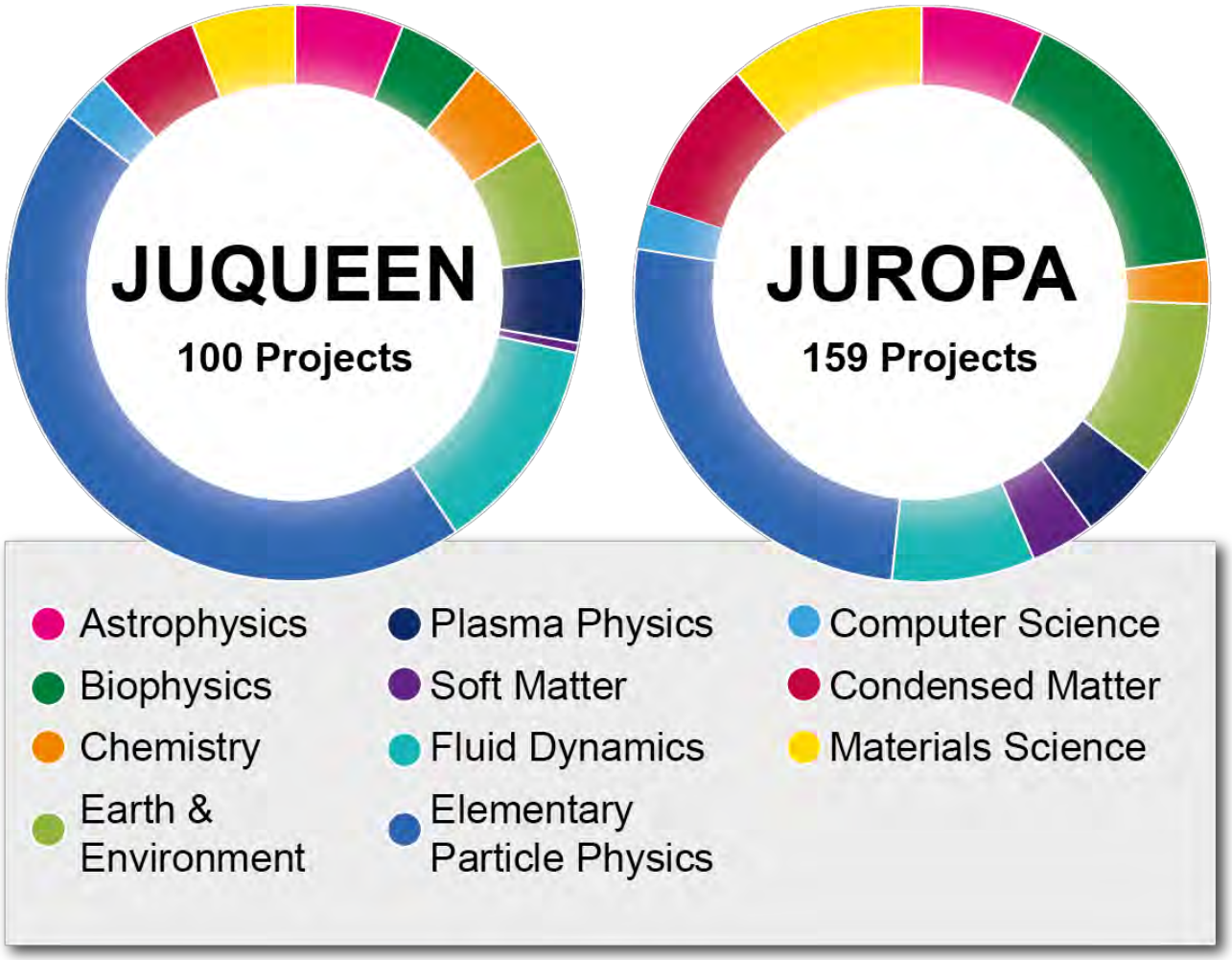
Astro, HEP, and plasma

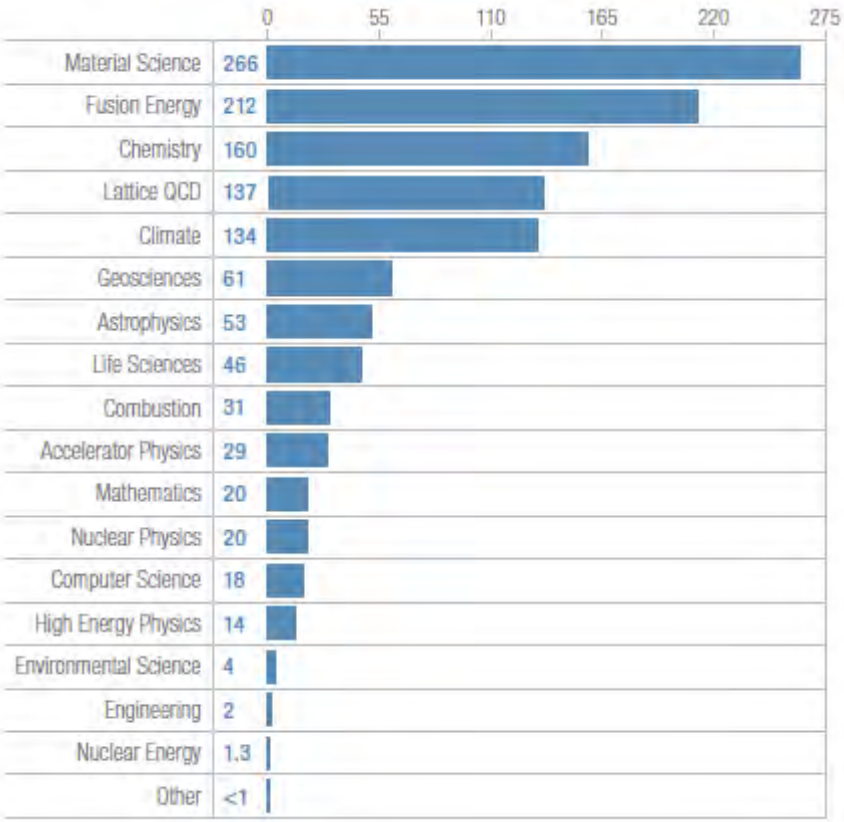
Data and computing needs

Stefan Krieg-Venghaus | Jülich Supercomputing Centre

Present usage: JSC

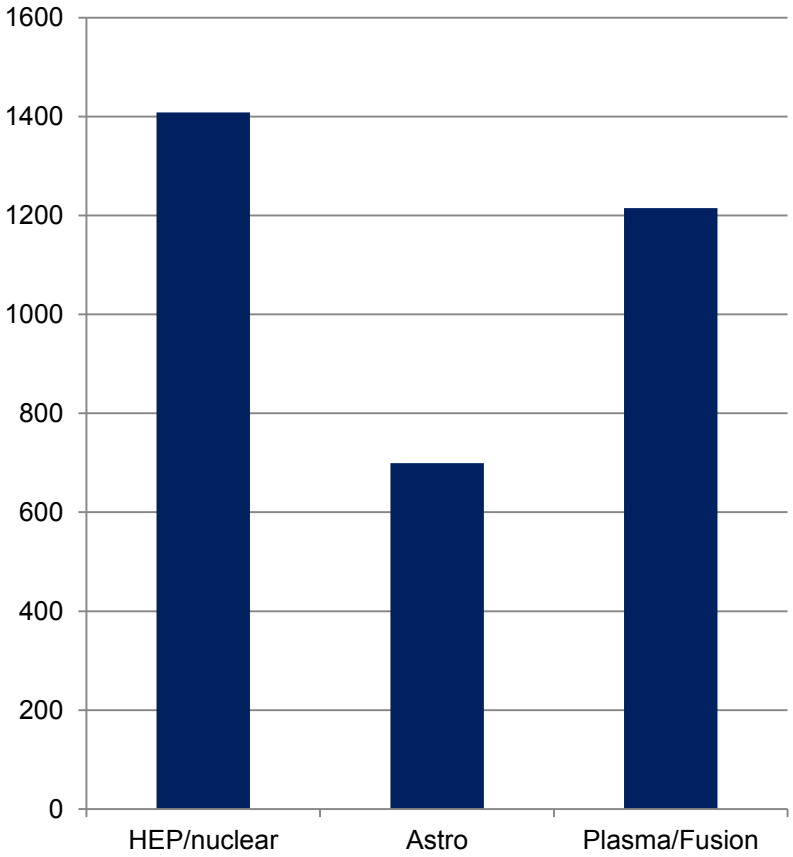


Present usage: US



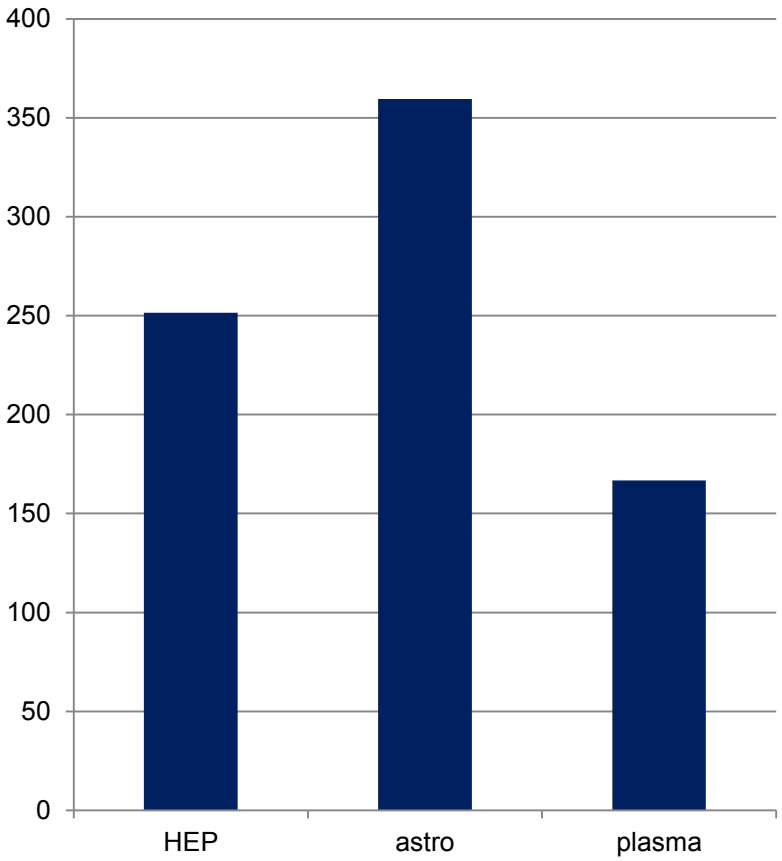
NERSC 2013

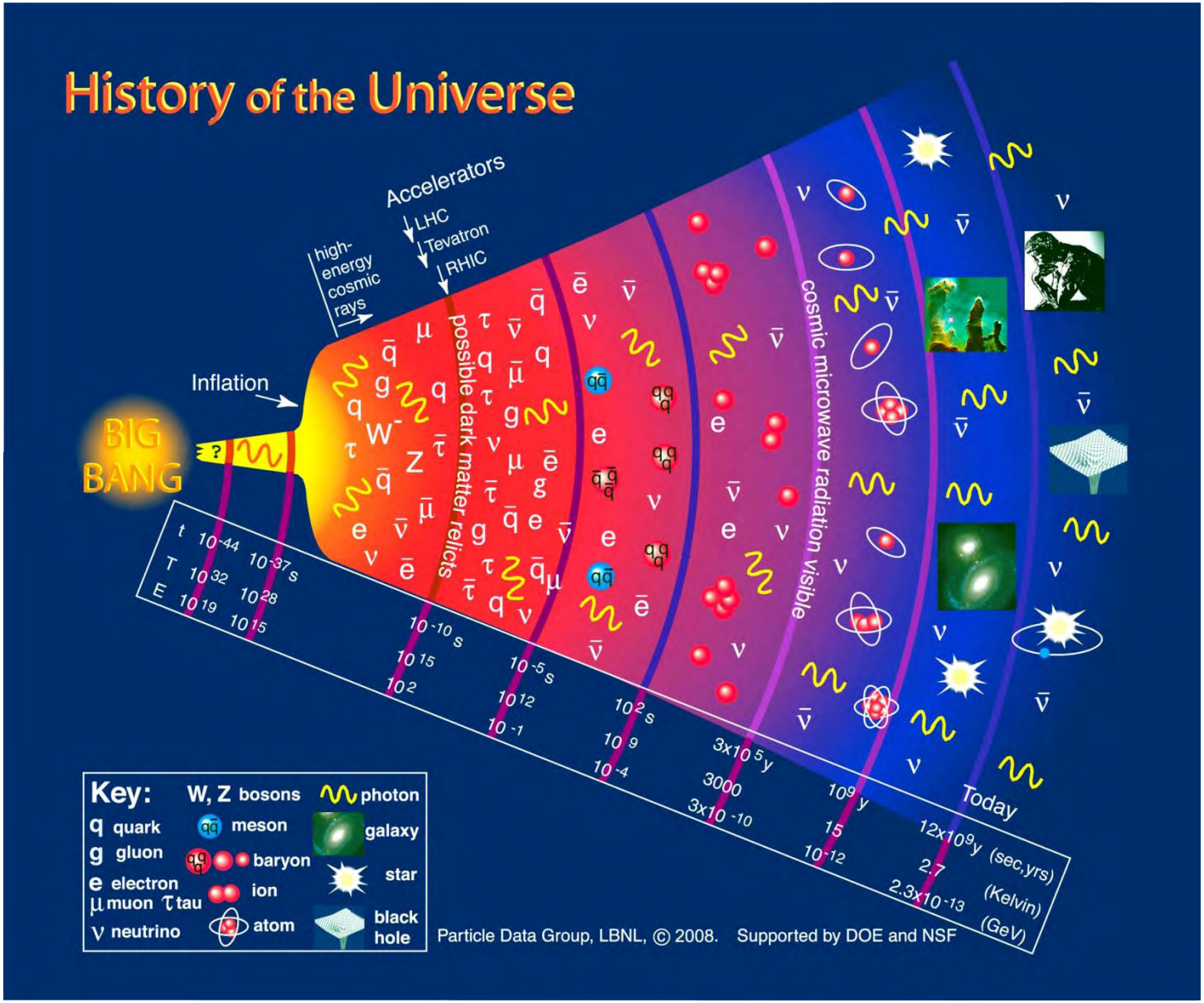
DoE INCITE 2014+2015 allocations



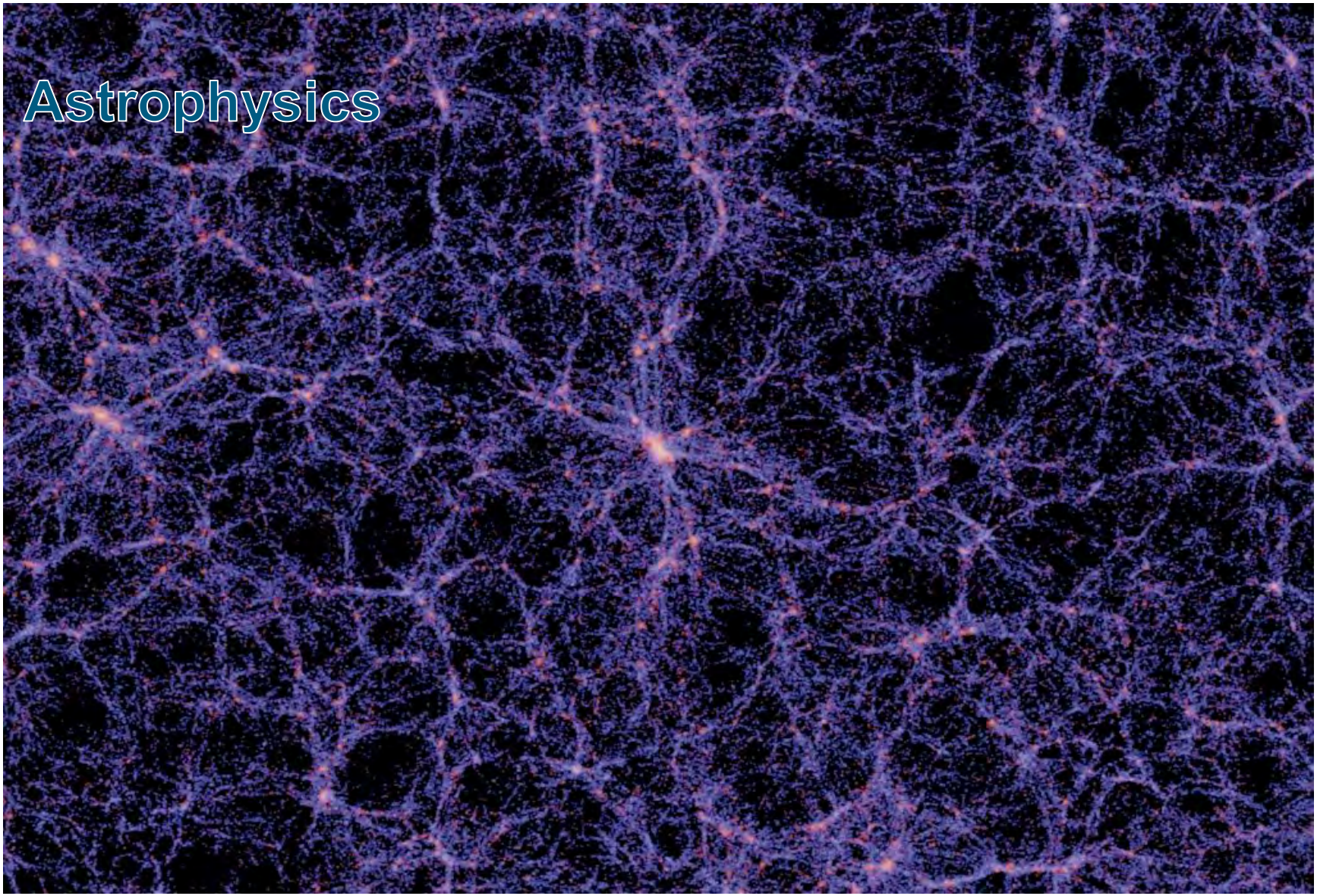
Present usage: PRACE

PRACE 2014 (calls 8&9) allocations





Astrophysics



Astro: science case

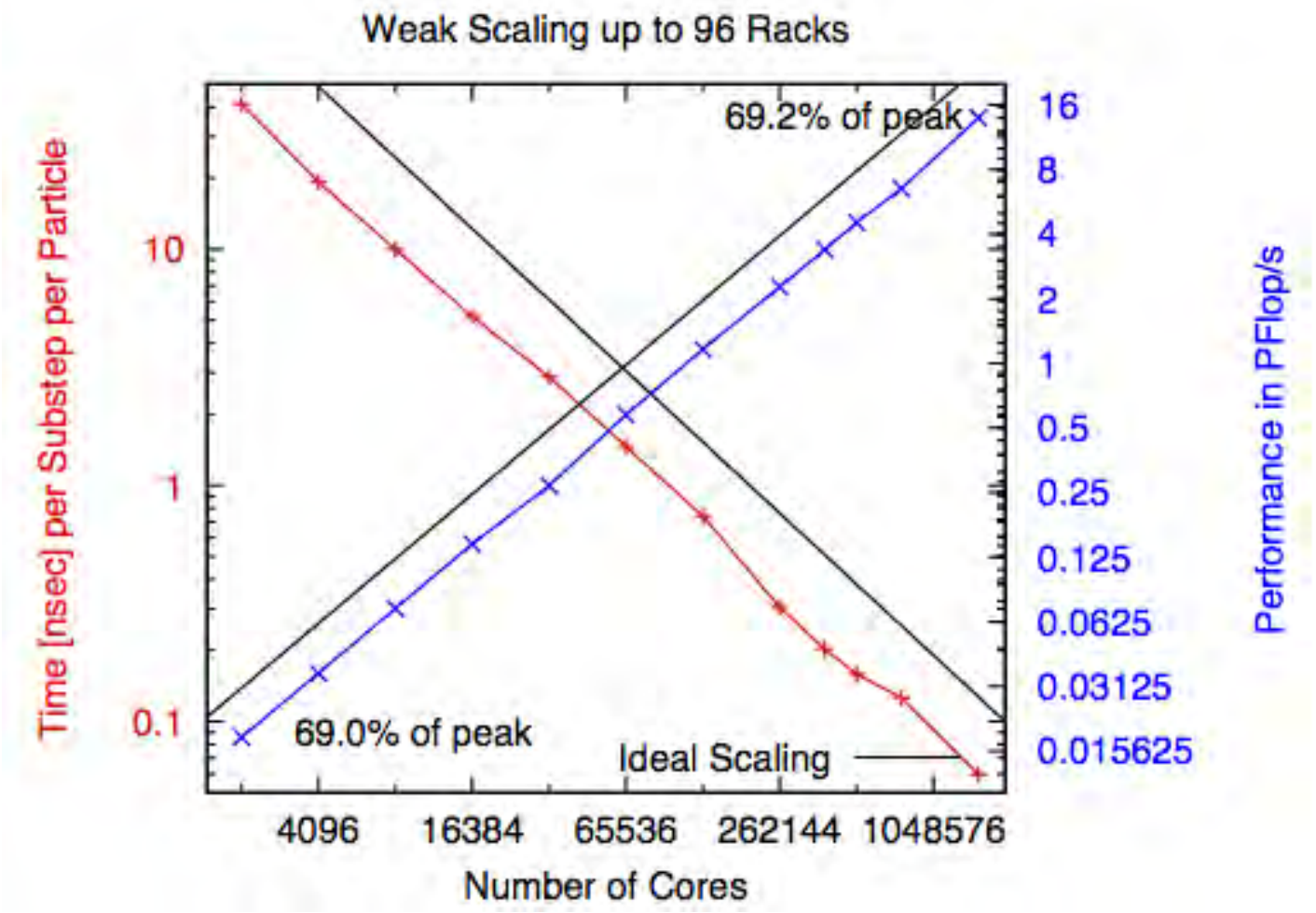
- Dark energy, dark matter
- Evolution of the universe and its structures:
  - Galaxies
  - Stars
  - Planets
- Study AGNs, black holes etc.
- "Map the sky"
- Etc.

Models(theory) and observations rely heavily on available computing and software infrastructure

Astro: structure of the universe

- Simulations:
  - Substantial memory requirements, O(PB) to match experiment
  - Realistic simulations of galaxies need Exascale resources (e.g. EAGLE resolution of the Milky Way)
  - Algorithms? (Grav.+ Hydrodynamics, decomposed?)
- Experiments: LSST, Euclid, JWST, LOFAR, SKA…:
  - Data centric
  - Require substantial computing resources (pre- and post-processing)
  - Comparable situation with LHC

Astro: scaling (HACC, N-body)



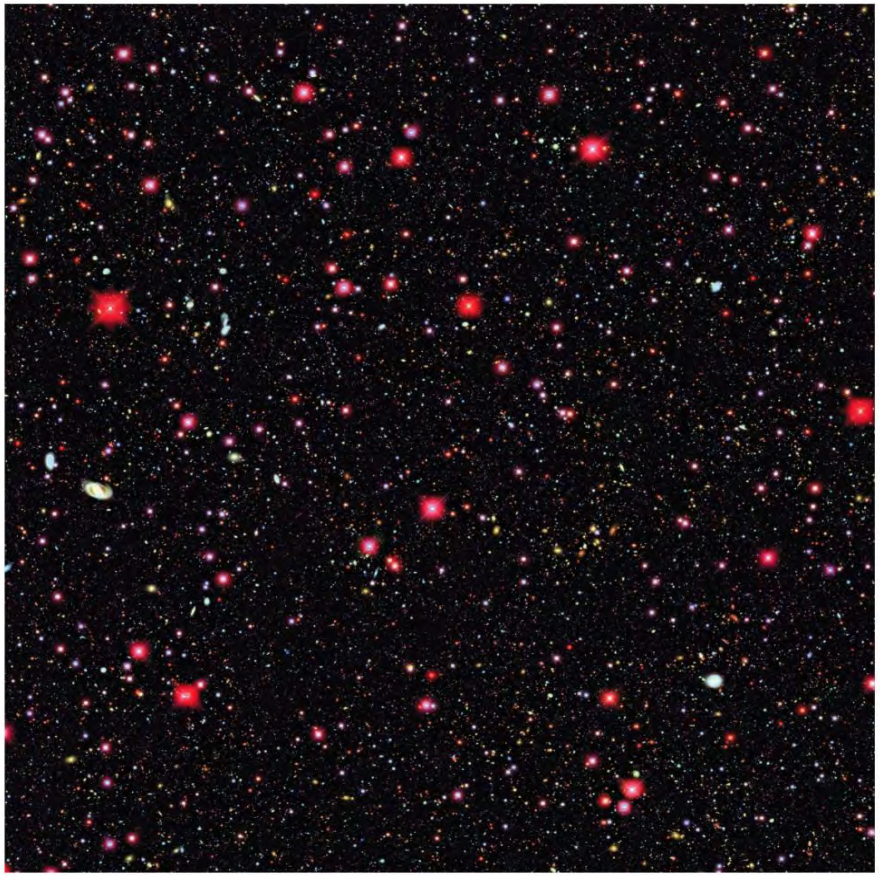
Astro: planets, stars, supernovae…

Examples:

- SN explosion
  - Resources: e.g. present PRACE call: 150 Mch
  - Understand the mechanism of the explosion
  - Predict neutrino and gravitational-wave signals
- Plantets, stellar systems
  - Turbulence of central importance in accretion disk
  - Resources: e.g. present PRACE call: 30 Mch
    Increased spatial resolution quickly reaches Exascale

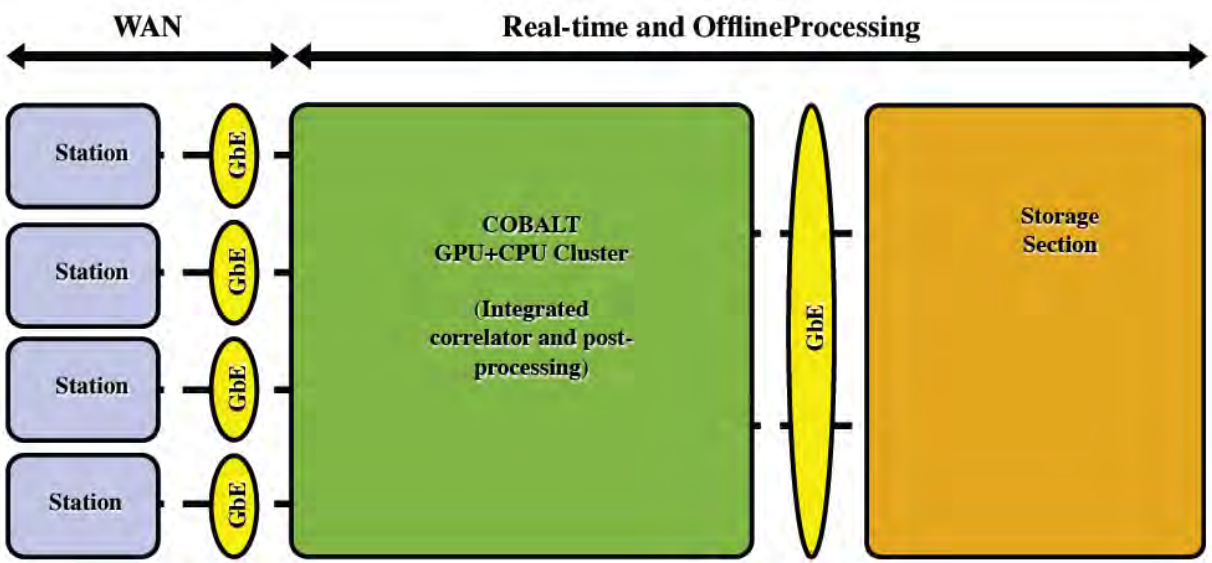
Astro: Large Synoptic Survey Telescope (LSST)

- Dark matter
- Mapping the Solar System & Milky Way
- Data 1.3 PB/a
- Computing:
  - 100 Tflop/s initially
  - 250 Tflop/s long term

