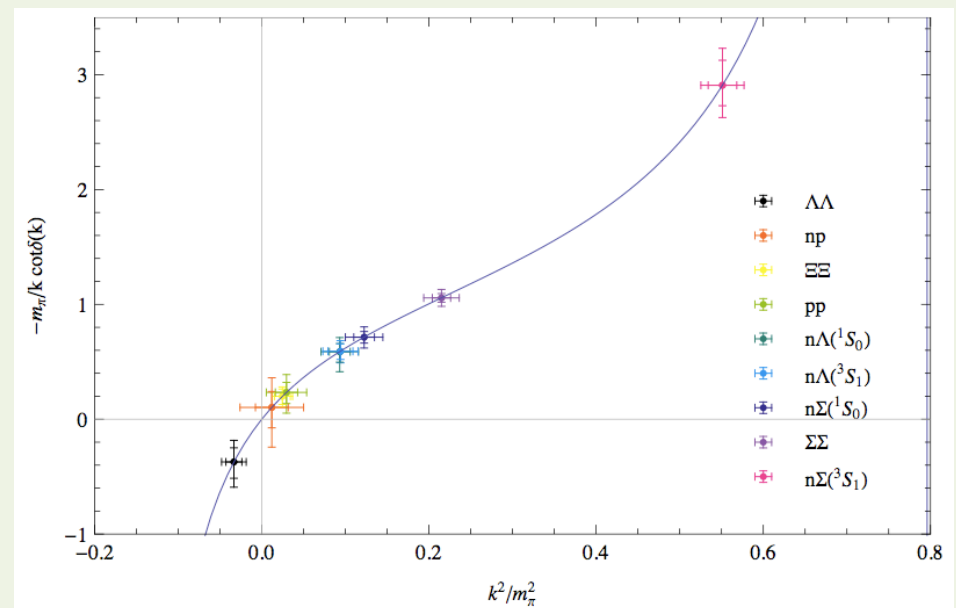
(but only asymptotically)

system with A nucleons

$20^3 \times 128$   $b \approx 0.123$  fm  $m_\pi \sim 390$  MeV



Phys. Rev. D. 80, 074501 (2009)



Phys. Rev. D 81, 054505 (2010)

# H-dibaryon

$I=0 \ J=0 \ s=-2 \ uuddss$

## Evidence for a Bound $H$ Dibaryon from Lattice QCD

S. R. Beane, E. Chang, W. Detmold, B. Joo, H. W. Lin, T. C. Luu, K. Orginos, A. Parreño, M. J. Savage, A. Torok, and A. Walker-Loud (NPLQCD Collaboration)

Phys. Rev. Lett. **106**, 162001 (Published April 20, 2011)

## Bound $H$ Dibaryon in Flavor $SU(3)$ Limit of Lattice QCD

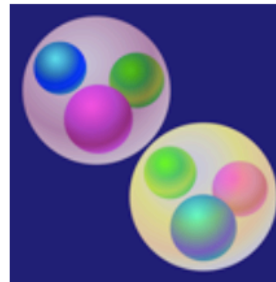
Takashi Inoue, Noriyoshi Ishii, Sinya Aoki, Takumi Doi, Tetsuo Hatsuda, Yoichi Ikeda, Keiko Murano, Hidekatsu Nemura, and Kenji Sasaki (HAL QCD Collaboration)

Phys. Rev. Lett. **106**, 162002 (Published April 20, 2011)



