HPC for Lattice QCD Applications to Nuclear Physics

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University of Tsukuba CCS-LBNL Joint Workshop HPC for Lattice QCD Applications to NP

• Science Goals and need for HPC

• Some details of calculations & challenges

• Some progress: Big Bang Nucleosynthesis and QCD



Low-Energy Nuclear Physics

• Understanding Nuclear Physics from QCD

• Testing the Standard Model at lowenergy in nuclear environments

Nuclear Physics from QCD

• QCD is The fundamental theory of the strong interactions $\mathcal{L}_{QCD} = \bar{q}_{a,\alpha,f}(x) \left[D_{\mu}\gamma_{\mu} + m \right]_{a,\alpha,f}^{b,\beta,f'} q_{b,\beta,f'}(x) - \frac{1}{4} G_{\mu\nu} G_{\mu\nu}$

 $q_{b,\beta,f'}(x)$ Quark of *color* b, *spin* β , *flavor* f flavors = $\begin{array}{c} up(u), & strange(s), top(t) \\ down(d), charm(c), bottom(b) \end{array}$

colors = red, green, blue

quarks transform under the fundamental representation of SU(3) color (unitary 3x3)

spin = 4 spin states, 2 particle, 2 antiparticle

Nuclear Physics from QCD

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Nuclear Physics from QCD QCD is The fundamental theory of the strong interactions $\mathcal{L}_{QCD} = \bar{q}_{a,\alpha,f}(x) \left[D_{\mu} \gamma_{\mu} + m \right]_{a,\alpha,f}^{b,\beta,f'} q_{b,\beta,f'}(x) - \frac{1}{\Lambda} G_{\mu\nu} G_{\mu\nu}$ $q_{b,\beta,f'}(x)$ Quark of *color* b, *spin* β , *flavor* f For Nuclear Physics: $flavors = \begin{array}{l} up(u), & (strange(s)) \\ down(d), & \end{array}$ neutron proton u d d $M_p = 938.272046 \text{ MeV}$ $M_n = 939.565379 \text{ MeV}$ $M_n - M_p = 1.29333217(42) \text{ MeV}$ $M_e = 0.511 \,\,{\rm MeV}$

Nuclear Physics from QCD QCD is The fundamental theory of the strong interactions $\mathcal{L}_{QCD} = \bar{q}_{a,\alpha,f}(x) \left[D_{\mu} \gamma_{\mu} + m \right]_{a,\alpha,f}^{b,\beta,f'} q_{b,\beta,f'}(x) - \frac{1}{\Lambda} G_{\mu\nu} G_{\mu\nu}$ $[D_{\mu}]^{b}_{a}q_{b}(x) = \delta_{a,b}\partial_{\mu}q_{b}(x) + ig[A_{\mu}]^{b}_{a}q_{b}(x)$ gluons adjoint rep. of SU(3) color - 8 gluons $\frac{1}{4}G_{\mu\nu}G_{\mu\nu}$

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Nuclear Physics from QCD

QCD is The fundamental theory of the strong interactions $\mathcal{L}_{QCD} = \bar{q}_{a,\alpha,f}(x) \left[D_{\mu}\gamma_{\mu} + m \right]_{a,\alpha,f}^{b,\beta,f'} q_{b,\beta,f'}(x) - \frac{1}{4} G_{\mu\nu} G_{\mu\nu}$

QCD is a remarkably simple theory to write down. At low energies (will define) QCD is a theory of only 3 or 4 parameters: m_u mass of the up quark (dimensionfull) m_d mass of the down quark (dimensionfull) (m_s) mass of the strange quark (dimensionfull) g gauge coupling between quarks and gluons (dimension-less)

Once these parameters are fixed - everything else is a prediction! - proton mass, He binding energy, neutron star equation of state (maximum neutron star mass), ...