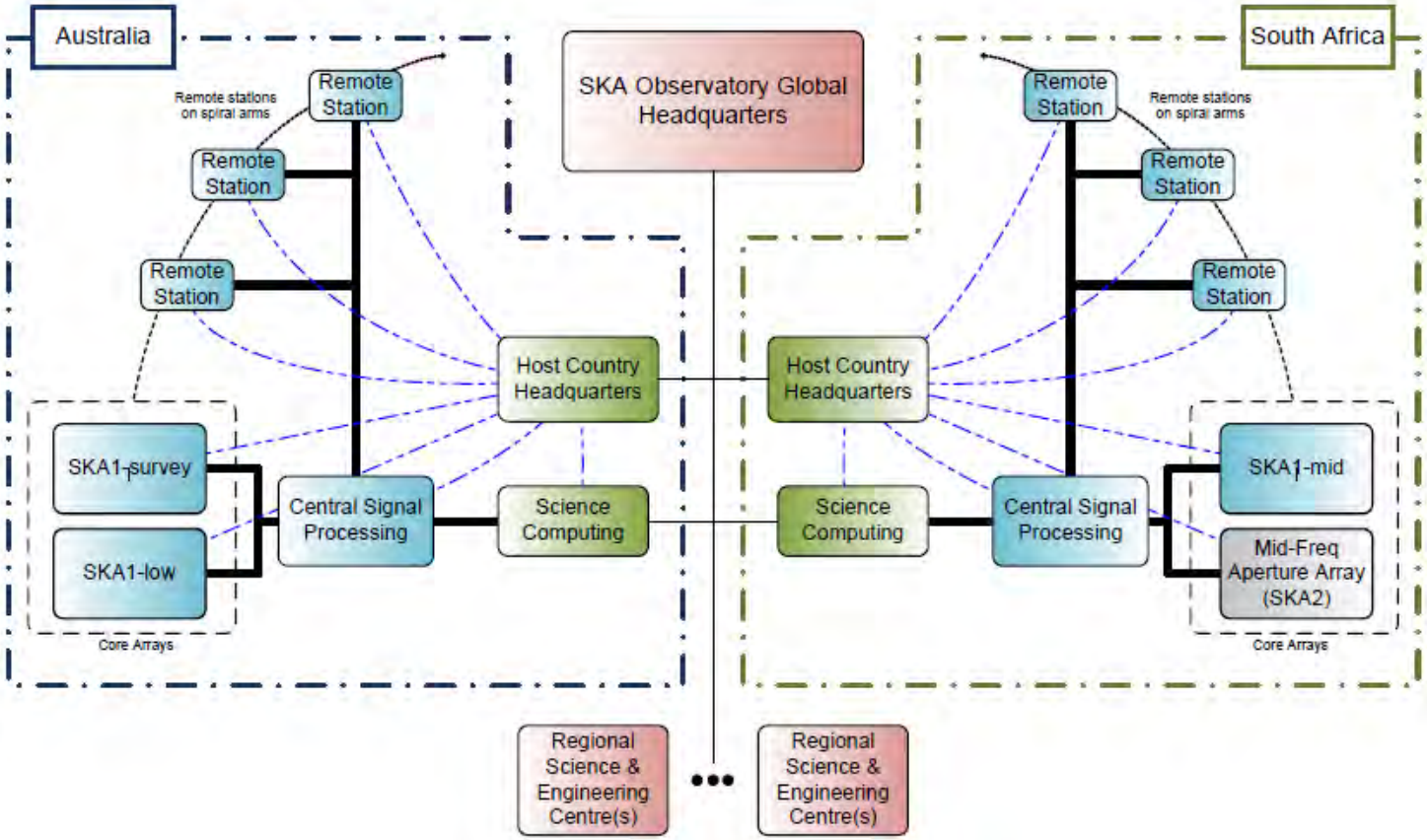


Astro: LOFAR

- 400 TB/d, reduced to 40 TB (post-proc.essing)
- Frequency parallel, mem. size limited, I/O bound
- Post-proc. can be parallelized,



Astro: SKA



Astro: SKA

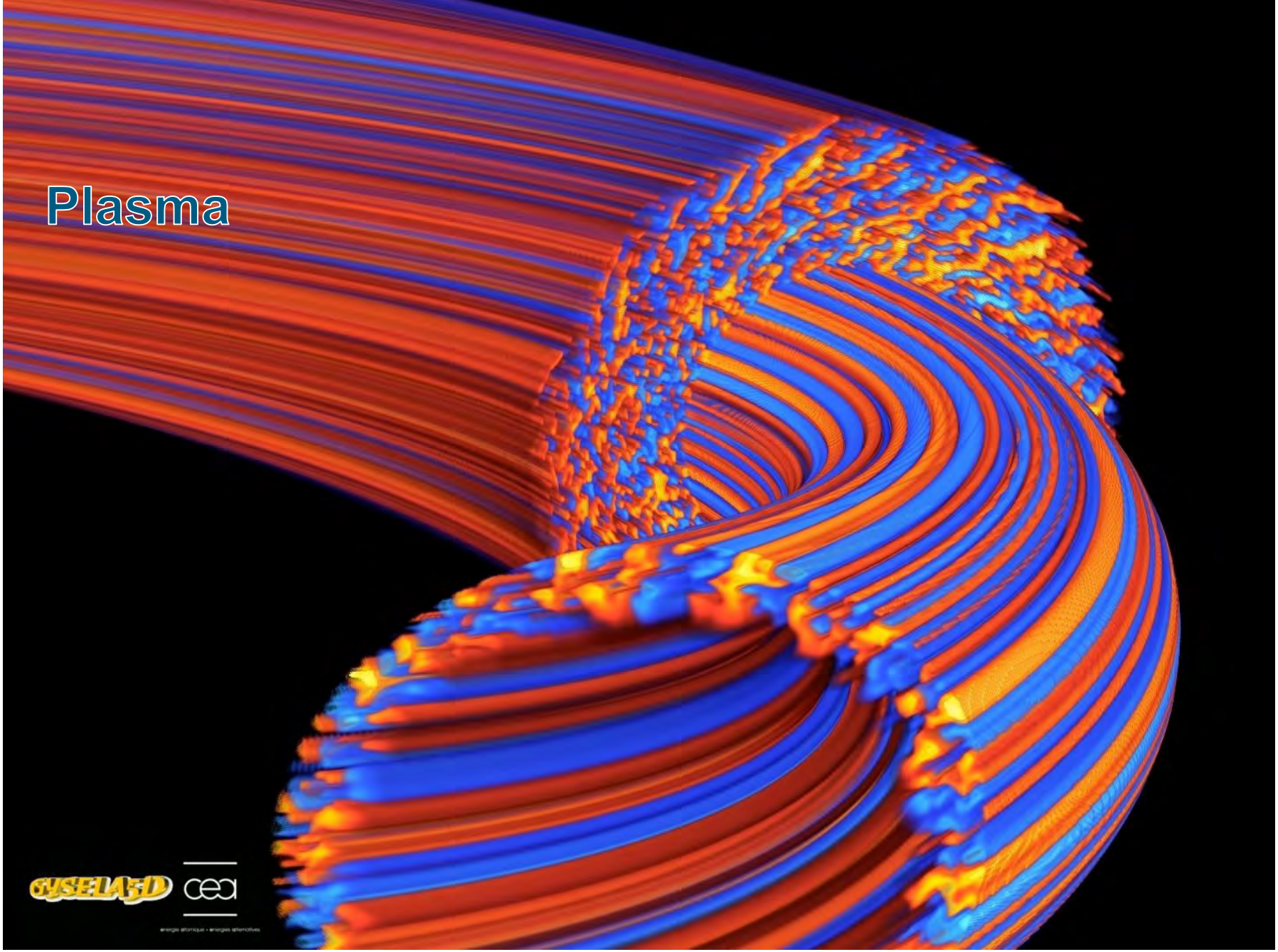
Processing (O(100) Pflop/s = 4*Tianhe-2 = 71MW)

- CSP (central signal processor)
  - Real time data processing 12 TB/s (SKA1)
- SDP (science data processor)
  - Data parallelism (position, polarization, frequency, time)
  - Limited inter-process communication (some global ops required)
  - Data locality to minimize data movement
  - Accelerator design considered for compute nodes
  - Partial HPC network for global ops

