Expression of Interest for a Centre of Excellence

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THE CYPRUS INSTITUTE

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The Cyprus Institute: Computation-based Science and Technology research center (CaSToRC)

CaSToRC:

- Promotes High Performance Computing and Computational Sciences in Cyprus and through the EU infrastructure project LinkSCEEM, in the Eastern Mediterranean region.
- Activities include:
  - Operation of the national supercomputing facility of Cyprus
  - Representation of Cyprus to PRACE - leads Lattice QCD applications in WP8 of PRACE-2IP and WP7 of PRACE-3IP, participates in prototyping in WP9 of PRACE-2IP and WP11 of PRACE-2IP
  - A PhD program in computational sciences
  - Training courses in HPC and code development
  - A Simulation Lab in Nuclear and Particle Physics with JSC and DESY-Zeuthen

Group at CaSToRC collaborates closely with the one at the University of Cyprus

Scientific areas of interest

- Hadron structure - need exascale for attaining 1% precision at physical point
- Algorithms and code development
- Lattice Perturbation theory
- Topology and simulation of SU(N)

Systematic uncertainties

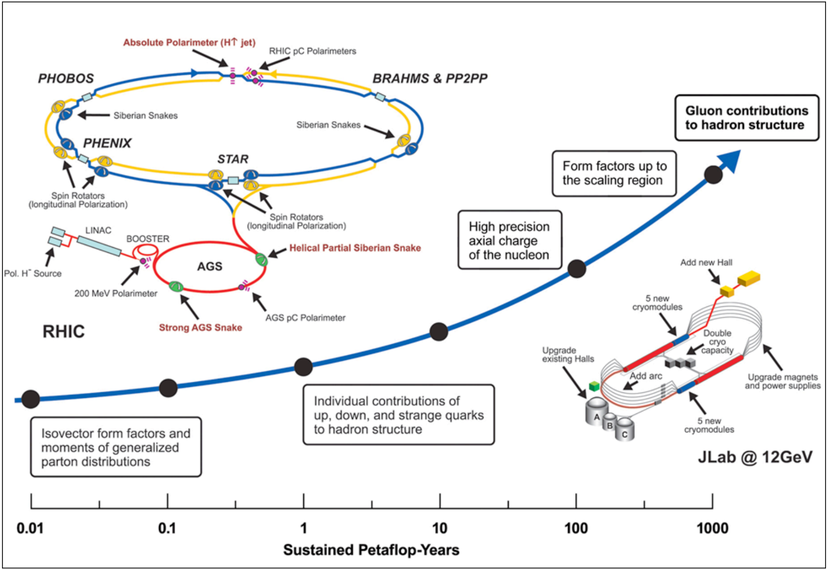
For precision hadron physics:

- Finite lattice spacing a - take the continuum limit $a \to 0$
- Finite volume L - take infinite volume limit $L \to \infty$
- Identification of hadron state of interest or excited state contributions - g_A, $\langle x \rangle$ and nucleon σ-terms
- Simulation at physical quark masses - now feasible
- Inclusion of quark loop contributions in hadronic observables - now feasible

$\Longrightarrow$ exascale computer resources

Computational resources

Report on Nuclear Physics, Extreme Computing, Washington D.C., USA, Jan. 26-28, 2009.



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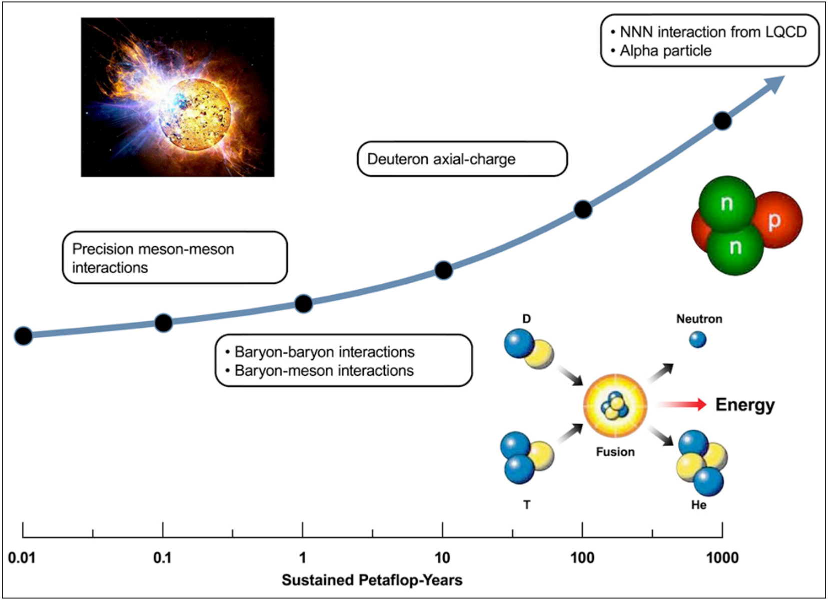

