

André Walker-Loud

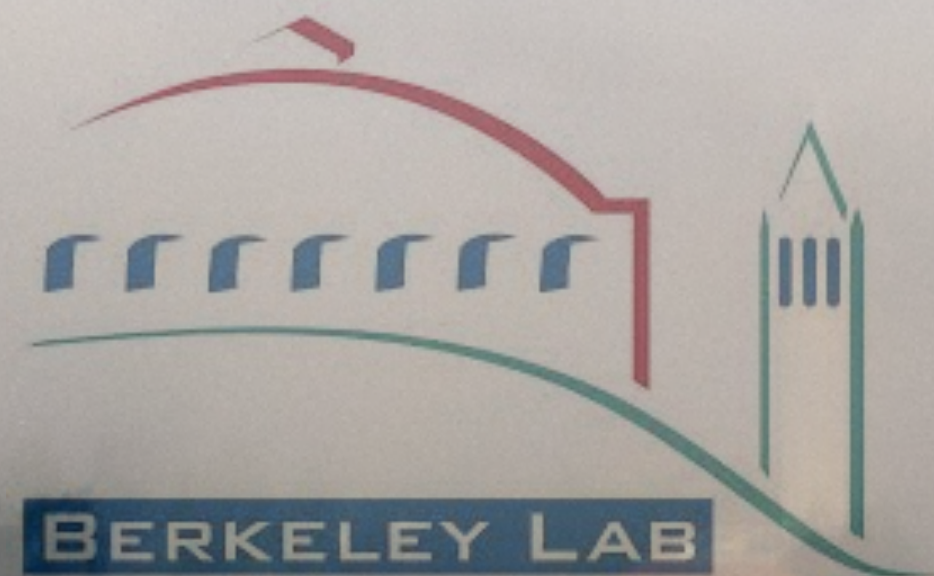
Staff Scientist

Lawrence Berkeley National Laboratory

S91010 - Accelerating our Understanding of the Nuclear Physics and the Early Universe

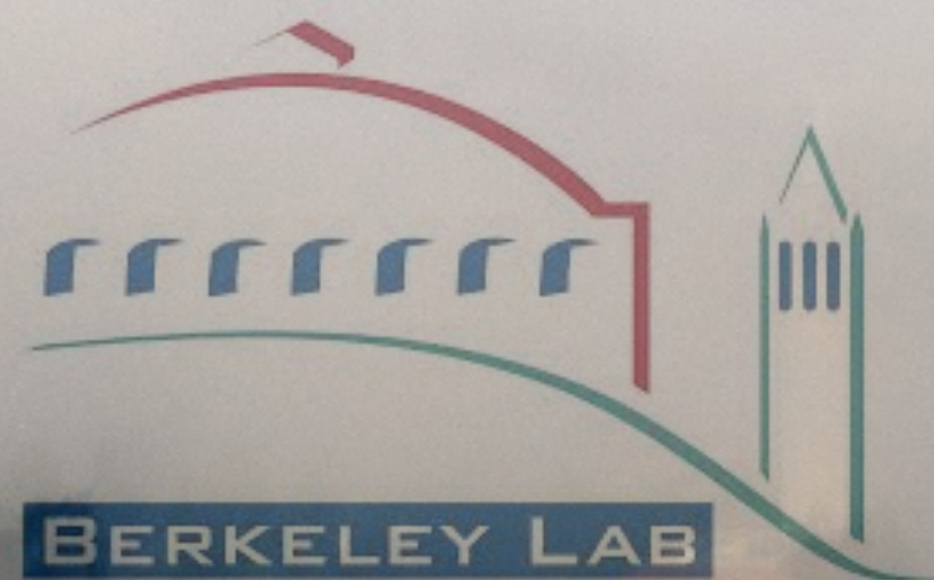
Accelerating our Understanding of the Nuclear Physics and the Early Universe

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Accelerating our Understanding of ~~the~~ Nuclear Physics and the Early Universe