Lattice QCD



Lattice QCD



Asymptotic Freedom Feynman Path Integrals Wilson Lattice Field Theory Monte Carlo methods



allows numerical solution

$\mathcal{N}uclear Physics from QCD$ $\mathcal{L}_{QCD} = \bar{q}_{a,\alpha,f}(x) \left[D_{\mu}\gamma_{\mu} + m \right]_{a,\alpha,f}^{b,\beta,f'} q_{b,\beta,f'}(x) - \frac{1}{4} G_{\mu\nu} G_{\mu\nu}$ $E_{N,Z,S}^{(i)} = \Lambda_{QCD} \times f_{N,Z,S}^{(i)} \left(\frac{m_u}{\Lambda_{QCD}}, \frac{m_d}{\Lambda_{QCD}}, \frac{m_s}{\Lambda_{QCD}}, \alpha_{f.s.}, \Lambda_{QCD}^2 G_F \right)$

these energy levels range from a few KeV to MeV to many GeV (eV = atomic energy scales)

- Λ_{QCD} QCD dynamics generates a mass scale (even if all quark masses were 0) $\Lambda_{QCD} \sim 250 \text{ MeV}$ to normalize this: proton mass = 938 MeV
- $\alpha_{f.s.}$ electromagnetic coupling constant: how strong does photon couple to quarks
- G_F Fermi's weak coupling

$$\mathcal{N}uclear Physics from QCD$$

$$\mathcal{L}_{QCD} = \bar{q}_{a,\alpha,f}(x) \left[D_{\mu}\gamma_{\mu} + m \right]_{a,\alpha,f}^{b,\beta,f'} q_{b,\beta,f'}(x) - \frac{1}{4} G_{\mu\nu} G_{\mu\nu}$$

$$E_{N,Z,S}^{(i)} = \Lambda_{QCD} \times f_{N,Z,S}^{(i)} \left(\frac{m_u}{\Lambda_{QCD}}, \frac{m_d}{\Lambda_{QCD}}, \frac{m_s}{\Lambda_{QCD}}, \alpha_{f.s.}, \Lambda_{QCD}^2 G_F \right)$$

these energy levels range from a few KeV to MeV to many GeV (eV = atomic energy scales)

- Λ_{QCD} QCD binds quarks/gluons into protons and neutrons, it binds protons and neutrons into nuclei strong nuclear force fusion
- $\alpha_{f.s.}$ E&M + QCD responsible for fission

$$G_F \qquad Weak \text{ decay:} \quad n \to p \qquad \qquad \tau_n = 881.5s$$

Nuclear Physics from QCD

• There are well known fine-tunings in nature that have a significant impact on our existence

 $M_n - M_p$, B_d , triple alpha process and ${}^{12}C$, ...

How sensitive are these fine-tunings to variations of fundamental parameters in the Standard Model?

How sensitive is the Universe as we know it to variations in these fundamental parameters?



need a solution to QCD

Nuclear Physics from QCD

 What is the weak fusion rate p+p→d+ν_e+e⁺ as a function of parameters in the Standard Model?
 What is the composition and equation of state of dense nuclear matter in neutron stars?

- With the discovery of the Higgs boson, the Standard Model (SM) is now complete
- However, the LHC has turned up only one hint of any physics beyond the Standard Model (BSM)
 - Further, there is almost NO terrestrial experimental hints for any physics BSM
 - the exceptions: muon anomalous magnetic moment proton radius puzzle

high-energy physics colliders are one way to search for BSM physics - but it is not clear this will be possible in the near future

this helps emphasize the important role low-energy precision nuclear physics can play in searching for new physics (in addition to muon g-2 and proton size)

While we have no direct confirmation of any BSM physics - we have very strong indirect evidence:



The SM describes only $\sim 5\%$ of the mass of the Universe

~25% of the mass of the Universe is believed to be Dark Matter

~70% of the mass of the Universe is believed to be Dark Energy

Standard Model

The assumed existence of Dark Matter (DM) comes from several sources:

Velocity curves of rotational galaxies require significantly more gravitating mass than observed



The assumed existence of Dark Matter (DM) comes from several sources:

N-body simulations of galaxy formation (assuming cold-dark matter) DM gives rise to observed structure of galaxies and galaxy clusters (simulations without DM do not)



The assumed existence of Dark Matter (DM) comes from several sources:

Bullet-Cluster: two colliding galaxies gravitational lensing shows COM moved right through collision and is not observable while visible matter "collided"



What do we know about Dark Matter?