## Physics: Binding baryons on the lattice

April 26, 2011

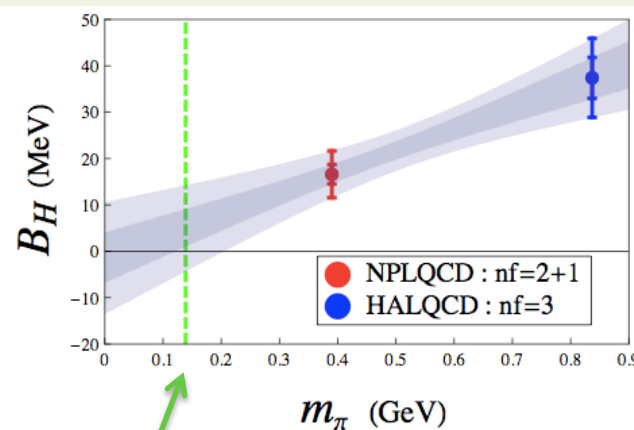
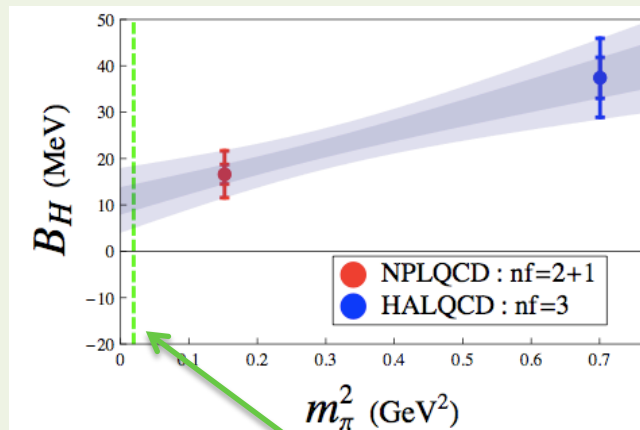
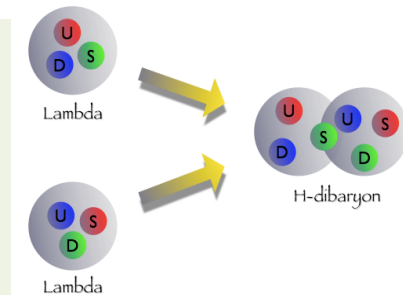


State of the art computer simulations provide the first indication of a dibaryon bound state.

[Synopsis on Phys. Rev. Lett. **106**, 162001 (2011)]

[Synopsis on Phys. Rev. Lett. **106**, 162002 (2011)]

[Read Article](#) | [More Synopses](#)



physical pion mass

$$B(m_\pi) = B_0 + d_1 m_\pi^2$$

$$B_H^{quad} = +11.5 \pm 2.8 \pm 6 \text{ MeV}$$

$$B(m_\pi) = B_0 + c_1 m_\pi$$

$$B_H^{lin} = +4.9 \pm 4.0 \pm 8.3 \text{ MeV}$$

e-Print: arXiv:1103.2821 [hep-lat]

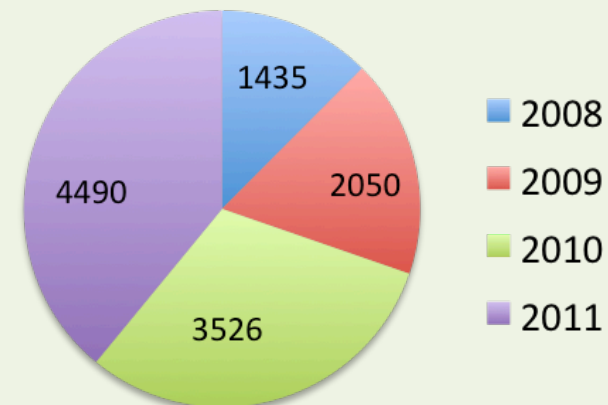


# Project SAIL in MN (BSC)

- NPLQCD Coll in MN  
PowerPC Cluster, 10k cores, Myrinet interconnect.  
Partnership 2006 to present day (15 periods)
- Current period ~ 5% share of total resource.
- Steady increase in time allocated over the years.
- Computing power in the upcoming years ?

The more the merrier?