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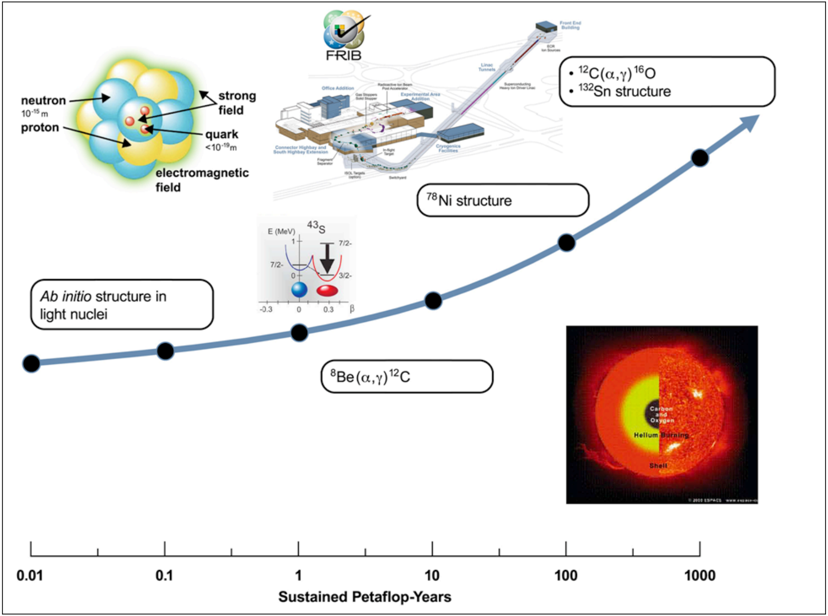
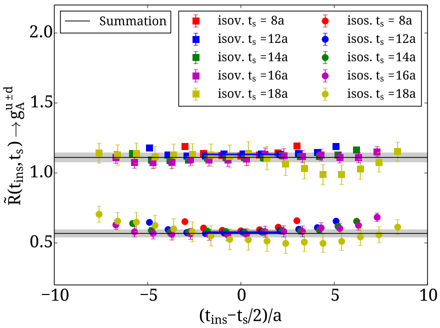
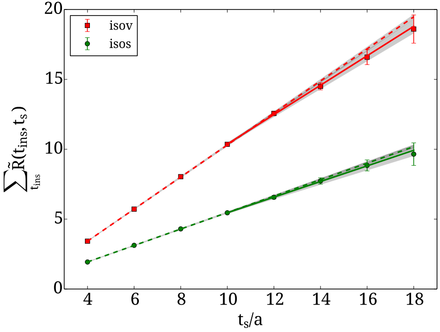


Axial charge g_A

Axial-vector FFs: $A^3_\mu = \bar{\psi}\gamma_\mu\gamma_5\frac{\tau^3}{2}\psi(x) \Longrightarrow \frac{1}{2}\bar{u}_N(\vec{p}')\left[\gamma_\mu\gamma_5 G_A(q^2) + \frac{q^\mu\gamma_5}{2m}G_p(q^2)\right]u_N(\vec{p})|_{q^2=0}$
$\rightarrow$ yields $G_A(0) \equiv g_A$: i) well known experimentally, & ii) no quark loop contributions

$N_f = 2+1+1$ twisted mass, a = 0.082 fm, m_π = 373 MeV, 1200 confs





- No detectable excited states contamination
- Consistent results between summation and plateau methods

For this study we used PRACE Tier-0 resources (JUQUEEN): 1.7 Tflops-years sustained making use of EigCG
$\rightarrow$ about 500 Tflops-years at the physical point for the same calculation keeping a the same and doubling L

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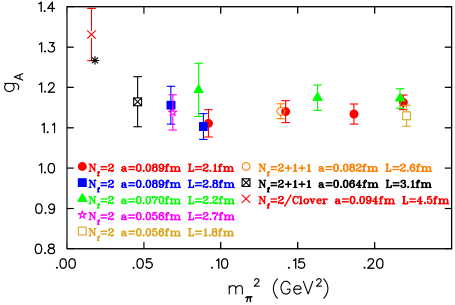