DM interacts very weakly, if at all, with the SM except through gravity DM is weakly self-interacting: DM exists in halos rather than disks (matter accumulates to a disk through collisions) DM is cold (non-relativistic) since it clumps



The assumed existence of Dark Matter (DM) comes from several sources:

These three observations, in particular the bullet cluster, are very difficult to explain with modified gravity. Cold Dark Matter is the simplest explanation consistent with all observations



There are several significant experimental efforts underway to try and directly detect Dark Matter - through elastic collisions with matter

These detectors all use nuclei (e.g. Xenon-130) to search for elastic recoil

to interpret constraints/ observations we must understand QCD and possible interactions with DM!

LUX exclusion plot [arXiv:1405.5906]



To the best of our knowledge, the SM matter in the Universe is comprised entirely of matter and not anti-matter

A measure of the excess matter in the Universe is given by the primordial ratio of the number of baryons to photons - from the CMB, we know this number to be

$$\eta \equiv \frac{X_N}{X_{\gamma}} \simeq 6.2 \times 10^{-10}$$

However, the SM is nearly symmetric in matter and antimatter. While this observed asymmetry is small, it is orders of magnitude larger than allowable by the SM

To produce a matter/anti-matter asymmetry, we need the three Sakharov conditions:

- baryon number violation
- C-symmetry and CP-symmetry violation
- interactions out of thermal equilibrium
- C = charge conjugation: $e^- \leftrightarrow e^+$ particle to anti-particle symmetry
- P = Parity: mirror symmetry (physics in the mirror should be the same)
- T = Time-reversal symmetry: laws of physics going forwardand backwards in time is the same

These discrete symmetries are almost perfectly respected by the SM with small violations.

Quantum Mechanics + special relativity ---> C*P*T conserved

To produce a matter/anti-matter asymmetry, we need the three Sakharov conditions:

- baryon number violation
- C-symmetry and CP-symmetry violation
- interactions out of thermal equilibrium

CP violation implies T violation which implies there will be permanent electric dipole moments (EDMs) for SM fermions. There are significant experimental efforts to search for permanent electric dipole moments in electrons, protons, neutrons, deuterium, \dots ¹⁹⁹Hg, ²²⁵Ra , \dots

In order to relate constraints/measurements on permanent EDMs in nucleons/nuclei to BSM physics,

we must be able to solve QCD!

Feynman Path Integrals $\mathcal{Z} = \int DA_{\mu}D\psi D\overline{\psi}e^{iS_{QCD}}$ $S_{QCD} = \int d^4x \mathcal{L}_{QCD}$ $\langle \Omega | \hat{\mathcal{O}}(y) \hat{\mathcal{O}}^{\dagger}(x) | \Omega \rangle = \frac{1}{\mathcal{Z}} \int DA_{\mu}D\psi D\overline{\psi}e^{iS_{QCD}} \mathcal{O}(y) \mathcal{O}^{\dagger}(x)$

The path-integral gives us a relation between matrix elements of operators and a high dimensional integral over field configurations.

- We know how to do the integral on the right (in principle at least). The beginning of lattice QFT is to discretize the universe so that we can compute the path-integral representation directly with a computer.
- Suppose we chop the universe into size $32 \times 32 \times 32 \times 64 = 2^{21}$
- our path integral goes over all field configurations on all sites, $n^{2^{21}}$ terms!



Feynman Path Integrals $\mathcal{Z} = \int DA_{\mu} D\psi D\overline{\psi} e^{iS_{QCD}}$ $S_{QCD} = \int d^4x \mathcal{L}_{QCD}$ $\langle \Omega | \hat{\mathcal{O}}(y) \hat{\mathcal{O}}^{\dagger}(x) | \Omega \rangle = \frac{1}{\mathcal{Z}} \int DA_{\mu} D\psi D\overline{\psi} e^{iS_{QCD}} \mathcal{O}(y) \mathcal{O}^{\dagger}(x)$ How can we actually perform this integral? If we Wick-rotate to Euclidean time, $t \rightarrow it_E$, then we have $\langle \Omega | \hat{\mathcal{O}}(y_E) \hat{\mathcal{O}}^{\dagger}(x_E) | \Omega \rangle = \frac{1}{\mathcal{Z}} \int DA_{\mu} D\psi D\overline{\psi} e^{-S_{QCD}^E} \mathcal{O}(y_E) \mathcal{O}^{\dagger}(x_E)$