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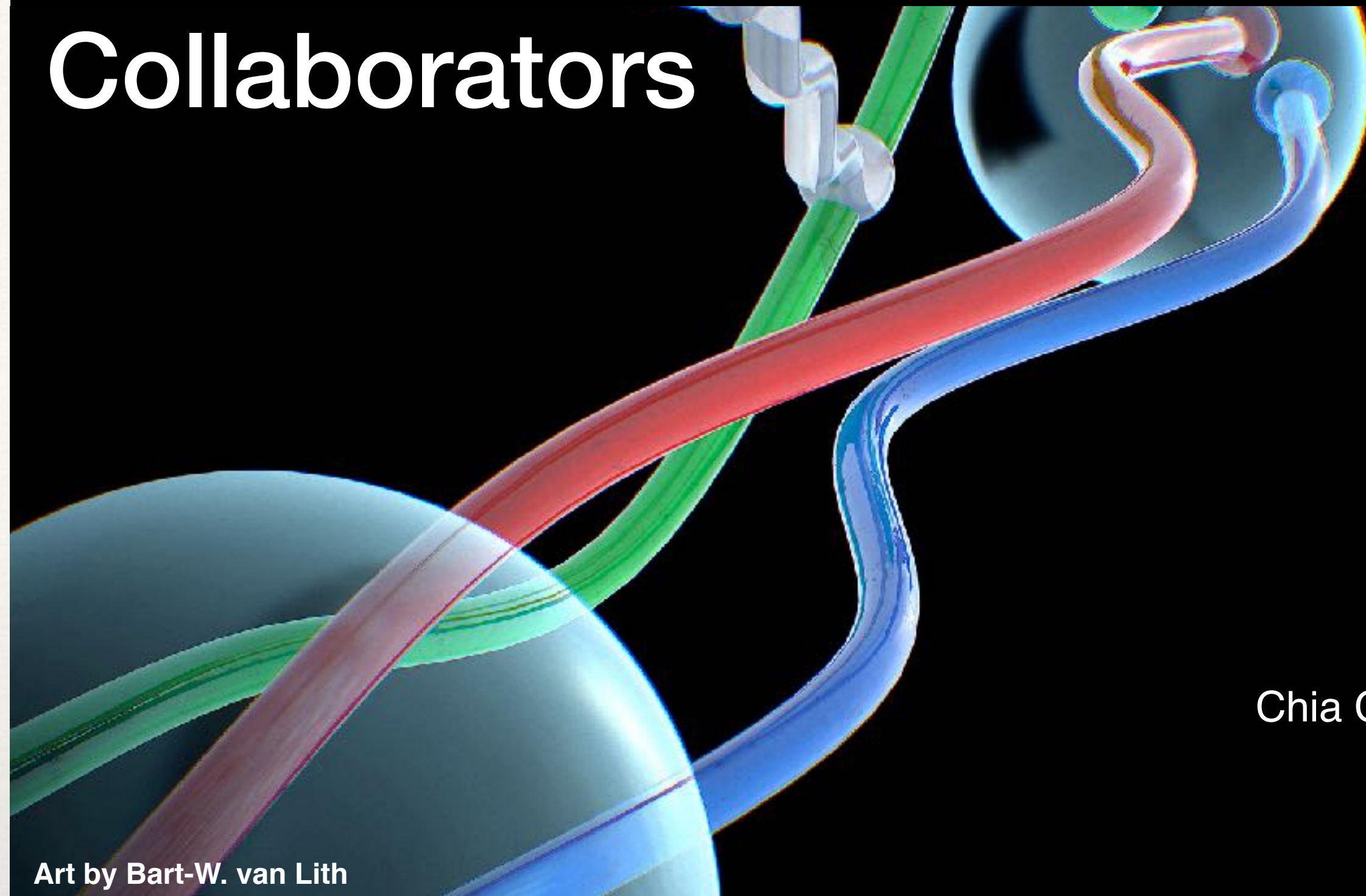
This Talk

- What are the driving science questions we are trying to understand?
- Why do we need High-Performance-Computing?
- How do we make optimal use of the Leadership Class Supercomputers (like Summit at Oak Ridge National Laboratory)?
- Preliminary new results from new machines

Acknowledgements

- I would like to thank **Jack Wells** for suggesting us for this talk
- We would like to thank the Lawrence Livermore CORAL team **Scott Futral, Greg Tomaschke, Adam Bertsch, John Gyllenhal, Py Watson** for providing us early access to Sierra and help understanding how to use the machine
- We would like to thank the Oak Ridge Leadership Computing Facility team **Jack Wells, Tjerk Straatsma, Chris Fuson, Gustav Jansen, ...** for providing us early access (and an Early Science Award) on Summit and help understanding how to use the machine