We needed 5.5 Tflops-years for 6% in g_A at the physical point with $L = 48$ and $a \sim 0.1$ fm $\rightarrow \sim 200$ Tflop/s-years for 1% error at sink-source separation of 1.1 fm

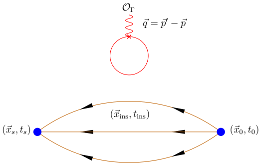
Results from ETMC, C.A., M. Constantinou, S. Dinter, V. Drach, K. Jansen, C. Kallidonis, G. Koutsou, arXiv:1303.5979

- Results at physical pion mass are now becoming available $\rightarrow$ need a dedicated study with high statistics, a larger volume and 3 lattice spacings
- A number of collaborations are engaging in systematic studies, e.g.
  - $N_f = 2+1$ Clover, J. R. Green *et al.*, arXiv:1209.1687
  - $N_f = 2$ Clover, R.Hosley *et al.*, arXiv:1302.2233
  - $N_f = 2$ Clover, S. Capitani *et al.* arXiv:1205.0180
  - $N_f = 2+1$ Clover, B. J. Owen *et al.*, arXiv:1212.4668
  - $N_f = 2+1+1$ Mixed action (HISQ/Clover), T. Bhattacharya *et al.*, arXiv:1306.5435

Disconnected quark loop contributions

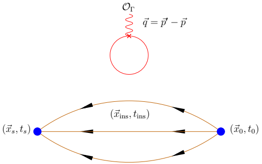
Notoriously difficult

- $L(x_{\rm ins}) = Tr\,[\Gamma G(x_{\rm ins}; x_{\rm ins})] \;\rightarrow$ need quark propagators from all $\vec{x}_{\rm ins}$ or L^3 more expensive as compared to the calculation of hadron masses
- Large gauge noise $\rightarrow$ large statistics



- Use special techniques that utilize stochastic noise on all spatial lattice sites $\rightarrow N_r$ more expensive that hadron masses with $N_r \ll L^3$
- Reduce noise by increasing statistics
  $\Longrightarrow$ take advantage of graphics cards (GPUs) $\rightarrow$ need to develop special multi-GPU codes

Disconnected quark loop contributions



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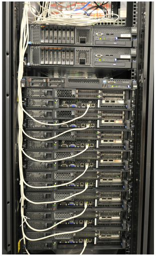
A Fermi card



Cluster of 8 nodes of Fermi GPUs at the Cyprus Institute

C. A., M. Constantinou, S. Dinter, V. Drach, K. Hadjiyiannakou, K. Jansen, G. Koutsou, A. Strelchenko, A. Vaquero arXiv:1211.0126
C.A., K. Hadjiyiannakou, G. Koutsou, A. O'Cais, A. Strelchenko, arXiv:1108.2473

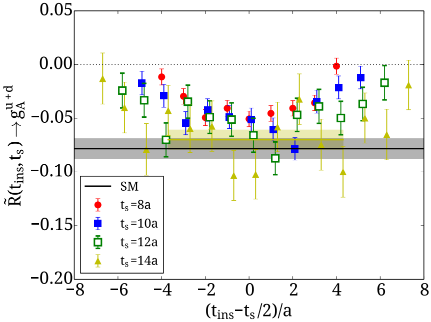
Axial charge g_A

To compute $\Delta\Sigma^q$ we need also the isoscalar g_A^{u+d}

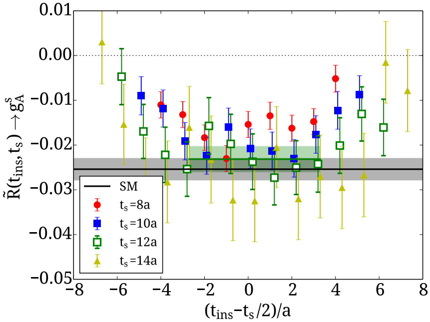
Dedicated high statistics study

Choose one ensemble to perform a high statistics analysis for all disconnected contributions to nucleon observables

$N_f = 2+1+1$ twisted mass, a = 0.082 fm, m_π = 373 MeV, $\sim$ **150, 000** statistics (on 2300 confs)
For the light, strange and charm loops we needed: 1.2 M2070 GPU-years or about 1.4 Tflop/s-months