• We can use this factor as a probability measure to importance sample the integral with Monte-Carlo methods for those field configurations that minimize S^E_{QCD}

Feynman Path Integrals $\langle \Omega | \hat{\mathcal{O}}(y_E) \hat{\mathcal{O}}^{\dagger}(x_E) | \Omega \rangle = \frac{1}{\mathcal{Z}} \int DA_{\mu} D\psi D\overline{\psi} e^{-S_{QCD}^E} \mathcal{O}(y_E) \mathcal{O}^{\dagger}(x_E)$

 We can make N_{cfg} different samples of the field configurations and then our correlation functions are approximated with finite statistics

 $\langle \Omega | \hat{\mathcal{O}}(y_E) \hat{\mathcal{O}}^{\dagger}(x_E) | \Omega \rangle = \lim_{N_{cfg} \to \infty} \frac{1}{N_{cfg}} \sum_{i=1}^{N_{cfg}} \langle \Omega | \hat{\mathcal{O}}(y_E) [A^i_{\mu}, \psi_i, \overline{\psi}_i] \hat{\mathcal{O}}^{\dagger}(x_E) [A^i_{\mu}, \psi_i, \overline{\psi}_i] | \Omega \rangle$

 $[A_{\mu}^{i}, \psi_{i}, \overline{\psi_{i}}]$ = the ith value of the fields on "configuration" i

 At finite statistics (finite N_{cfg}) we will have an approximation to the correlation functions with some computable statistical uncertainty that can be systematically improved (with more computing time) Feynman Path Integrals $\langle \Omega | \hat{\mathcal{O}}(y_E) \hat{\mathcal{O}}^{\dagger}(x_E) | \Omega \rangle = \frac{1}{\mathcal{Z}} \int DA_{\mu} D\psi D\overline{\psi} e^{-S_{QCD}^E} \mathcal{O}(y_E) \mathcal{O}^{\dagger}(x_E)$

• What do we expect our Euclidean spacetime correlation functions to look like? Let us take $x_E=0$ (without loss of generality – translation invariance lets us do this) and $\vec{y}_E = 0$ for simplicity

 $C(t) = \langle \Omega | \hat{\mathcal{O}}(t, \vec{0}) \hat{\mathcal{O}}^{\dagger}(0, \vec{0}) | \Omega \rangle$

Insert a complete set of states

Lattice QCD results are given by a sum of noisy exponentials – a challenging numerical analysis problem $C(t) = \sum_{n} \langle \Omega | \hat{\mathcal{O}}(t) | n \rangle \langle n | \hat{\mathcal{O}}^{\dagger}(0) | \Omega \rangle$ $= \sum_{n} \langle \Omega | e^{\hat{H}t} \hat{\mathcal{O}}(0) e^{-\hat{H}t} | n \rangle \langle n | \hat{\mathcal{O}}^{\dagger}(0) | \Omega \rangle$ $= \sum_{n} Z_{n} Z_{n}^{\dagger} e^{-E_{n}t}$ $Z_{n} = \langle \Omega | \hat{\mathcal{O}}(0) | n \rangle$

 $1 = \sum |n\rangle \langle n|$

 $\begin{array}{l} \textbf{Integrating the fermion fields} \\ \mathcal{Z}_F = \int \mathcal{D}\left[\psi\right] \mathcal{D}\left[\overline{\psi}\right] \exp\left\{-S_W\left[U,\overline{\psi},\psi\right]\right\} \quad S_W = a^4 \sum_x \overline{\psi}(x) \left[D_W + M\right] \psi(x) \end{array}$

This integral is quadratic in the quarks, so we can directly do the integral. We do this because the quarks are Grassmann numbers (anti-commuting)

$$= \det [D_W + M] = \prod_{q=1}^{N_f} \det [D_W + m_q]$$

$$\mathcal{Z}_{QCD} = \int DU_{\mu} \det \left[D_W + M \right] e^{-S_G[U_{\mu}]}$$

J

 $U_{\mu} = e^{iagA_{\mu}}$

How do we evaluate the determinant?

