HPC in QCD and Nuclear Physics

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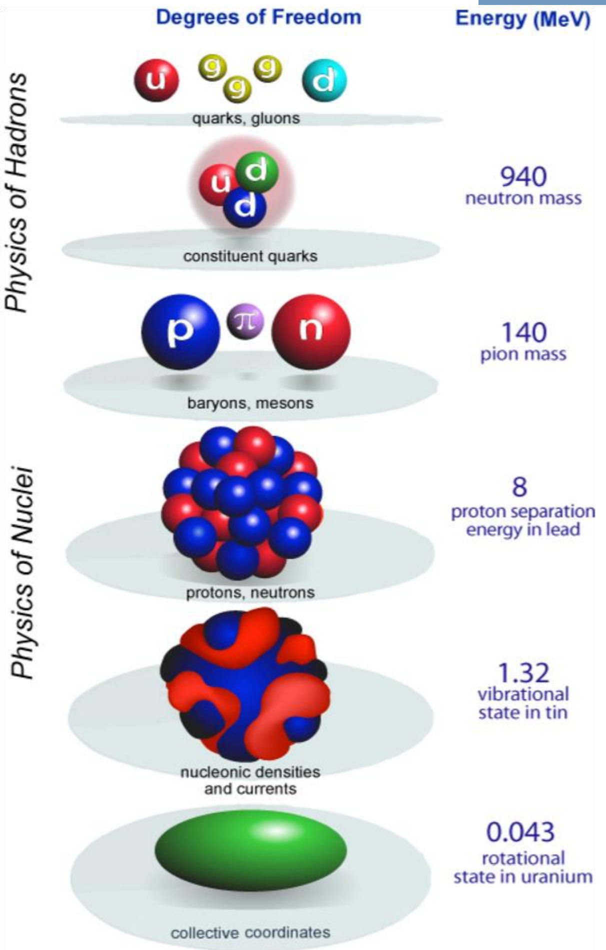
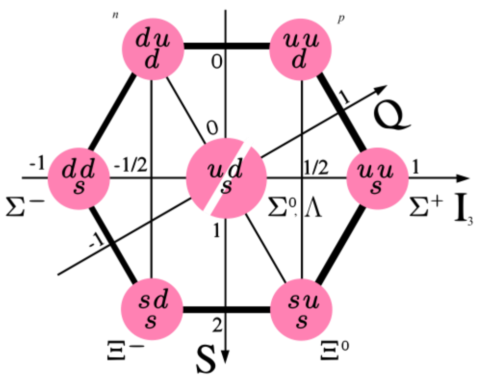
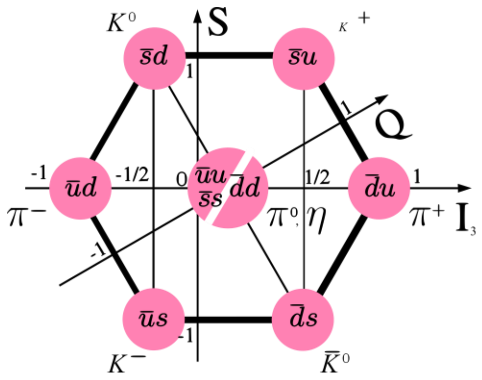
CNRS – IN2P3 – Conseil Scientifique calculs et données

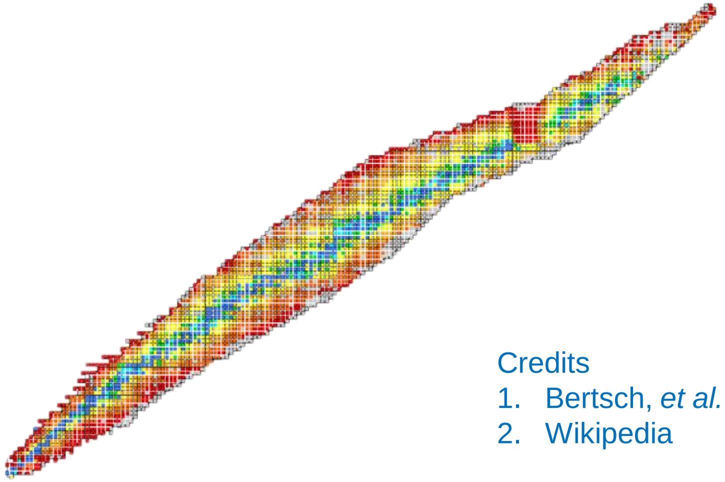
HPC in QCD and Nuclear Physics

Covering the physics of the two infinite









Credits
1. Bertsch, *et al.*
2. Wikipedia

Credits ESA

Structure of HPC applications for QCD and NP at IN2P3

PI & Projects self-reporting

Project	Personnel	Laboratory	HPC Center	Topic
IN2P3 project ENFIA	Nadya Smirnova	IP2iB	Mesocentre MCIA	Ab initio
				Nuclear structure
IN2P3 project BRIDGE	Guillaume Hupin	IJCLab	GENCI	Ab initio
ANR NECTAR			CC-IN2P3	Nuclear reactions
ANR NEWFUN	Michael Bender	IP2I	CC-IN2P3	Nuclear structure
	Karim Bennaceur		In-house cluster	
IN2P3 project PUMA	Rimantas Lazauskas	IPHC	GENCI	Ab initio
			CC-IN2P3	Nuclear reactions
IN2P3 project Speedy Charmonia	Benoît Blossier	IJCLab	PRACE	Lattice QCD
				Non-perturbative QCD
ANR LatHiggs			GENCI	
NC	Mariane Mangin-Brinet	LPCS		Nucleon structure and spectroscopy
NC	Vincent Morénas	LP- Clermont	CC-IN2P3	
				Flavor physics
NC	Marek Ploszajczak	GANIL	In-house cluster	Nuclear structure
NC	Hubert Hansen	IP2I	GENCI	Dense nuclear/QCD
	Jérôme Margueron		CC-IN2P3	Neutron stars
IN2P3 project EPOSHQ	Klaus Werner	Subatech	CC-IN2P3	Quark-gluon plasma
	Jörg Aichelin			
	Pol-Bernard Gossiaux			HE nuclei-nuclei collisions
	Marlène Nahrgang			

Key figures

15
Staff scientists or Professor/Tenure track

3
ANR

5
IN2P3 master projects

In brief

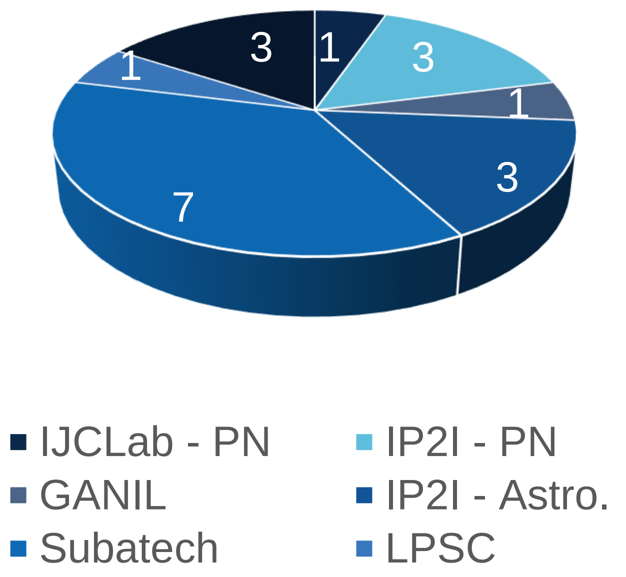
~70% of personnel either belongs to IN2P3 or an ANR project

- All IN2P3 projects are supporting experimental investigations (CERN/GANIL/ex. EU facilities);
- All IN2P3 applications have international contributors;
- CCIN2P3 serves as the institute mesocenter for HPC applications;
- Many IN2P3 theory teams are developing codes that are not ported to many-cores – many-nodes – or accelerated computing;
- So far all the HPC skills exist “in-house”.