RES-Mare Nostrum



# Example

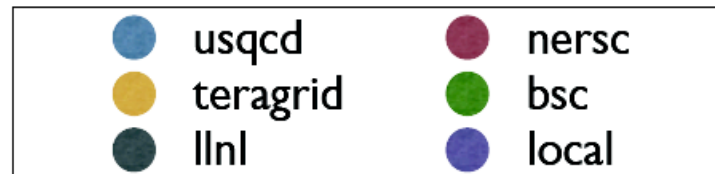
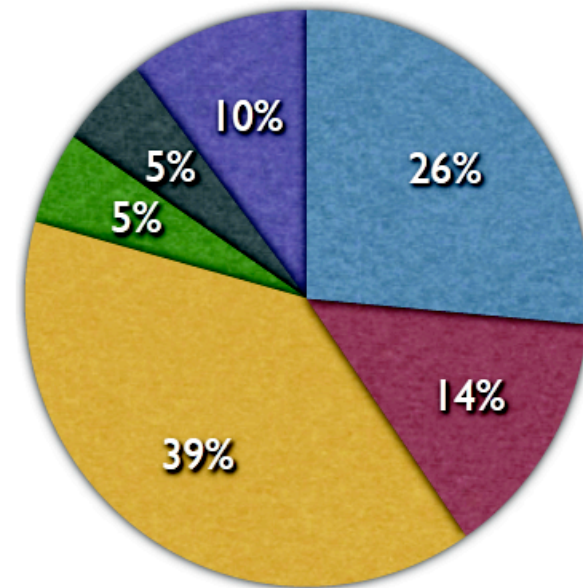
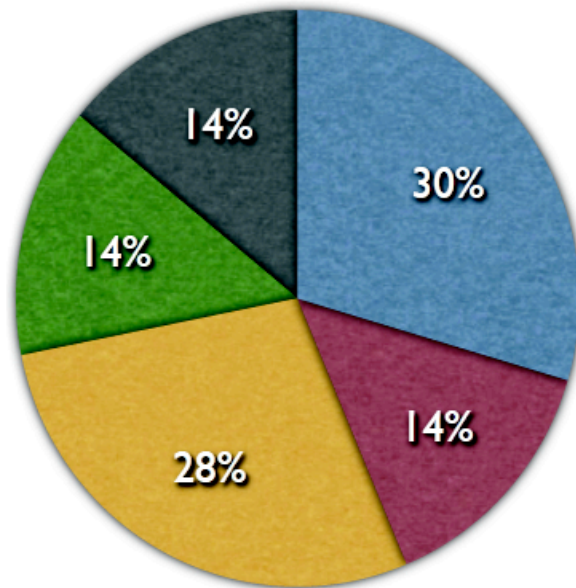
- Propagator generation :
  - solve a sparse matrix equation iteratively
$$M x = b, \quad \text{size of } M \sim L^4 \text{ by } L^4$$
  - 2400 configurations “M”
- 180 sources “b” at 4 volumes
  - ... at current rate (30 mins per prop / 256 cores)
    - 800 configurations x 90 inversions x 1 volume
    - ~ 5% (of total resource at BSC) => non-stop 2 years
- Factor of 20 increase in total resource at Mare Nostrum to reach 0.1% stats. error and perform volume extrapolation.