Integrating the fermion fields How do we evaluate the determinant? $Z_{QCD} = \int DU_{\mu} \det [D_W + M] e^{-S_G[U_{\mu}]}$

$$\begin{aligned} \mathcal{Z}_{\psi} &= \int D[\psi] D[\overline{\psi}] e^{-\int d^4 x \overline{\psi} [D_W + M] \psi} \\ &= \det[D_W + M] \\ &= \frac{1}{\det[[D_W + M]^{-1}]} \\ &= \int D[\phi] D[\phi^*] e^{-\int d^4 x \phi^* [D_W + M]^{-1}} \end{aligned}$$

Gaussian integral we can do exactly – for Grassmann variables, we get a determinant. For regular variables, we get the inverse determinant. Introduce pseudo-fermions

We need to invert a large, sparse matrix with small eigenvalues $[D_W + M]^{-1}$

this takes ~90% of CPU cycles for generating ensemble of configurations

Quark contractions: Making protons, pions, ...

$$[D_W + M] S(x, y; U) = \frac{1}{a^4} \delta_{xy}$$

Pion correlation function

Quark propagator

To solve for the quark propagator, S, we must invert a large sparse matrix

 $[D_W + M]^{-1}$

Then – we Wick-contract the quarks together to make states of interest: e.g. the pion

 $\left\langle \overline{u}(x)\gamma_5 d(x)\overline{d}(y)\gamma_5 u(y)\right\rangle_F = -\operatorname{tr}\left\{\gamma_5 S_{dd}(x,y;U)\gamma_5 S_{uu}(y,x;U)\right\}$



Quark contractions: Making protons, pions, ...

$$[D_W + M] S(x, y; U) = \frac{1}{a^4} \delta_{xy}$$

A proton has 2 u-quarks and 1 d-quark. The contractions are slightly more complex – we need to keep track of which u-quark from x goes to which u-quark at y - 2 contractions (Nu! * Nd!)

Proton correlation function



2 protons (proton-proton scattering) has 4! * 2! = 48 contractions He3 (ppn) has 5! * 4! = 2880 contractions He4 (ppnn) has 6! * 6! = 518400 contractions!

Symmetries can be used to largely reduce this growth Yamazaki, Kuramashi, Ukawa – Phys.Rev. D81 (2010) But this Wick-contraction cost can be dominant for multi-nucleon lattice QCD calculations

Signal-to-Noise

Calculations involving nucleons suffer a severe signal-to-noise problem

 $Signal = Ze^{-m_N t} \left[1 + \delta Z_n e^{-(E_n - m_N)t} \right]$

 $\frac{Signal}{Noise} \sim \sqrt{}$

$$\sqrt{N_{sample}} e^{-(m_N - \frac{3}{2}m_\pi)t}$$

 $\frac{Signal}{Noise} \sim \sqrt{N_{sample}} \ e^{-A(m_N - \frac{3}{2}m_\pi)t}$

Signal for a proton correlation function

Signal-to-noise for a proton correlation function $m_N \simeq 939 \text{ MeV}$ $m_\pi \simeq 135 \text{ MeV}$ Signal-to-noise for A nucleons

Solving this problem requires solutions at early Euclidean-time before the Noise becomes large – but this requires sophisticated "wave-functions" for the proton, which compounds the Wickcontraction cost mentioned above

Why exascale?

QCD is a 4-Dimensional theory. Our current best algorithms scale as

 $t_{MC} \sim \frac{1}{a^6}$

We require sufficiently small discretization scales, a, such that a continuum limit can be taken. Also, 3 or more discretization scales are needed for a controlled extrapolation

 $L/a = \{64, 128, 256, \dots\}$

The previously mentioned signal-to-noise problem requires millions of stochastically independent samples

With current strategies and algorithms, we can easily occupy an entire exascale-year

Role of QCD in the Evolution of the Universe

Big Bang Nucleosynthesis $T\simeq 1$ trillion K ightarrow 1 billion K $t\simeq 3 imes 10^{-5}s ightarrow 3$ min

when systems cool, they settle into the lowest energy state mass/energy n P

 $\tau_n \sim 15 \min$

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$\tau_n \sim 15 \min$

what prevented this from destroying all the neutrons?

if nothing else were to happen in the next few minutes, our universe would be full of only Hydrogen

when systems cool, they settle into the lowest energy state



Answer: formation of nuclei

a system with protons and neutrons can collapse to a compact bound state, the deuteron: the attractive binding of a neutron and proton allows neutrons to survive when embedded in nuclei