Losing CCIN2P3 HPC means that theory teams would need lab. financial support to use mesocenters.

1:1

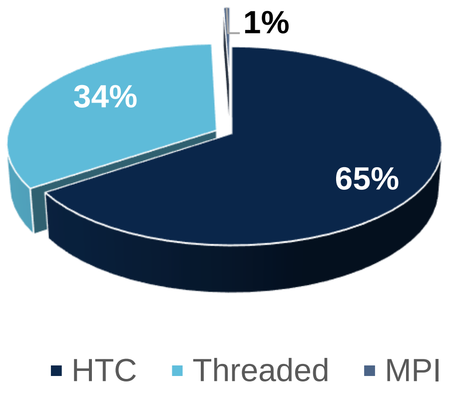
Ratio between staff to PhD students

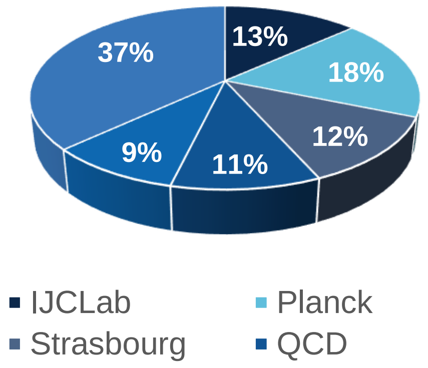


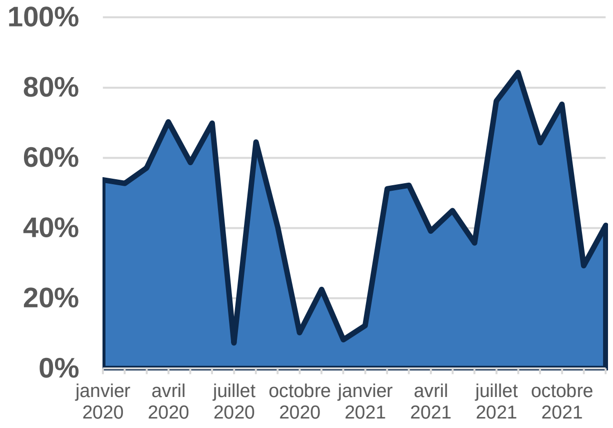
Technical reporting

GENCI usage at IN2P3
CCIN2P3 usage by PIs

HPC partition at CCIN2P3







Share per paradigm

- HPC only represents 1% of the total;
- pre- or post-processing are run on either HTC or HPC partitions;
- frontier between the two paradigm not clear in data driven era.

HPC per project

- no laboratory or project identifies as a key user of the resources;
- lack of institute wide policy on the topic;
- IN2P3 teams have not been renewed with junior scientists, so far.

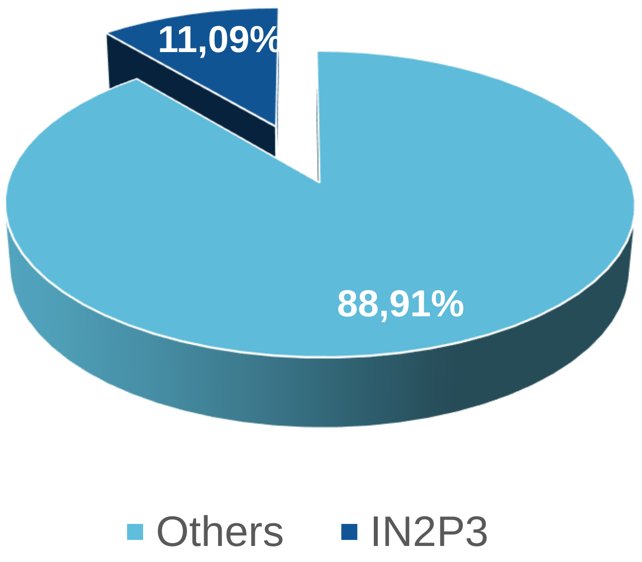
HPC yearly use

- the prototypical HPC usage: period of intense workload alternating with underuse;
- large fluctuations reflect small number of permanent or fixed-term staffs.

IN2P3 share of GENCI ressources

11% of the GENCI capabilities are either consumed or requested by IN2P3 PIs

- LQCD is the largest contributor to IN2P3 HPC applications;
- As of 2019 (cf. GENCI report), the share of others computing grant in the “Theoretical and plasma physics” section has increased to 20% and is continuously growing;
- Nuclear astrophysics projects are submitted to “Astrophysics and Geophysics” section;
- 100% of the applications performed on GENCI machines derived from either open-source codes or international collaborations;
- IN2P3 PIs contribute to code development, porting and continuous implementation of new formalism.