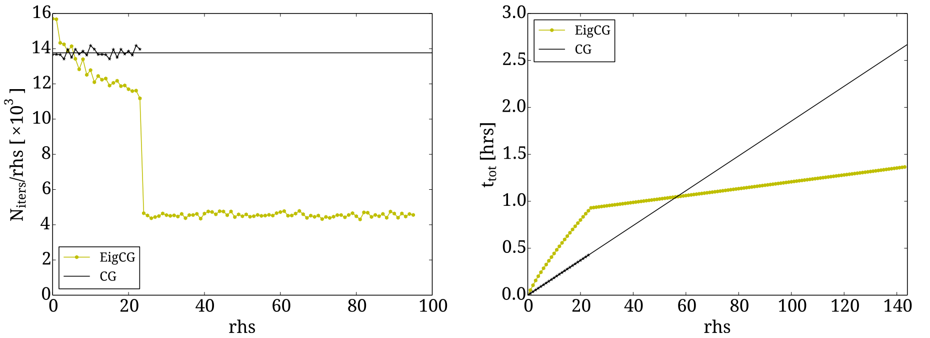
Disconnected isoscalar, agrees with Bali *et al.* (QCDSF), Phys.Rev.Lett. 108 (2012) 222001



Strange quark loop

Methods

EigCG (A. Stathopoulos & K. Orginos, SIAM J. Sci. Comput. 32 (2010) 439-462)



Accumulate EVs with every new rhs

- Approximate, lowest eigenvectors
- Used to provide next CG starting vector
- Speed-up in number of iterations $\sim$3.5
- Speed-up in runtime depends on total rhs, e.g. $\sim$3 for $N_{\text{rhs}} = 150$

Methods

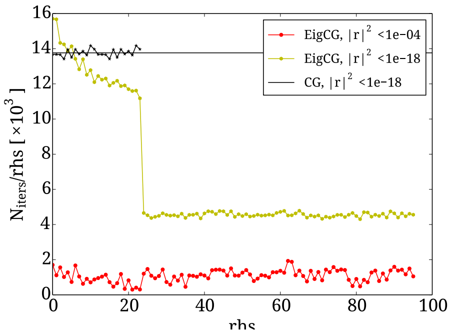
Further gains by using relaxed numerical precision

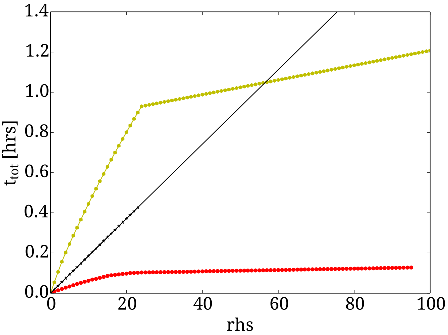
- Solver accuracy typically set much smaller than statistical accuracy
- Mixed precision
  - ★ Compute $N_{\rm HP}$ (expensive) correlation functions to full-precision C^H
  - ★ Compute $N_{\rm LP}$ (cheap) correlation functions to low-precision C^L
  - ★ Improved estimator:

$$C^{\rm I} = \frac{1}{N_{\rm HP}} \sum_i^{N_{\rm HP}} (C_i^{\rm H} - C_i^{\rm L}) + \frac{1}{N_{\rm LP}} \sum_j^{N_{\rm LP}} C_j^{\rm L}$$

- Error scales as $\sim \frac{1}{\sqrt{N_{\rm LP}}}$, namely $e \propto \sqrt{2(1-r) + \frac{1}{N_{LP}}}$
  with $r \simeq 1$ the correlation between $C_i^{\rm H}$, $C_i^{\rm L}$
- Truncated Solver Method:
  G. Bali, S. Collins & A. Schafer, Comput. Phys. Commun. **181** (2010) 1570
- Covariant Approximation Averaging:
  T. Blum *et al.*, Phys. Rev. **D88** (2013) 094503

Methods





Combined EigCG and CAA

- Small number of full-precision correlators
- Relaxed-precision correlators $5\times$ faster than full-precision EigCG
- Improvements due to combined EigCG+CAA $\simeq \times 10$

Interest in a CoE

As Simulation Lab we would have interest in the following WPs:

- WP1 - Community software development
- WP2 - New algorithms for large-scale simulations
- WP3 - Languages and programming models for heterogeneous architectures
- Some hardware related
- Would like to see an application-focused WP related to Lattice QCD
- ...