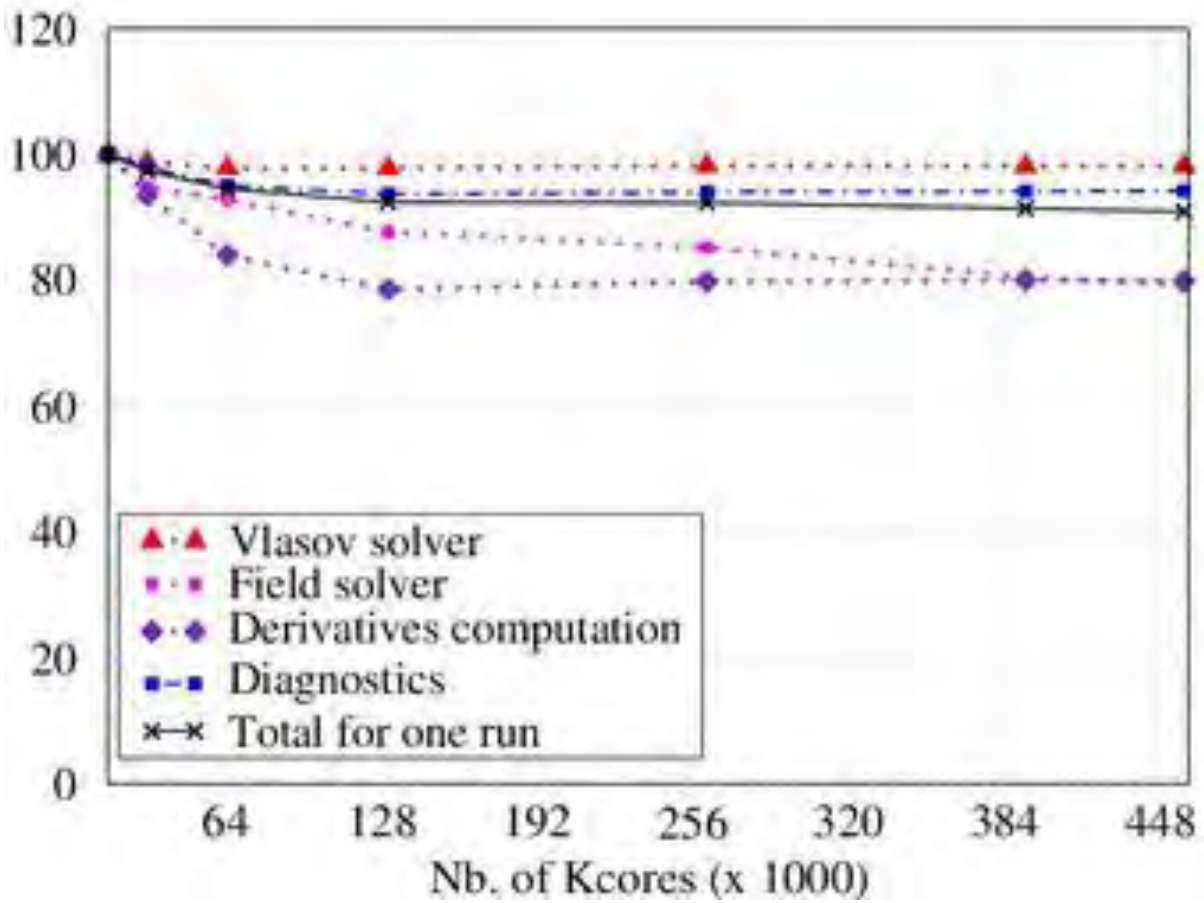
Astro: Summary

- Present allocations
  - O(1) Bch allocated
  - Single projects with O(100) can generate O(1) PB data
  - Moving towards “realistic” parameters immediately calls for Exasale resources
- Experiments
  - Require substantial computational resources: 100 Pflop/s (SKA)
  - Large data sets, O(1) PB/a LSST, O(100) PB/a SKA

Plasma



Plasma: Scaling (GYSELA)



Y. Sarazin et al, Nuclear Fusion **50**, 054004 (2010) http://gyseladoc.gforge.inria.fr/

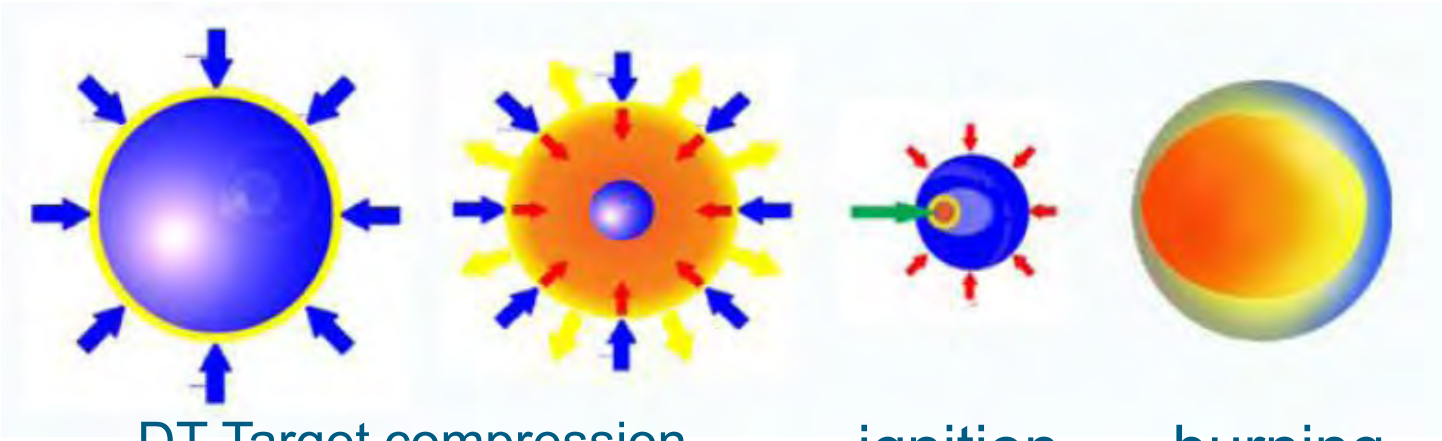
Plasma: core modelling requirements

Example: 5D gyrokinetic* simulation of plasma core transport in ITER, ¼ torus; 1 ms run time

	Grid Size	Cores	core-h	Data (per run)
Ion scale ¼ torus	300×10^9	80k	22×10^6	10 TB
Full torus	1.2×10^{12}	160	100×10^6	40 TB
Full confinement	1.2×10^{12}	16M	100×10^9	40 PB
Electron scale 1ms	10^{14}	2B	360×10^9	

Y. Sarazin et al, Nuclear Fusion **50**, 054004 (2010);
http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/Gysela/_node.html

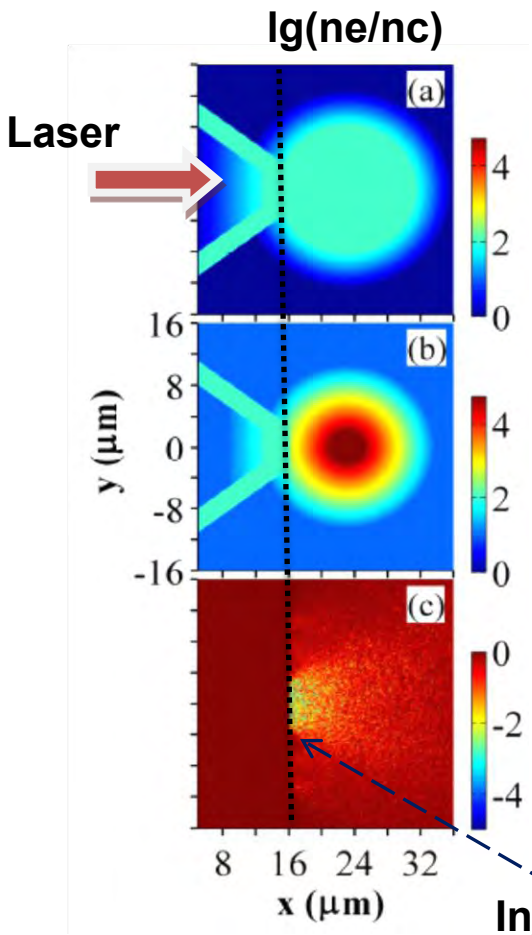
Plasma: laser fusion energy – fast ignition



Challenging simulation with large computation and complex physics:

- Plasma density of $6X10^4$ n_c for laser fusion
  - cf: 0.01 n_c for electron accelerator; 100 n_c for ion accelerator. ($n_c = 10^{21}$ cm^{-3})
- Multiple temporal scales: 3 fs for laser, 0.01 fs for plasma oscillation

Plasma: (hybrid) two-system Particle-in-Cell



First PIC system (maximum of ne =100 nc)

Second PIC system (real density profile ne up to 54000 nc = 300g/cm^3 for tritium target)

Ignition current (J_{fx}) in the second system

Injection point of fast electrons of E>0.1MeV and px>0.45mc (50keV)

Plasma: Fast ignition scenario req'nts

Example: hybrid PIC simulation of FI scheme; compressed target 300 gcm^{-3}, box size 200 µm x 100 µm; 2 ps run time*

	Resolution	Size (df)	Cores	10^6 core-h
2D	Δx=0.02 µm 50 particles/cell	50 M cells 2.5 B particles	16k	1
3D	Δx=0.02 µm 50 ppc	$5x10^9$ cells $250x10^9$ particles	16M	100
3D hi-res	Δx=2 nm 100 ppc	$5x10^{12}$ cells $500x10^{12}$ particles	16B	200 000

*Data from: Wang, Gibbon, Sheng & Li, Phys. Rev. Lett. **114**, 015001 (2015)

Plasma: Magnetic fusion (ITER)