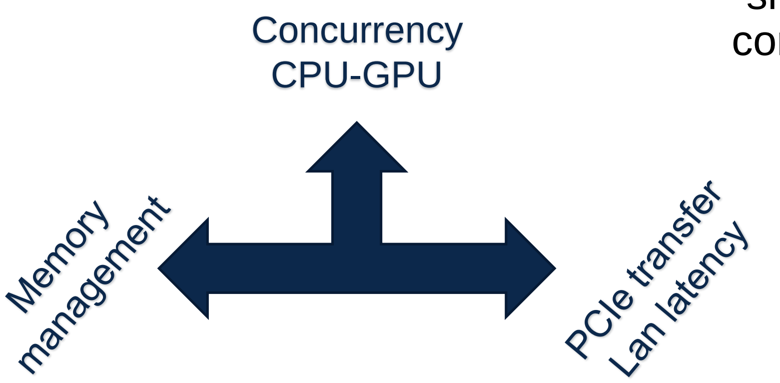


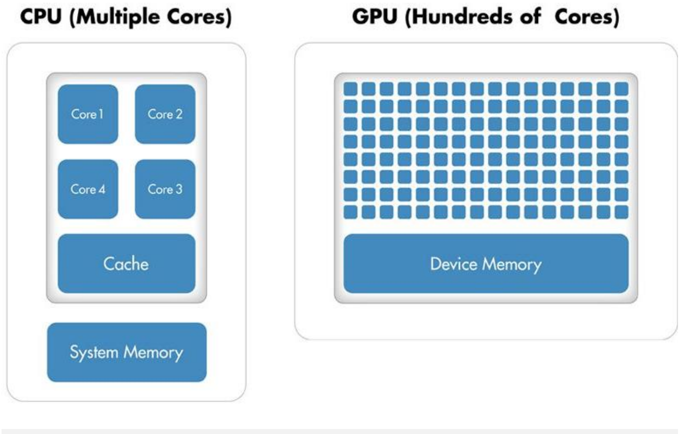
Porting to GPU

EuroHPC exascale project

Challenges

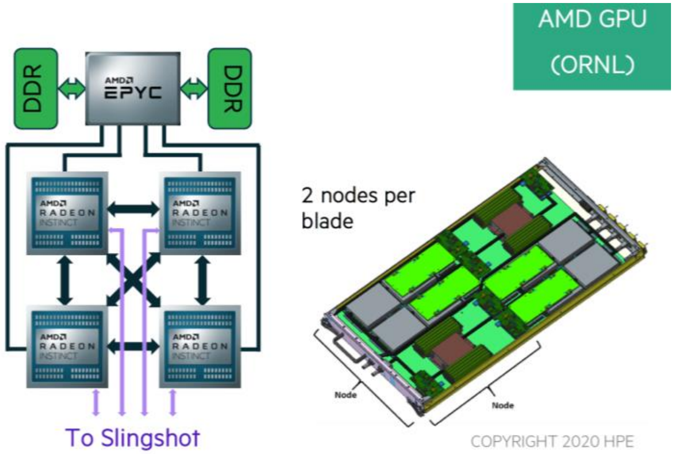
- **Porting code to GPUs:** requires significant man power as it often implies algorithm rewriting.
- **Code rewritting:** breaking complex algorithm to an ensemble of simple mathematical tasks.
- **Compatibility:** instruction based/language implementation for offloading to GPU (NVIDI/AMD).





CPU vs GPU

CPU: few flexible general purpose cores vs thousands of simple processing units where computing problems are broken into simple mathematical operations



Many GPUs nodes

Distributed tasks/shared memory over many GPUs communicating on single node via bus CPU-GPU-GPU itself within a network of nodes with distributed memory

Opportunities

Exascale: >1000 Pflop/s (ex. FRONTIER US/DOE) versus 61 Pflop/s (ADASTRA CINES)

Do not expect better scaling without algorithmic developments

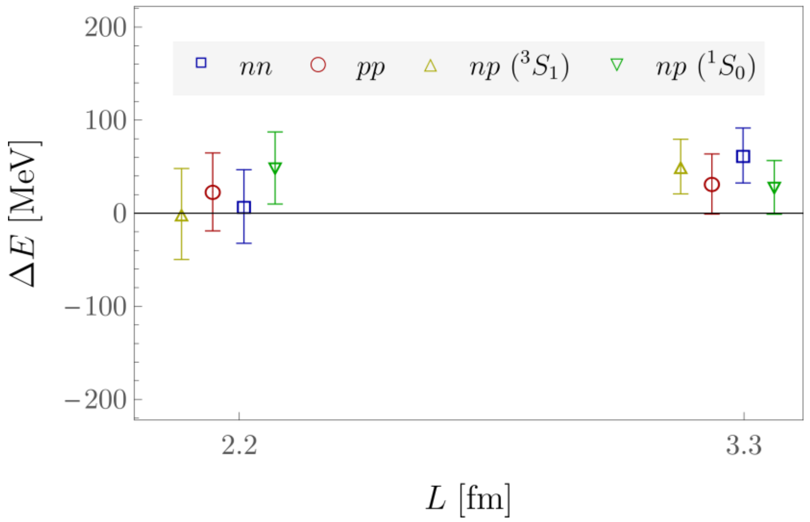
What can we expect from a gain of two orders of magnitude in computing capabilities ?

LQCD:

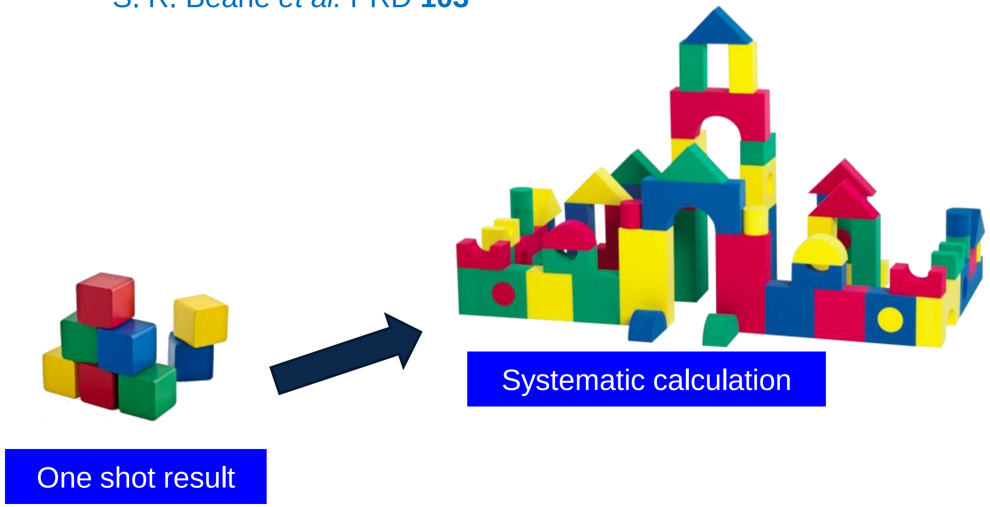
- Smaller lattice spacing/large.
- Many (≥ 6) quarks systems at physical π masses.

Nuclear Physics:

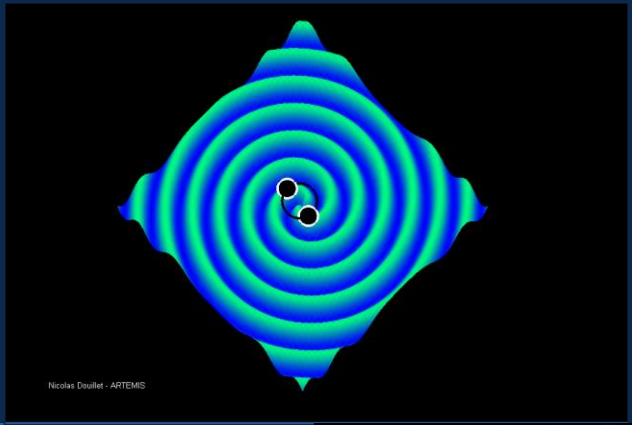
- Systematic calculations (uncertainty quantifications).