# NPLQCD Resources

6n node-hours

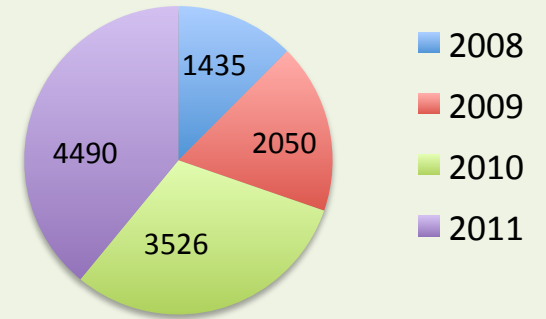
2007/8: 6.1 M

2008/9: 18.5 M



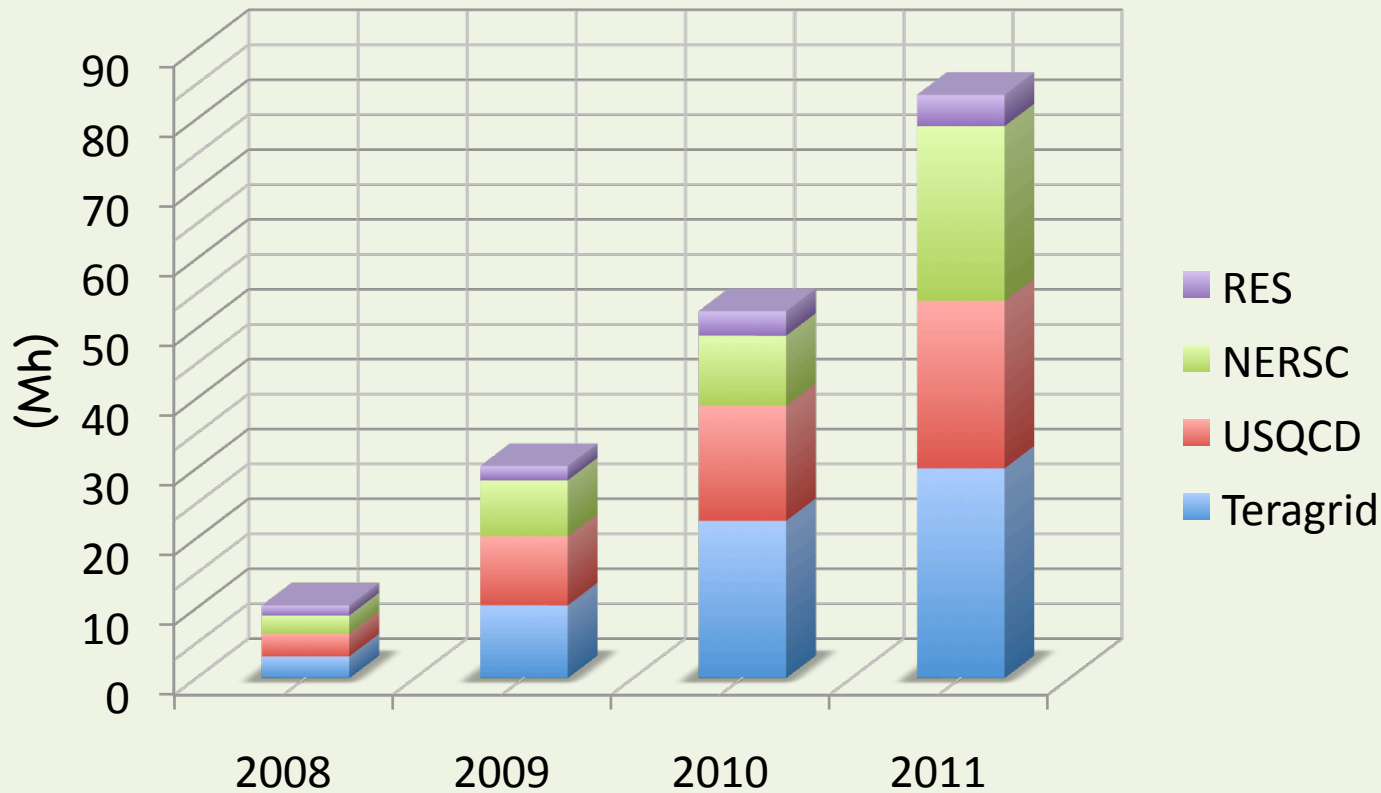
**Period from 1st Jan. to 31 Dec.**  
 (2011 projection based on current period  
 and application for next period)