Dedicated supercomputers for fusion community

2009-2013 HPC-FF (Jülich): 100TF

2013-2016 IFERC: 2PF / 72k cores = 0.03 GF/core

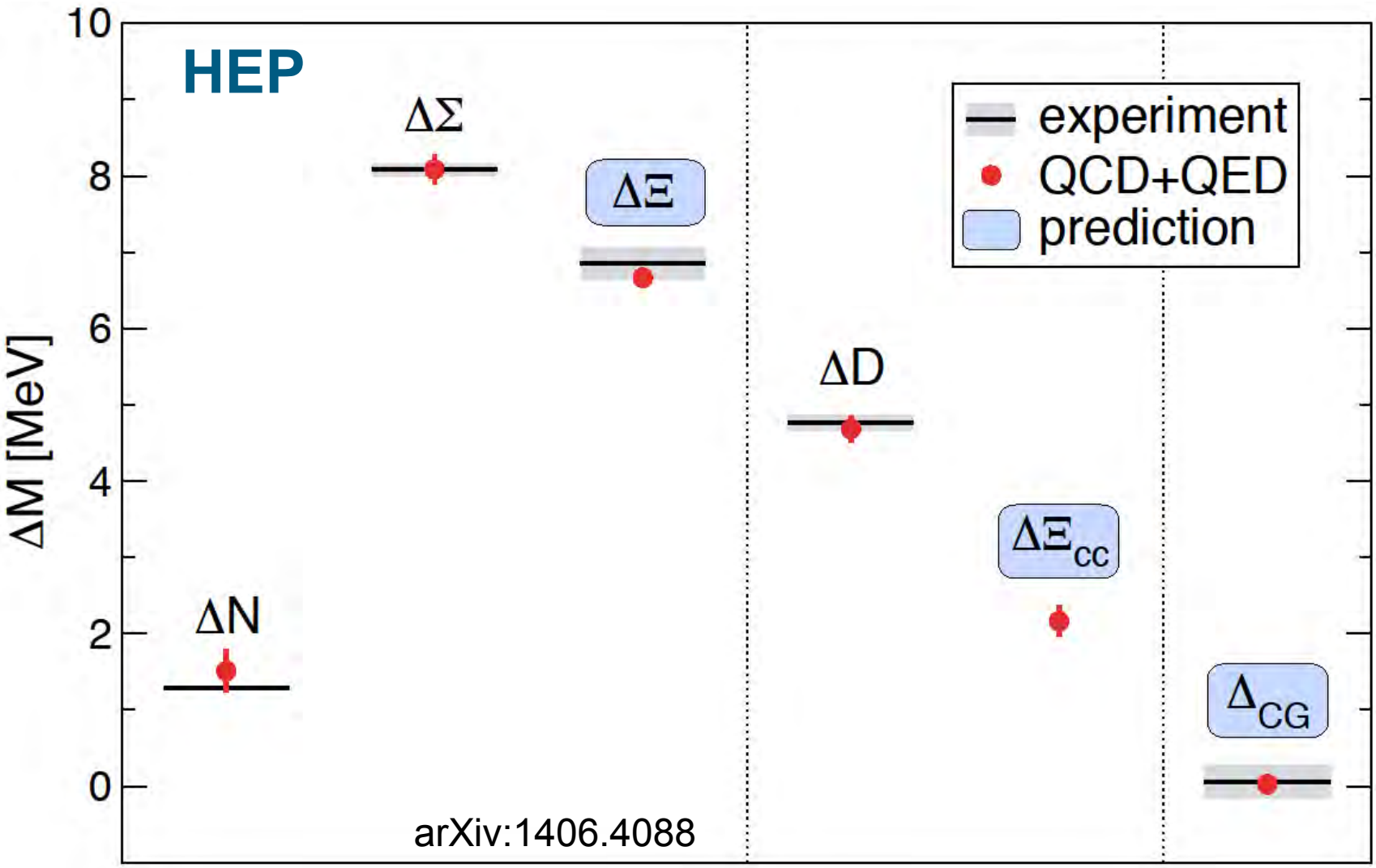
2017- Current Eurofusion call: 8PF /300k cores

Capacity: 2620 M core-h from 2017

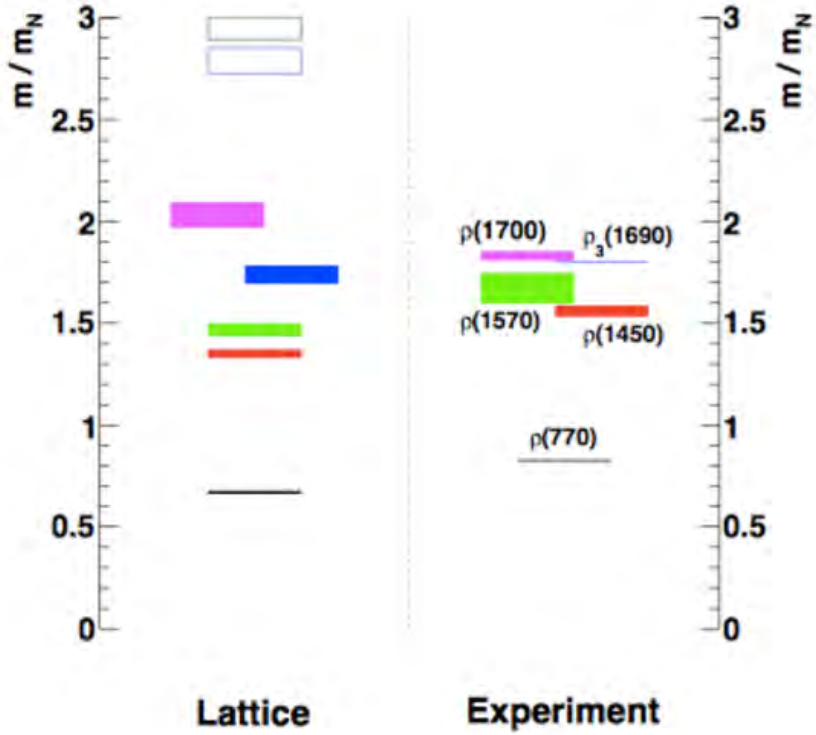
Plasma: HPC resources

	DoE INCITE Proposals (10^6 core-h)	PRACE + national EU (10^6 core-h)	EU facility-generated demand (10^9 core-h)	Projected demand >2020 (PF-y)*
Tokamak physics	500	500	ITER >2018: 5	15
Laser fusion (fast ignition)	300	100	HIPER >2020 1	3
Petawatt laser sources	250	400	ELI (x3) 5	15
Space/astro physics	200	200	ESA missions 2	6
Total	1200	1200	13	40

*Assumed 2 GF/core



HEP: LQCD spectrum



- Decays
- Fine-structure (iso-spin breaking)
- Multi-Nucleon systems: combinatorially and exponentially hard

→D, T, ^{3}He, ^{4}He, ^{6}Li,…

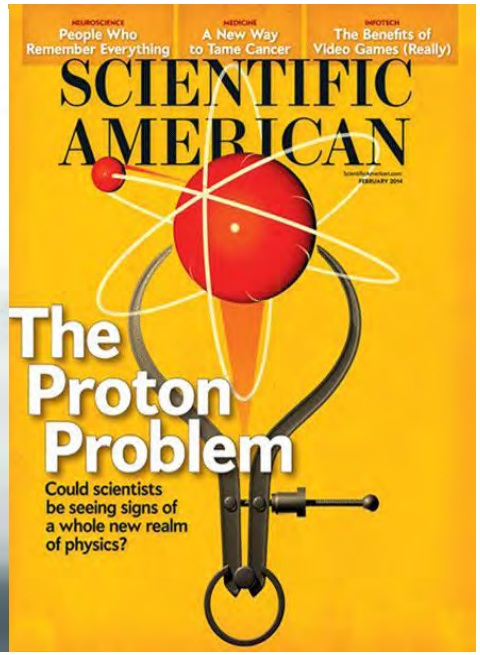
→NN, NNN forces

Price-tag:

>20 + O(100) Pflop/s-yrs

HEP: LQCD, zero temperature

- a_μ
- Matrix elements
- g_A
- GPDs, DAs, TMDs
- Bag parameters
- CKM physics
- Transition form factors
- etc.