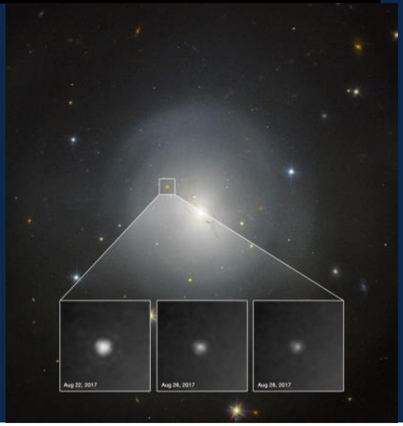


S. R. Beane *et al.* PRD **103**



Nuclear Astrophysics

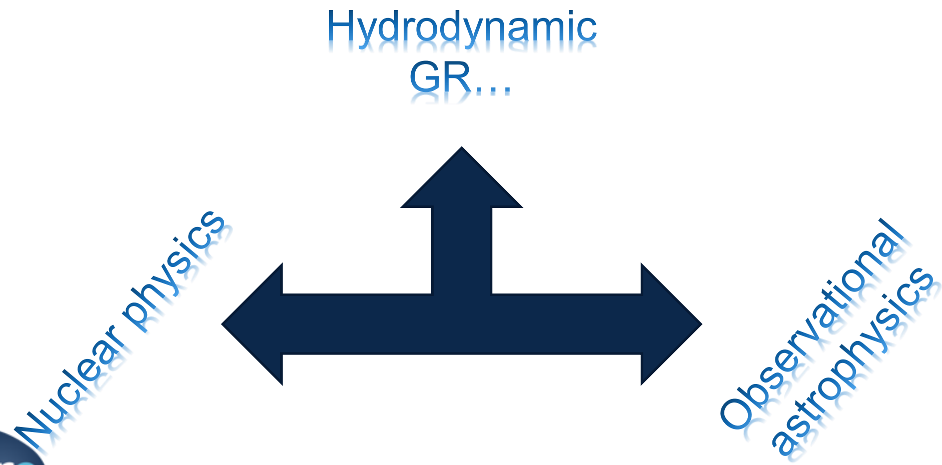


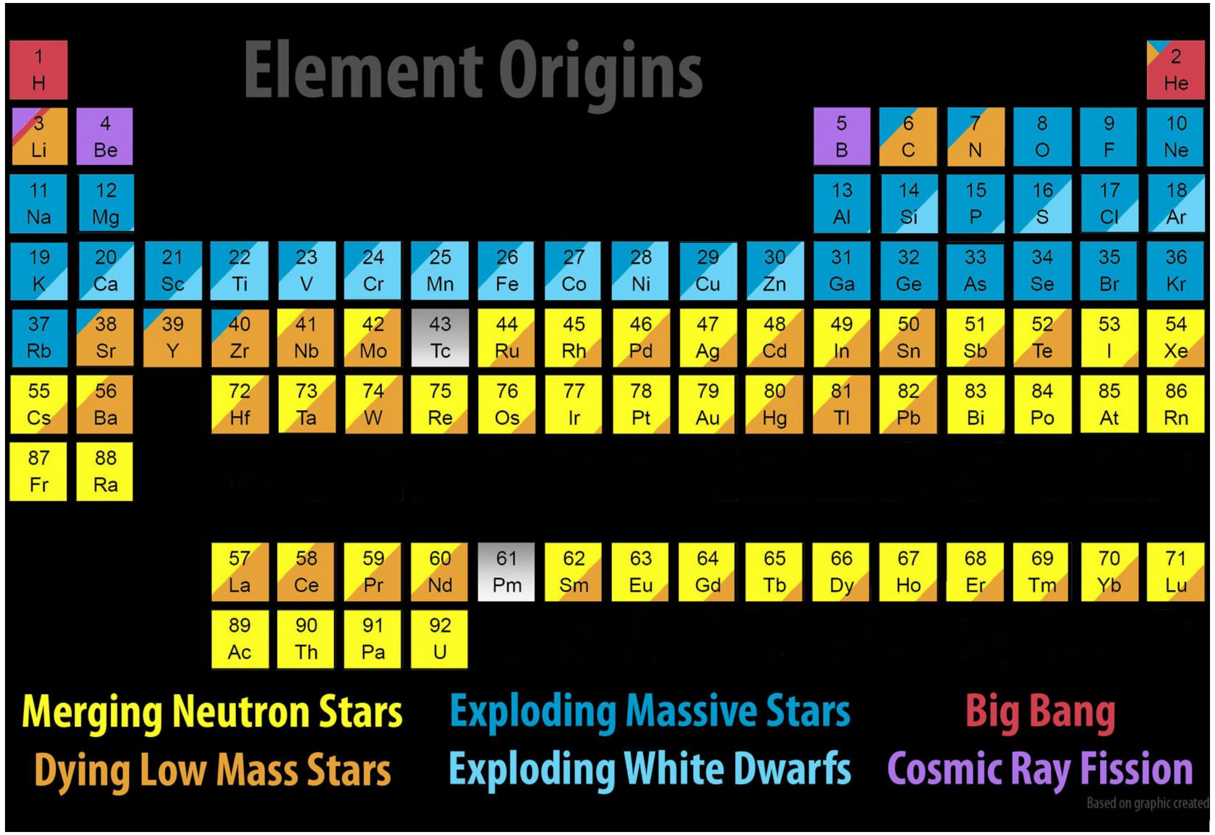


Wikipedia, NASA

Nuclear Astrophysics

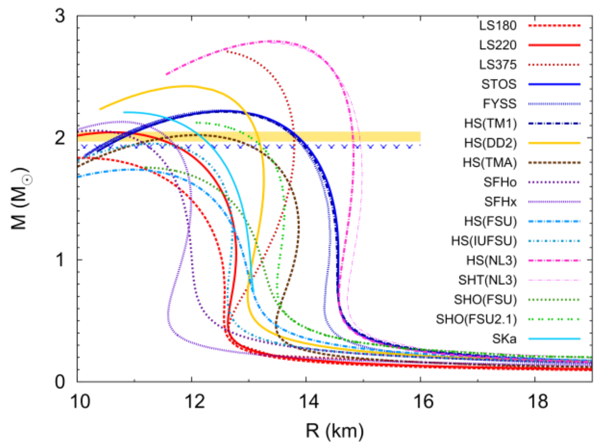
- nuclear reactions and their rates in cosmic environments, directly explain the **origin** of the **chemical elements** and isotopes;
- nuclear astrophysics probes the limits of bound nuclei and those of our knowledge in nuclear physics.