**RES-Mare Nostrum  
 (in Kh)**



*"half" estimate*

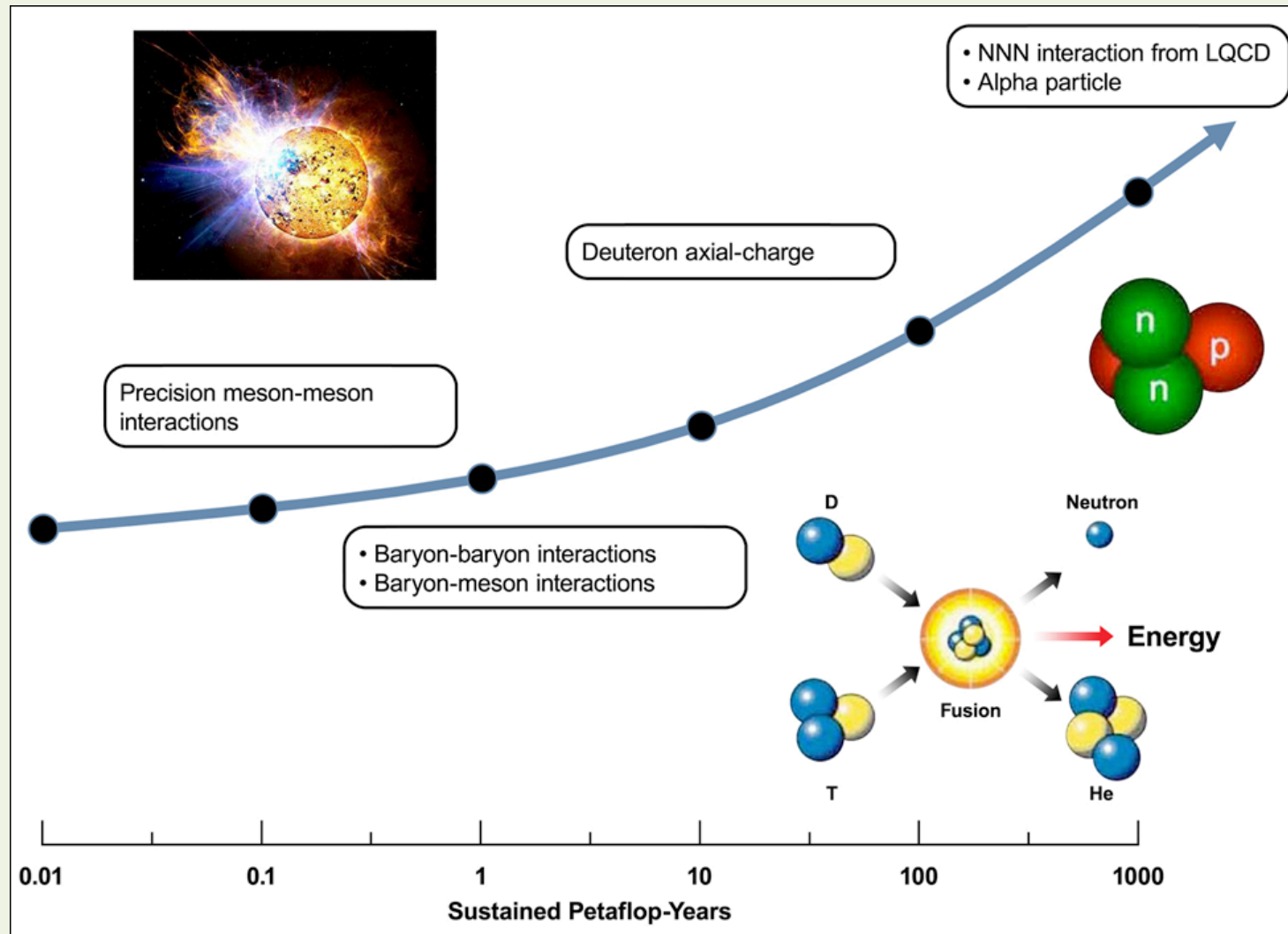
NPLQCD Resources





# From QCD to Nuclei

Resource requirements



*Scientific Grand Challenges: Forefront Questions in Nuclear Science and the Role of Computing at the Extreme Scale, <http://extremecomputing.labworks.org/nuclearphysics/report.stm>*