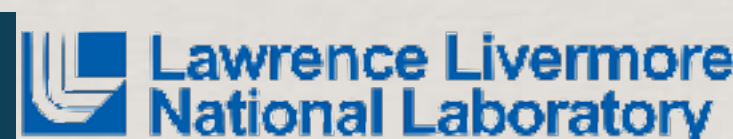
Collaborators



Art by Bart-W. van Lith

Gordon Bell
 Evan Berkowitz
 Kate Clark
 Arjun Gambhir
 Ken McElvain
 Amy Nicholson
 Enrico Rinaldi
 Pavlos Vranas
 André Walker-Loud
 Chia Cheng (Jason) Chang
 Balint Joó
 Thorsten Kurth
 Kostas Orginos

Nucleon Axial Coupling
 Chia Cheng (Jason) Chang
 Amy Nicholson
 Enrico Rinaldi
 Evan Berkowitz
 Nicolas Garron
 David Brantley
 Henry Monge-Camacho
 Chris Monahan
 Chris Bouchard
 Kate Clark
 Balint Joó
 Thorsten Kurth
 Kostas Orginos
 Pavlos Vranas
 André Walker-Loud



*not all in California

These calculations are made possible by



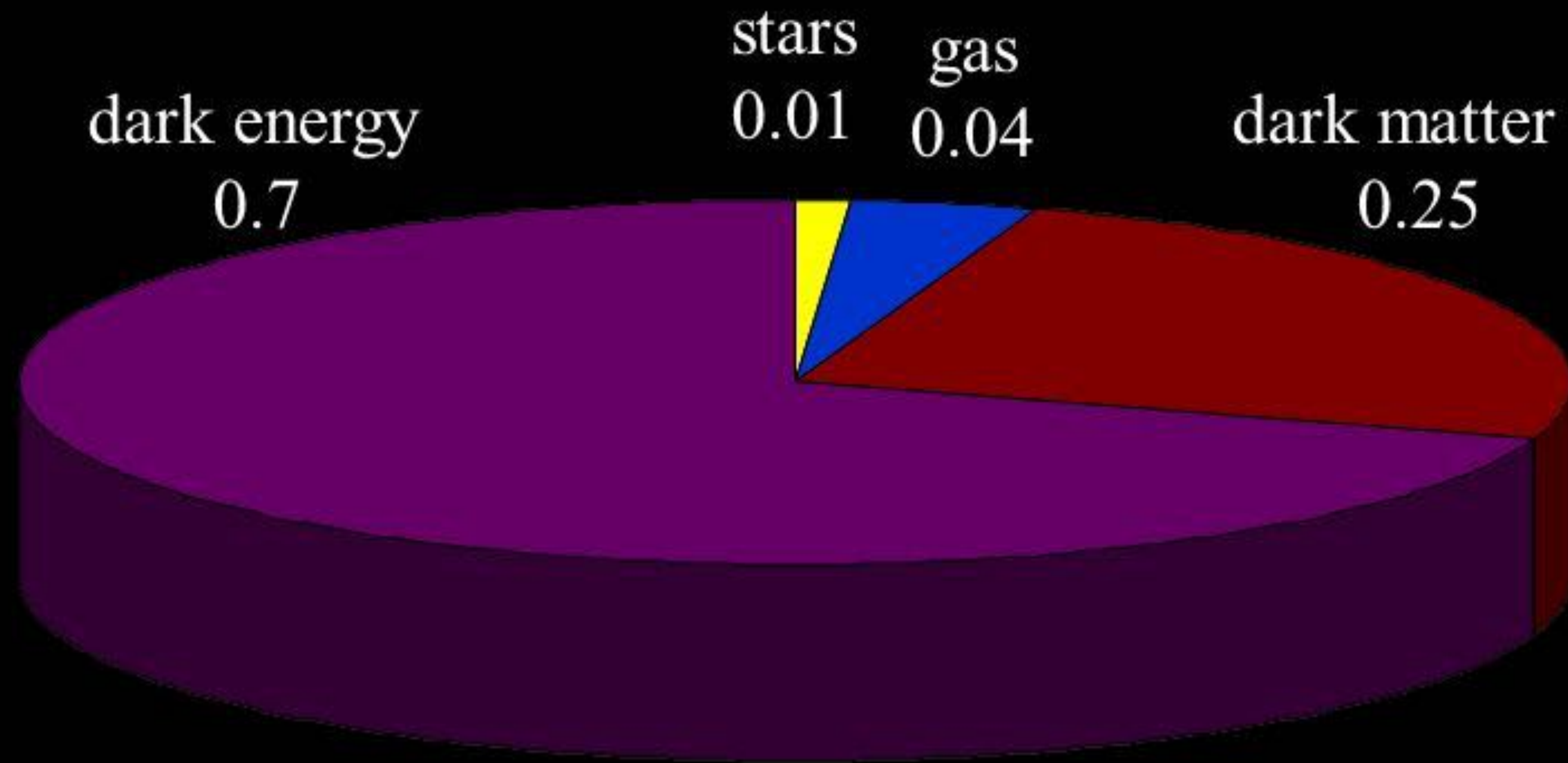
DOE Topical Collaboration
 Double Beta Decay