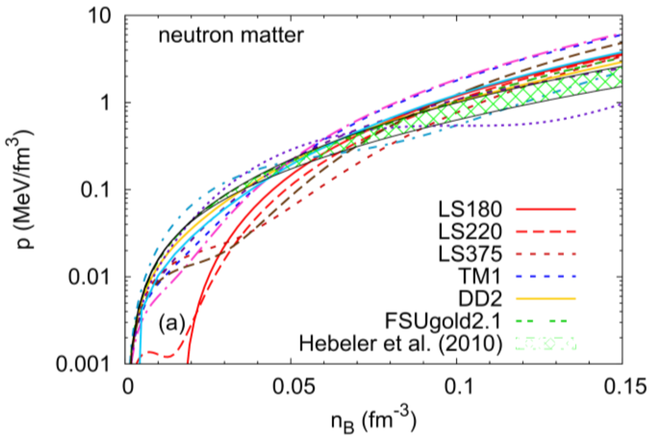
Nucleosynthesis. NASA

Probing the nuclear equation of state in the stars



NS Mass-to-radius

1-1 correspondence between dense matter EoS and static properties of NSs



Neutron EoS

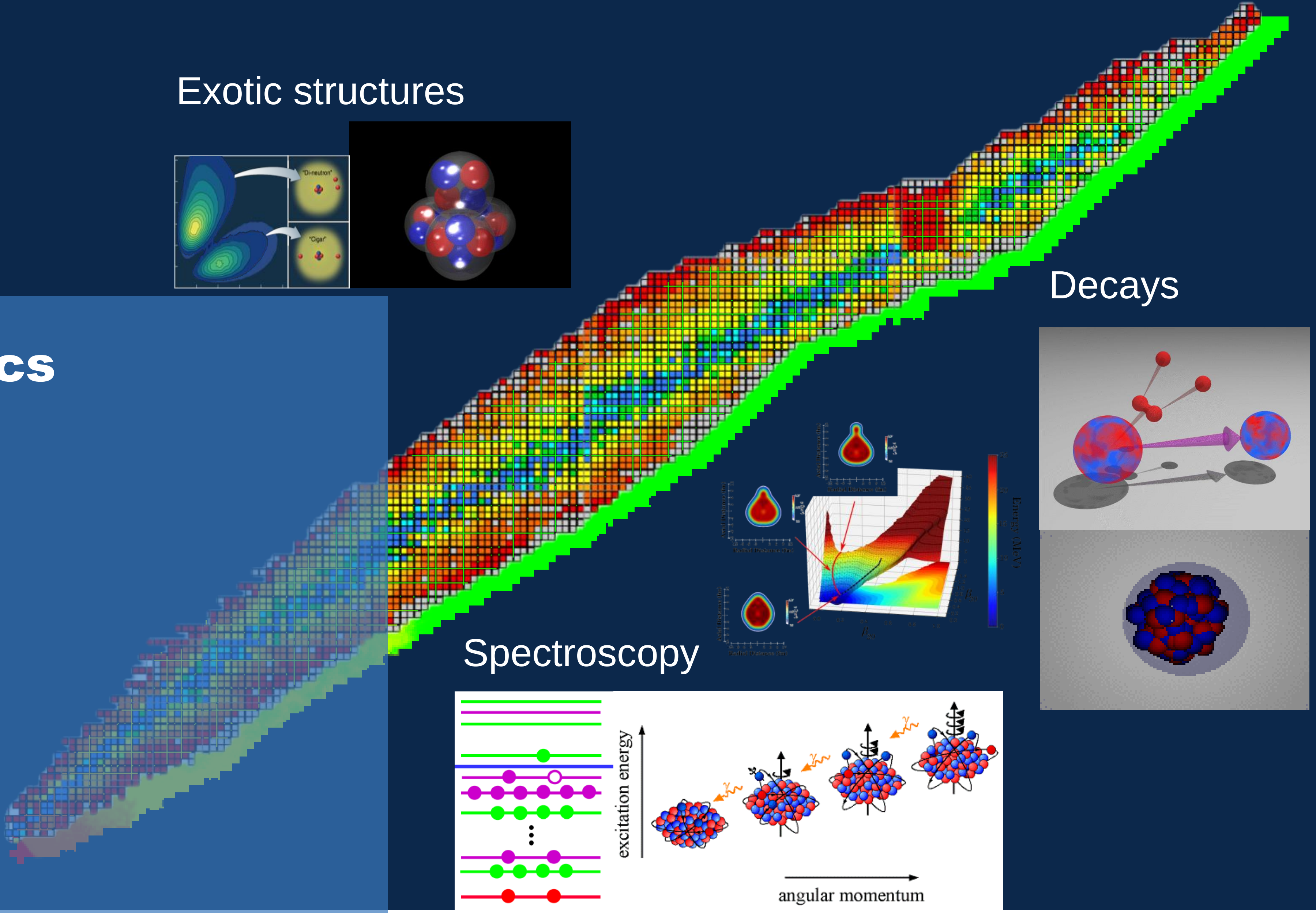
Nuclear EoS strongly depends on models at $\rho > \rho_0$, far from the region of confidence of the fits

- **GW** observations have shown their ability to globally constrain the **EoS of dense matter**;
- **MagnetoHydroDynamic simulations** of neutron star mergers can **probed** the effects of different nuclear **EoS**.

1. is the matter still largely composed of nucleons, as in the external region of the core?
2. do new degrees of freedom appear, such as quarks?
3. if so, what signatures in the GW and electro-magnetic signals would be made by hadronization during the BNS coalescence?

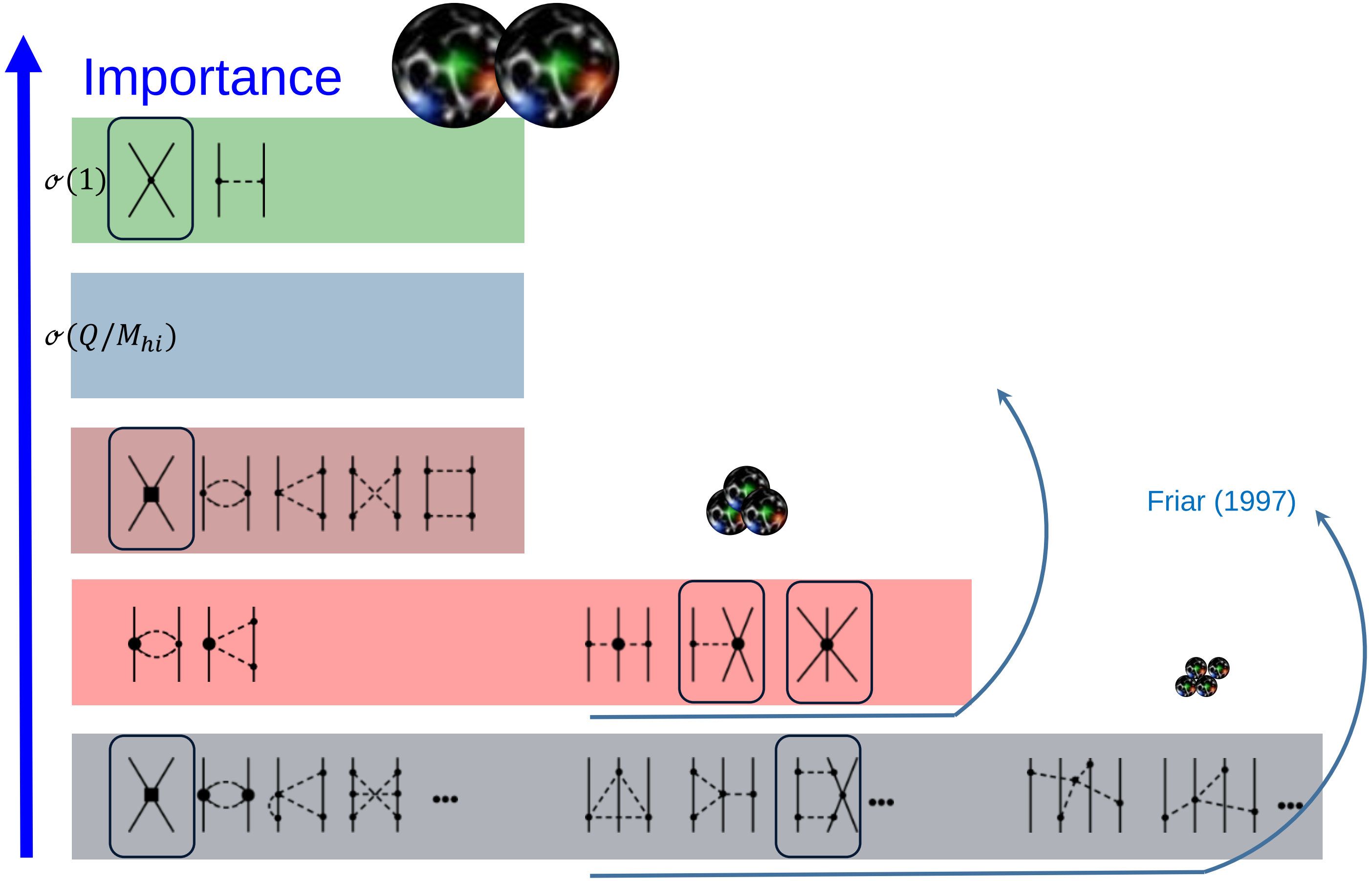
M. Oertel, et al. Rev. Mod. Phys. **89**