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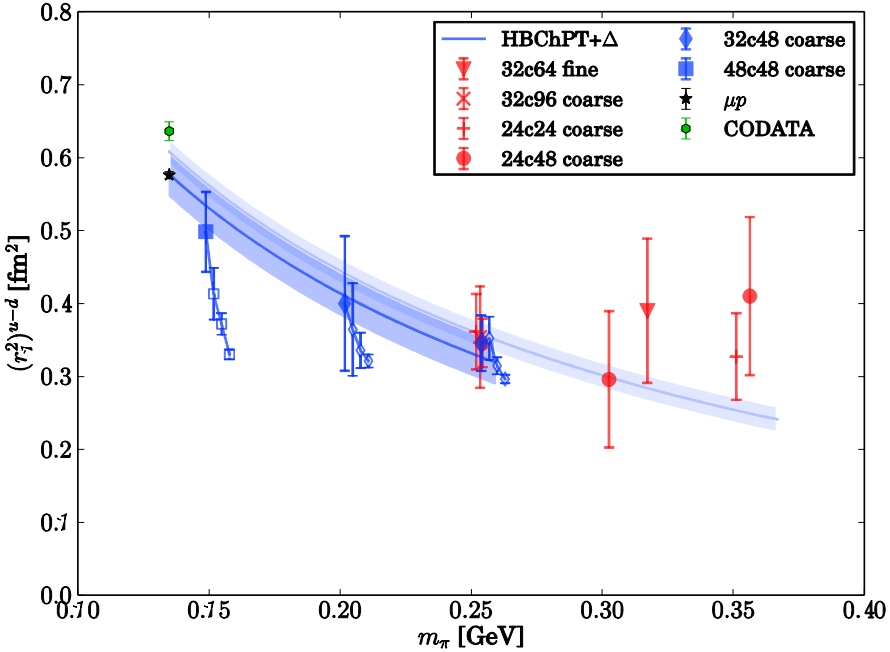
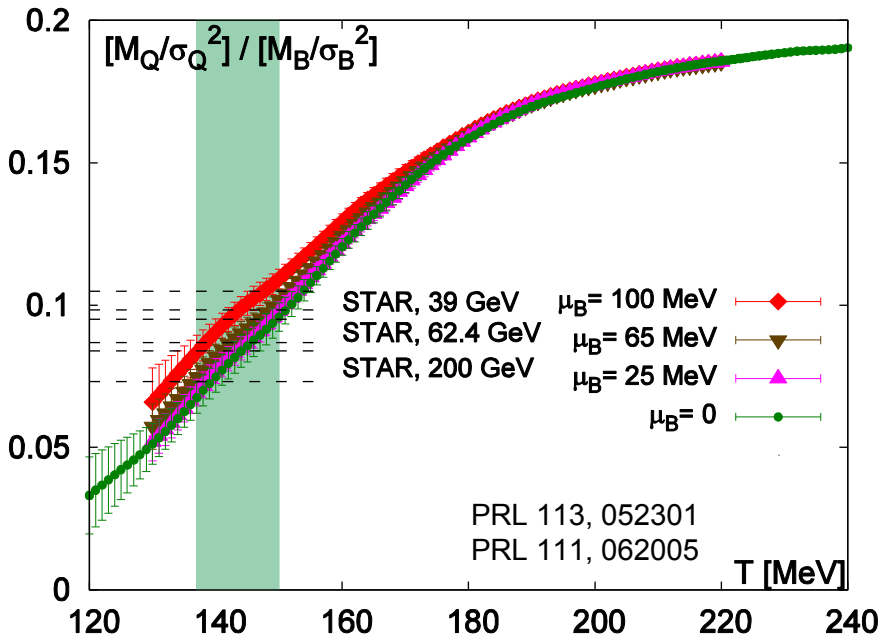
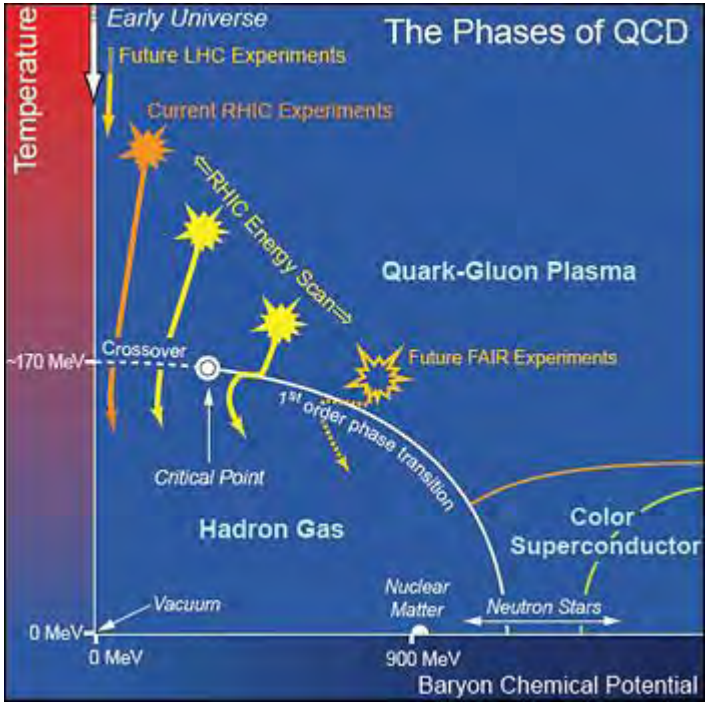


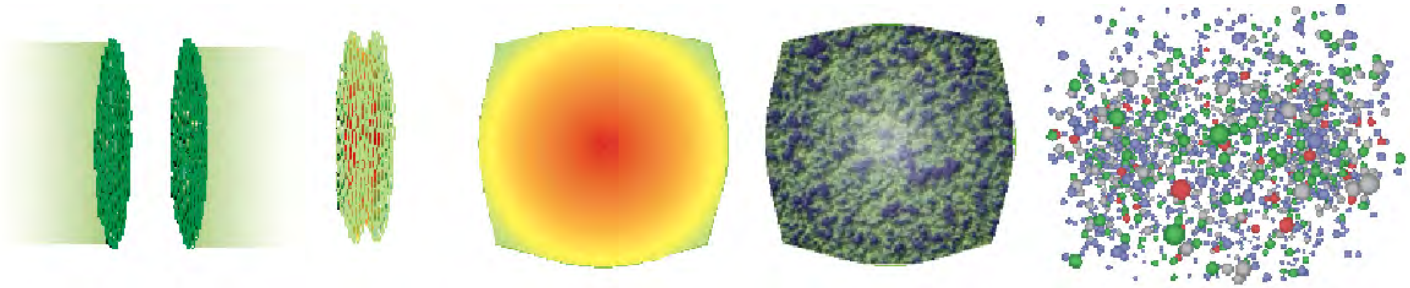
Price tag:

O(100) Pflop/s-yrs

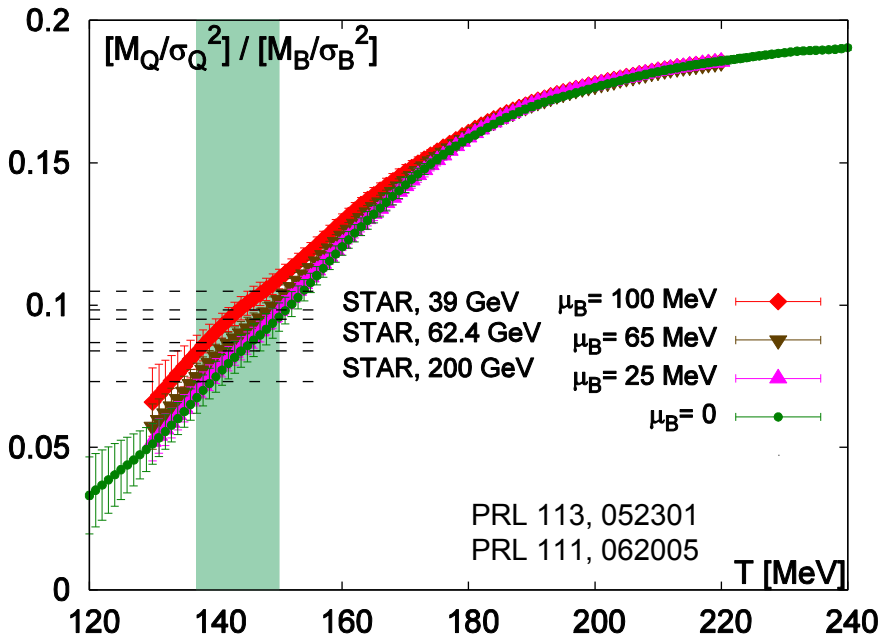
HEP: LQCD, finite T and μ







HEP: LQCD, finite T and μ

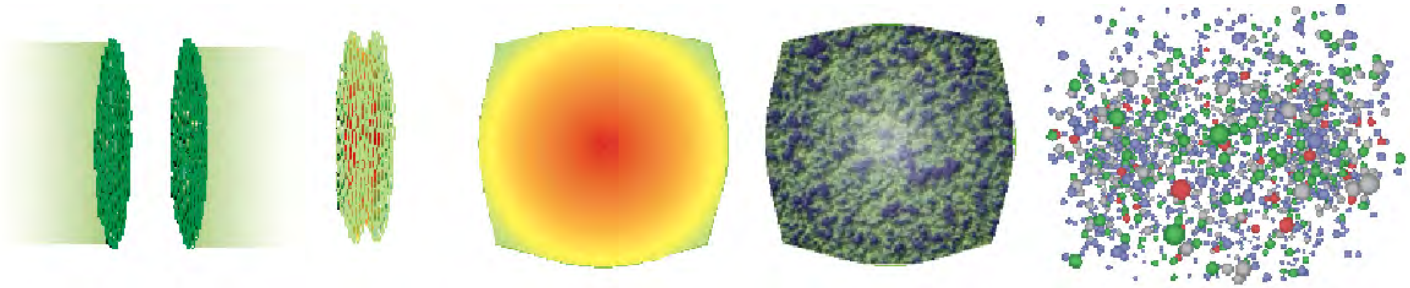


Finite temperature:

- Equation of state
- Critical point
- Freeze-out conditions
- Strangeness
- Fluctuations of con. charges
- Backgrnd. magnetic fields
- etc.