The deuterium "bottleneck"



The deuterium "bottleneck" is broken, neutrons flow into He



He stability: \uparrow,\downarrow protons and \uparrow,\downarrow neutrons can be packed together



The early universe contains 75% H and 25% ⁴He by mass fraction ("all" deuterium converted to ⁴He)

this picture very sensitive to binding energy of deuterium which is finely tuned (most nuclei have ~8 MeV binding per nucleon)!

$$B_d = 2.22$$
 MeV

What if

- $B_d \ll 2.22 \text{ MeV}$ more finely tuned all neutrons decay - no helium mostly hydrogen stars?
- $B_d \gg 2.22 \text{ MeV}$ natural scenario
- all neutrons captured in deuterium and helium - no hydrogen no stars like ours!

Turns out BBN abundances are also very sensitive to

$$m_n - m_p \propto \begin{cases} m_d - m_u \\ e^2/4\pi \end{cases}$$



How does QCD impact light element synthesis in the early Universe? (Will come back to this later)



Light lon reactions in early universe produce primordial abundances of light nuclei reactions dominated by radiation absence of bound A=5,8 nuclei limit synthesis (no ^{12}C)

Alpher, Gamow; Fermi, Turkevich; Hayashi; Alpher; Peebles; Hoyle, Tayler; Wagoner, Fowler, Hoyle; Kawano; Olive; ...





initial conditions for ratio of neutron to protons exponentially sensitive to mass splitting

$$\frac{X_n}{X_p} = e^{-(m_n - m_p)/kT}$$

neutron lifetime very sensitive to mass splitting

$$\frac{1}{\tau_n} = \frac{(G_F \cos\theta_C)^2}{2\pi^3} m_e^5 (1 + 3g_A^2) f\left(\frac{m_n - m_p}{m_e}\right)$$

$$f(a) \simeq \frac{1}{15} \left(2a^4 - 9a^2 - 8 \right) \sqrt{a^2 - 1} + a \ln \left(a + \sqrt{a^2 - 1} \right)$$

Griffiths "Introduction to Elementary Particles"

10% change in $m_n - m_p$ corresponds to ~100% change neutron lifetime

$$m_n - m_p = 1.29333217(42) \text{ MeV}$$

two sources of isospin breaking in the Standard Modelquark massquark electric charge $m_q = \hat{m}\mathbf{1} - \delta\tau_3$ $Q = \frac{1}{6}\mathbf{1} + \frac{1}{2}\tau_3$

at leading order in isospin breaking

$$m_n - m_p = \delta M_{n-p}^{\gamma} + \delta M_{n-p}^{m_d - m_u}$$
$$< 0 \qquad > 0$$

•
$$\delta M_{n-p}^{m_d - m_u} = \alpha (m_d - m_u) + \dots = 2.44(17) \text{ MeV}$$



determine electromagnetic contribution through Lattice QCD computation or by comparing with experiment

$$\delta M_{n-p}^{\gamma} = m_n - m_p - \delta M_{n-p}^{m_d - m_u} = -1.15(17) \text{ MeV}$$

Big Bang Nucleosynthesis highly constrains variation of $M_n - M_p$ and hence variation of fundamental constants

considering $\alpha_{f.s.}$ and $m_d - m_u$ simultaneously relaxes constraints (not yet simultaneously considered)

for now - freeze electromagnetic coupling and just look at effects of quark mass splitting



PRELIMINARY



A precise determination of α + BBN can constrain $m_d - m_u$ $\delta M_{n-p}^{m_d - m_u} \equiv \alpha (m_d - m_u)$





Big Bang Nucleosynthesis and $m_n - m_p \stackrel{\text{P. Banerjee, M. Heffernan,}}{\text{AVVL}}$



Conclusions

- Understanding nuclear physics from the fundamental theory of strong interactions, QCD, is exciting and important for these and other reasons:
 - 0
- Quantitative connection between QCD and the rich nuclear phenomenology
- Understanding precision low-energy nuclear physics to constrain the SM and searches for BSM physics
- The growth of computing power and algorithms means that TODAY is the beginning of a renaissance in nuclear physics where these exciting things are just becoming possible!