Nuclear Physics

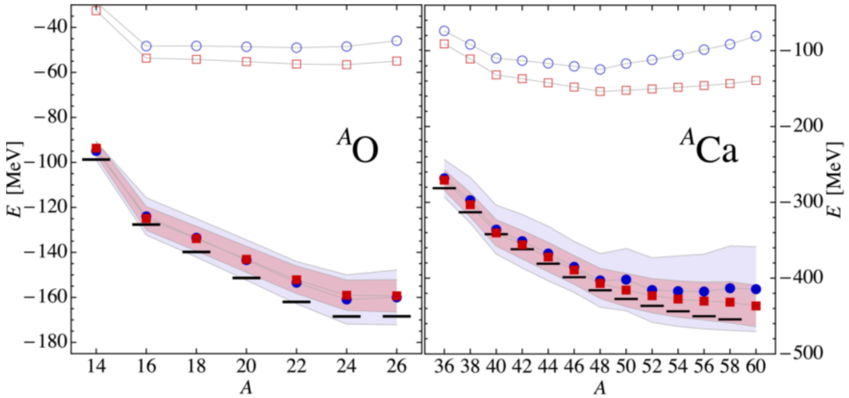


Courtesy T. Duguet *et al.*

EFTs: Chiral or other



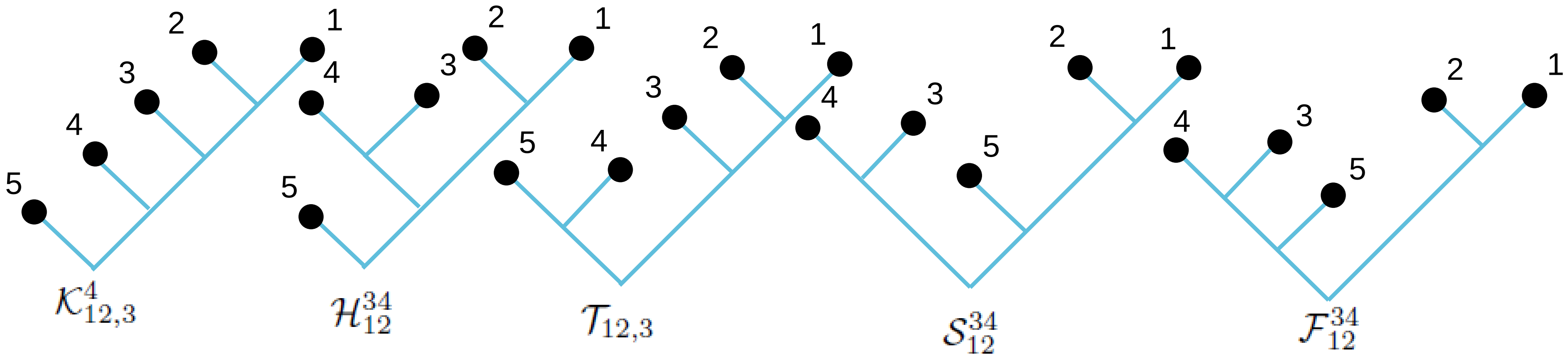
Weinberg (1990-2); Ordóñez and vK (1992); etc…



A. Tichai, *et. al.* Front. Phys. **8**, 164 (2020)

- ☺ **High quality** nuclear interactions (at N^{3}LO).
- 😐 **Various** fits and successes.
- ☹ Weinberg PC wrong: no **renormalizability**.
- ☺ Correct power counting: active research

Exact Faddeev-Yakubovsky method



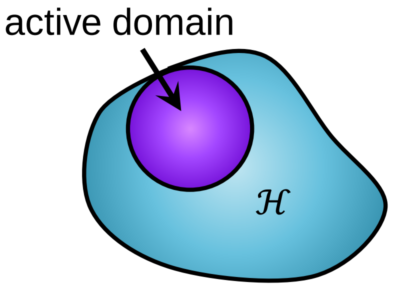
R. Lazauskas and J. Carbonell Few-Body Syst. **60**, 62 (2019)

System	Number eq. (= particles)	Number eq. (≠ particles)
$A = 2$	1	1
$A = 3$	1	3
$A = 4$	2	18
$A = 5$	5	180
$A = 6$	15	2700
$A = N$	$\mathrm{nint}\left(\frac{2(N-1)!}{\left(\frac{\pi}{2}\right)^N}\right)$	$\frac{N!\,(N-1)!}{2^{(N-1)}}$