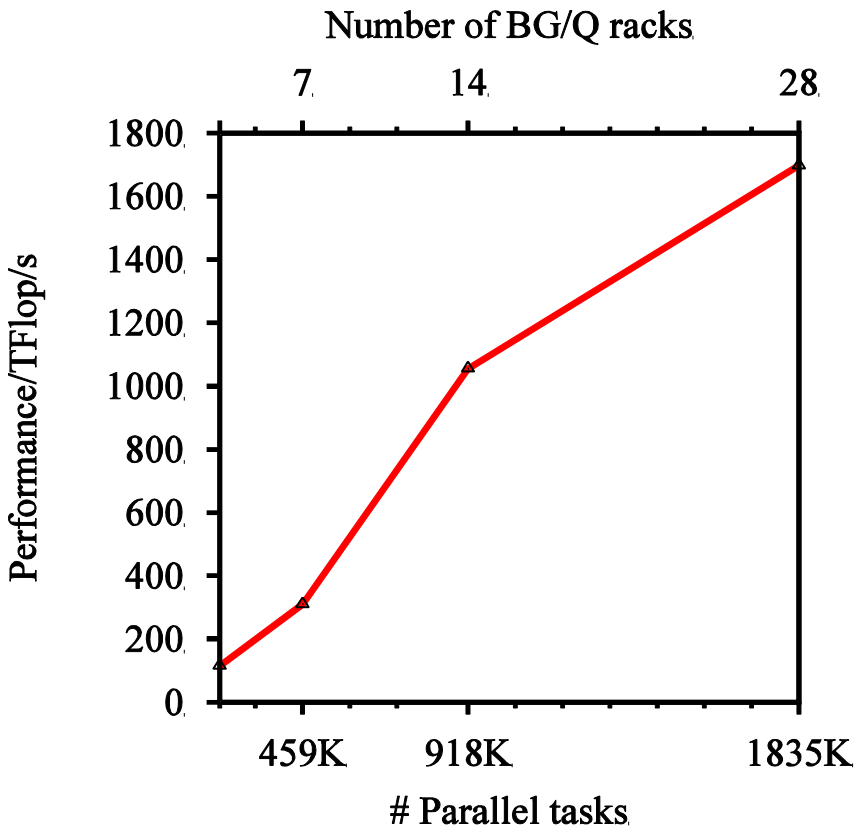
Price tag:

>100 Pflop/s-yrs



HEP: LQCD

- Highly scalable codes: O(10^6) strong scaling demonstrated (e.g. “High-Q club, JSC”)
- No “no-go” scaling hazards at this point
- Efficient solvers less scalable: used in (naively parallel analysis)



HEP: LQCD computers

QPACE @ Jülich

Blue Gene/Q @ EPCC

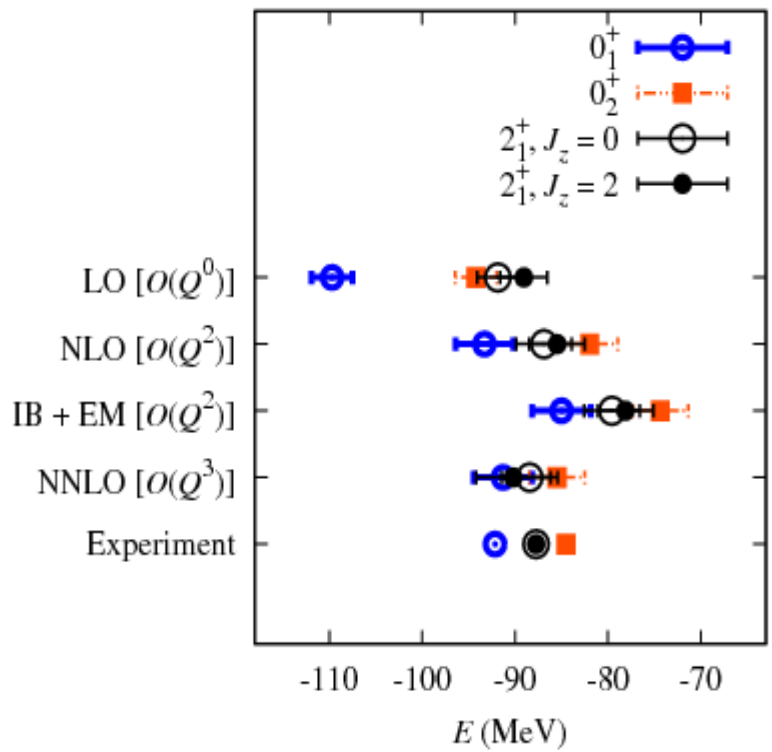
→ QPACE 2 (SFB TRR 55), XeonPhi based

HEP: LQFT, EFT

- Nuclei states
- Nuclear physics input for nucleosynthesis in supernovae
- Supersymmetric models
- Technicolor

Price tag:

$\approx$20 Pflop/s-yrs



Hoyle-state (red), PRL 106, 192501

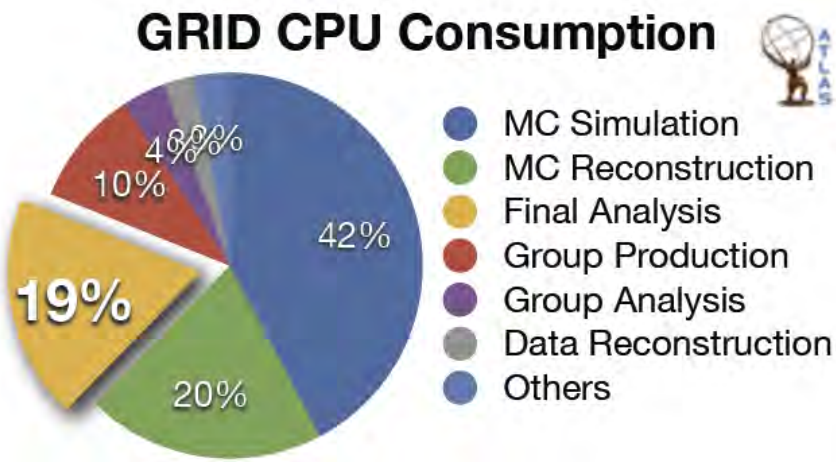
HEP: LHC

- 2 stage Trigger system, 40M events/s → 1K events/s
- 4 Experiments: Atlas: 320MB/s, CMS: 220MB/s, ALICE: 100MB/s, LHCb: 50 MB/s (2010)
- Total data: 15 PB/yr (2010), 27PB/yr (2012)
- Data storage and analysis in tier-ed grid (WLCG):
  - Tier-0: @CERN, 5.5+17PB storage, 6000 CPUs
  - Tier-1: distributed, 11 centers, 1+10 PB storage, archive
  - Tier-2: distributed, 150 centers, analysis, no storage
  - Tier-3&4: WLCG access points

HEP: LHC

Data processing

- Streaming
- Serial execution (few cases of threading due to mem restrictions)
- Simulation code is being vectorized



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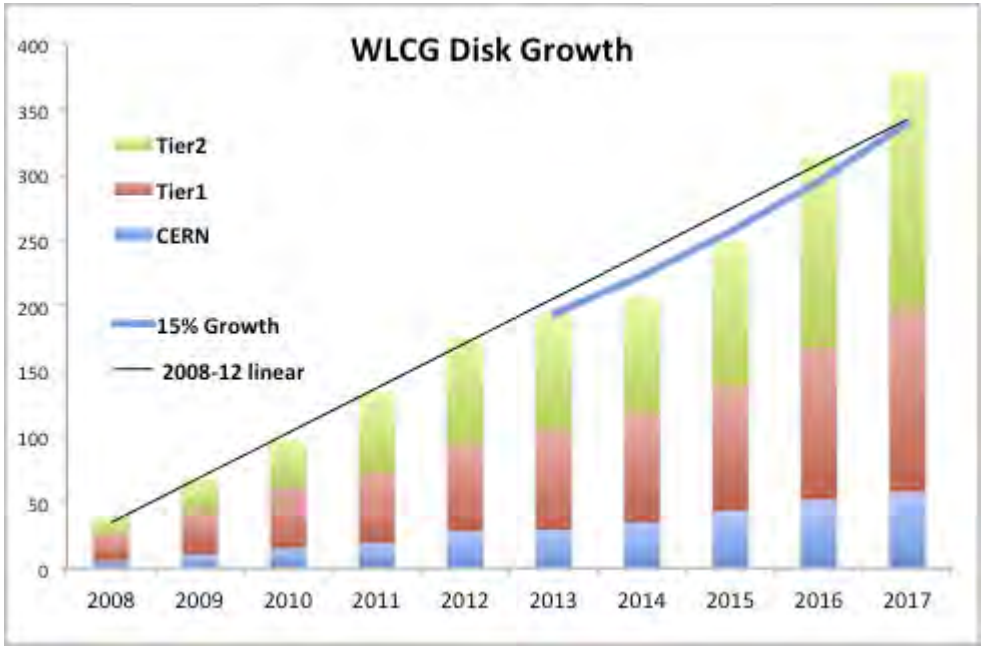

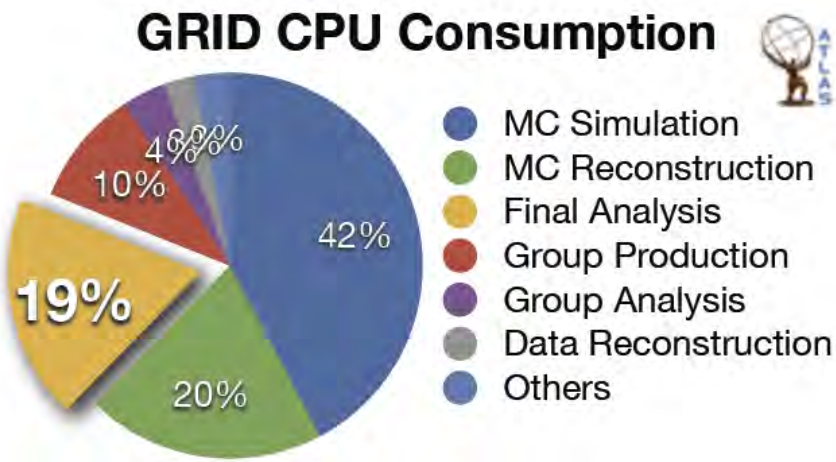

HEP: Summary

	present	2016-2020
LQCD, computing	ca. 5 Pflop-yrs	>500 Pflop-yrs
LQCD, data	O(200) TB	O(20) PB
LHC, computing	ca. 1 Pflop-yr	ca. 10 Pflop-yrs (extrapolated)
LHC, data	250 PB installed	ca. 600 PB (extrapolated)