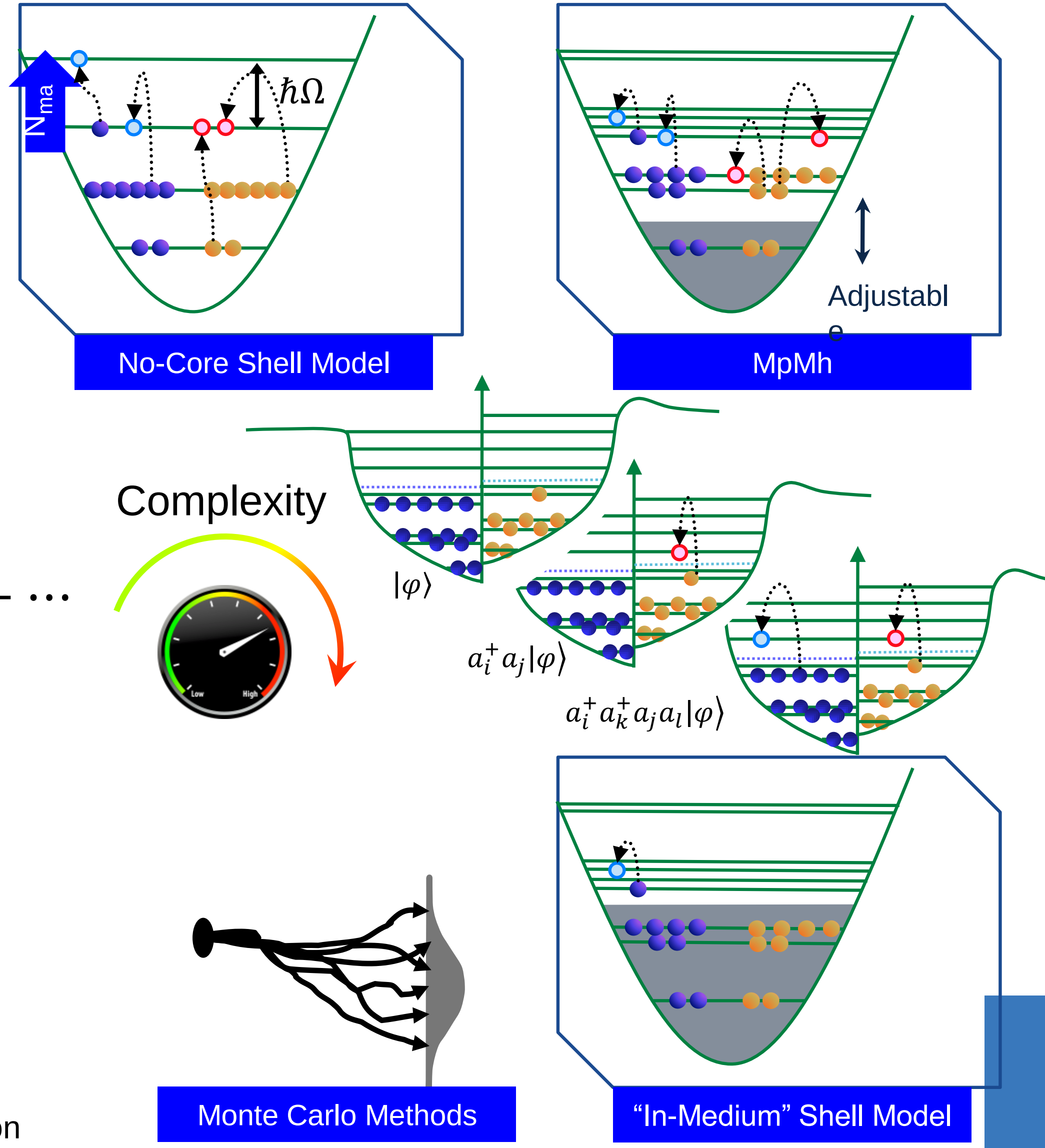
Applications

- Very **accurate**:
  1. Predictions for atomic systems;
  2. Coupling constant fit to data: nuclear, molecular, particle physics;
- Defines references ("calibration free");
- **CERN:** GBAR, PUMA; **NIST.**

Configuration interaction methods



- Variational.
- Orthonormal basis.
- Controllable parameters ($N_{\max}$, $E1_{\max}$ etc…)
- UV/IR convergence.

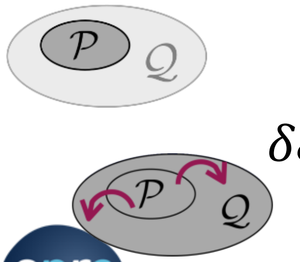


Superposition of Slater determinants:

$$|\Psi^A\rangle = \sum_\alpha c_\alpha \Phi_\alpha^\varphi(\vec{r}_1, \dots, \vec{r}_A) = A_0 \left|\Phi^0_{0p0h}\right\rangle + \sum_{\alpha'} A_{\alpha'} \left|\Phi^{\alpha'}_{1p1h}\right\rangle + \cdots$$

NCSM
IM-SH
MpMh

Optimization of mixing coefficients, one-body Hilbert space:

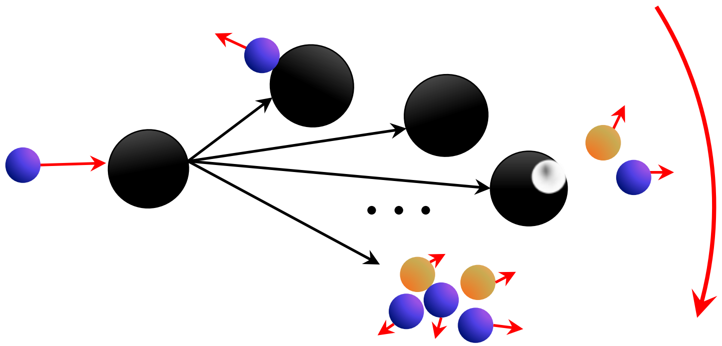


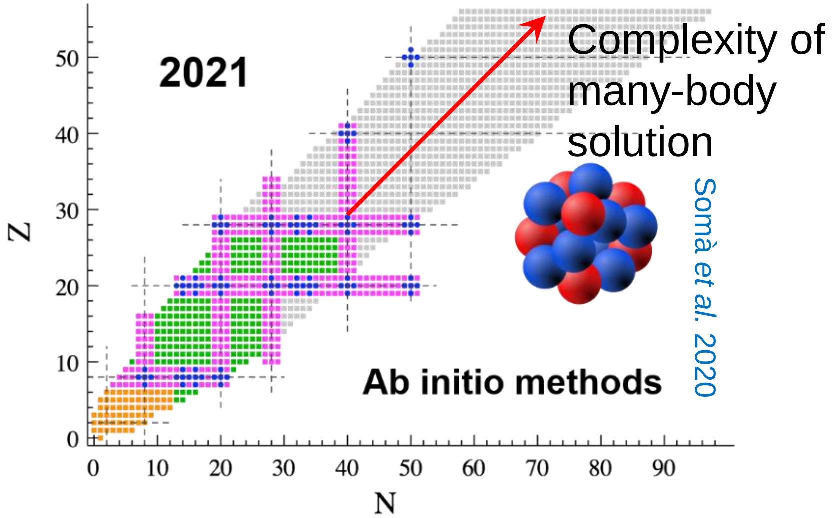
$$\delta\mathcal{E}[\Psi]_{/\{A_\alpha^*\}} = 0 \Rightarrow \sum_\beta A_\beta \langle \Phi_\alpha | \hat{H} | \Phi_\beta \rangle = E A_\alpha$$

$$\delta\mathcal{E}[\Psi]_{/\{\varphi_\alpha^*\}} = \langle \Psi | [\hat{H}, \hat{T}] | \Psi \rangle = 0 \Leftrightarrow [\hat{h}(\rho), \hat{\rho}] = \hat{G}(\sigma)$$

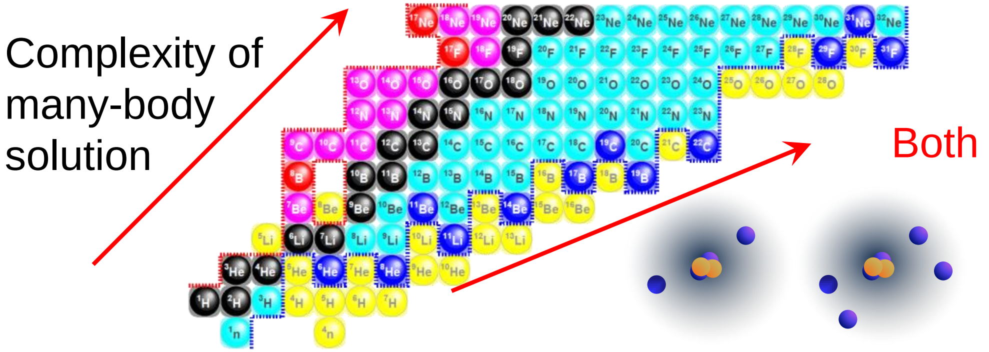
Generalized Brillouin (GB) equation

Scalability: new algorithms/more computing power





1. Computation of complex nuclear reaction mechanics
2. Ab initio structure for heavier systems
3. Drip lines physics



QCD and High-Energy physics

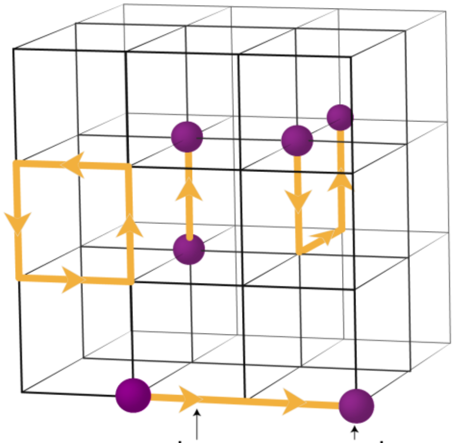
Wikipedia, NASA

Lattice QCD: Basics

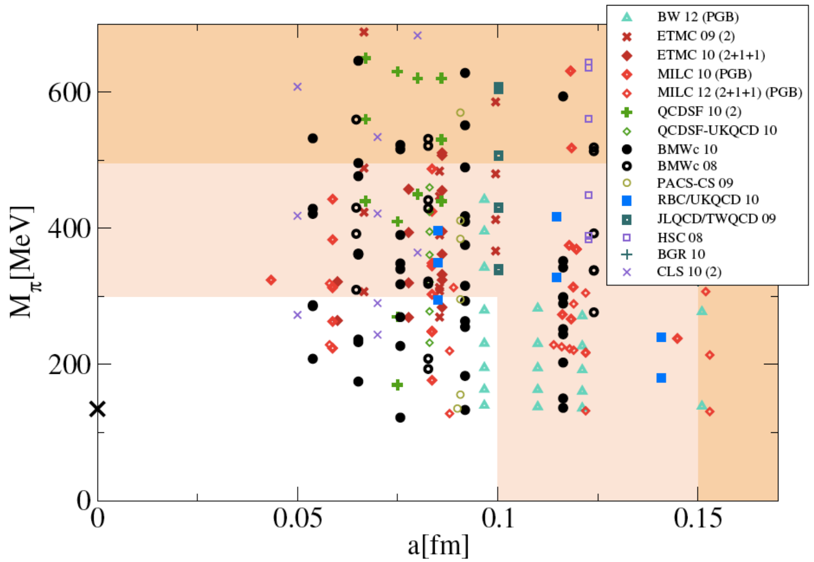
$$\mathcal{L} = \frac{1}{2} Tr[F_{\mu\nu}F^{\mu\nu}] + \sum_{f=1}^{N_f} \bar{\psi}_f(x)(i\not{D} - m_f)\psi_f(x)$$

Use Monte-Carlo on many configuration evaluate observable

$$\langle \mathcal{O}(\Phi) \rangle = \frac{1}{z} \int D[\Phi]\, \mathcal{O}(\Phi) e^{-iS(\Phi)}$$



- $L^3 \times T = 48^3 \times 96$
- 800×10^6 degrees of freedom
- $a \in [0.04, 0.1]$ fm ($L \in 2 - 6$ fm)



Generation of gauge configurations

☹ very expensive ($n = \mathcal{O}(10^3)$)

☺ need to be done **once**

Computation of the observable

☹ involves huge matrix

Lattice QCD: Searching for NP in support of experimental programs at CERN

Lepton Flavour Universality tests are now extensively performed to reveal possible tensions with Standard Model expectations.

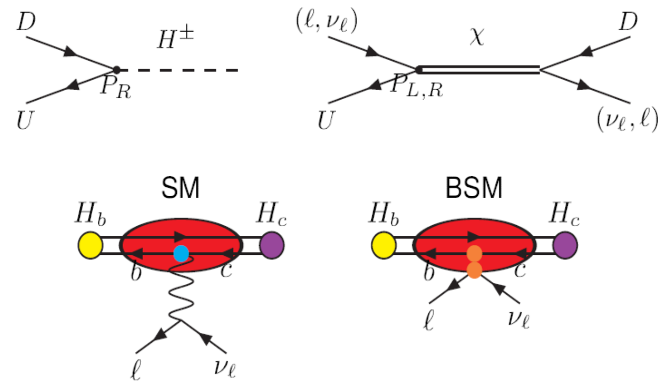
Form factors of $B_c \rightarrow J/\psi\, \ell \nu_l$

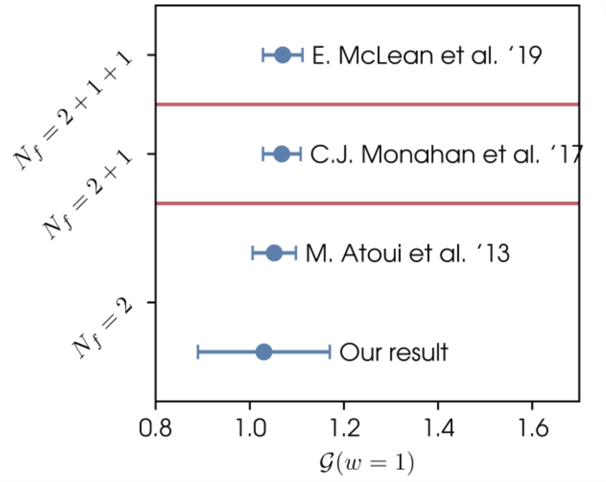
$B_s \rightarrow D_s^{(*)} \ell \nu_l$

from Lattice QCD

✓ Computation on ensembles with 2 + 1 dynamical quarks at the physical point.

$100^3 \times 200$ lattices: 500 Mch required in terms of computer time.
Port codes on GPUs?





Relativistic Ion Collisions

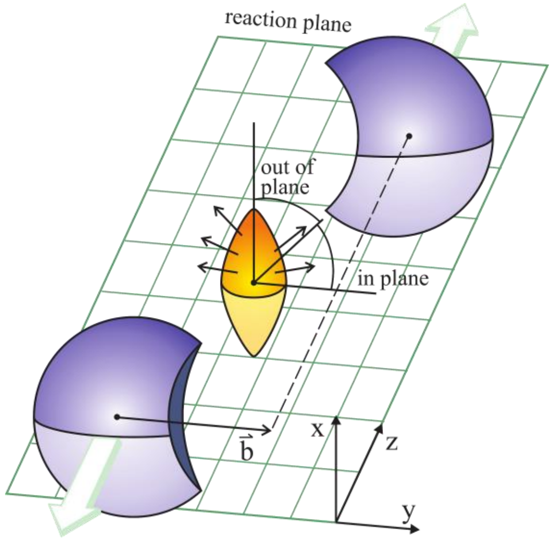
EPOS is an event generator for the simulation of collisions relevant at

- ATLAS, CMS, ALICE, LHCf... pp, heavy ions collision
- AUGER cosmic-ray air shower simulation
- RHIC (STAR, PHENIX)

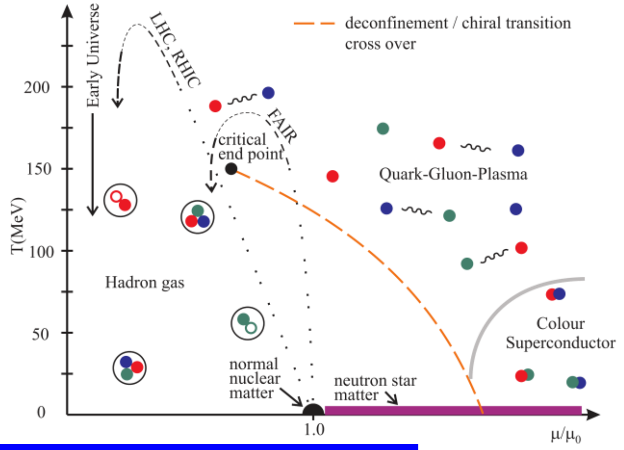
Hydrodynamical equations are solved to obtain the evolution of the quark-gluon plasma.

EPOS generates large data files (~To).

Contributes to interpretation of data.



Geometry of a heavy-ion collision



QCD phase diagram

B. Betz ArXiv 0910.4114

Thank you

www.cnrs.fr