Science Drivers

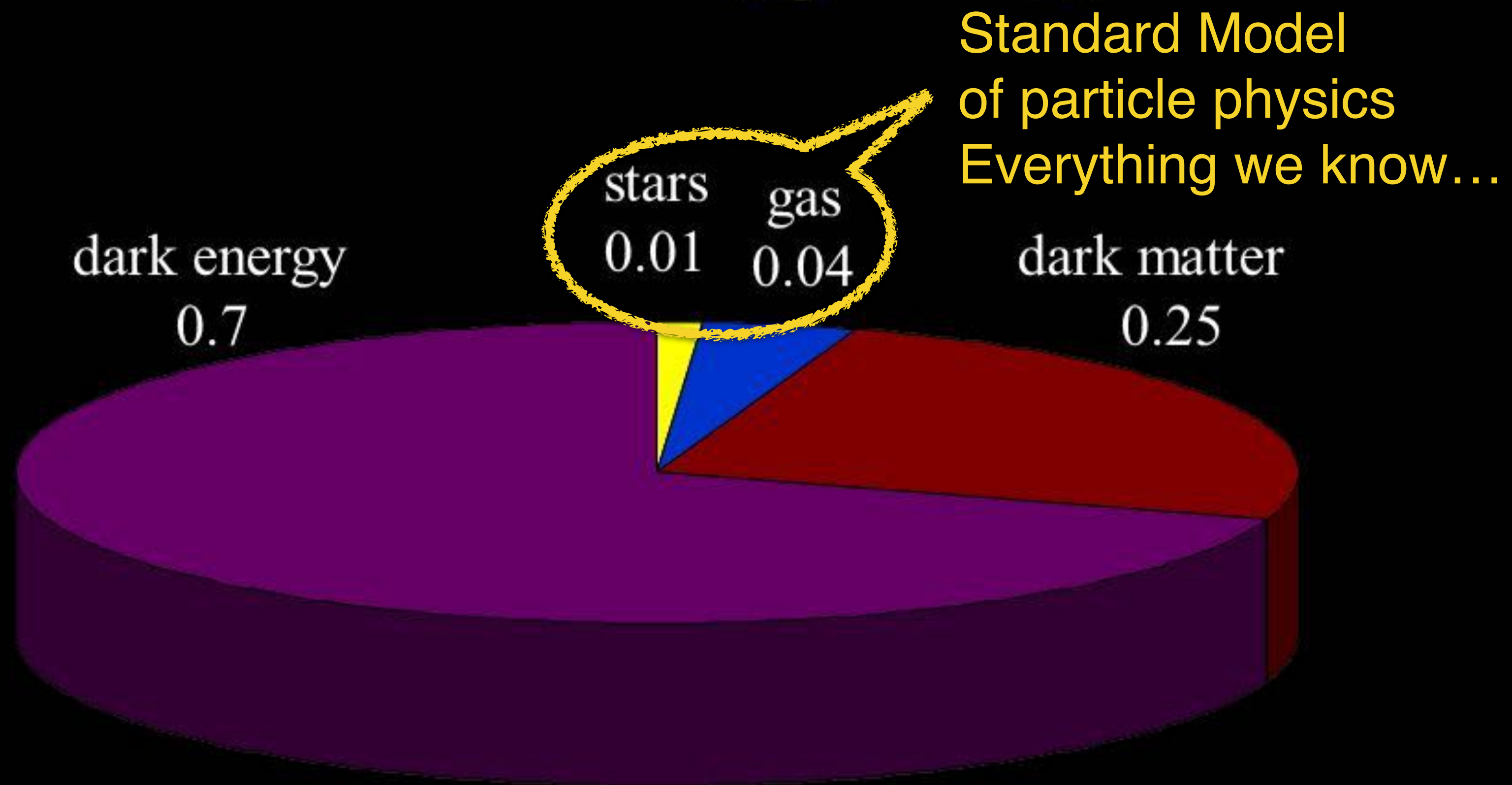
- Can we understand the properties of matter (protons, neutrons, atomic nuclei) directly from the Standard Model of particle physics?
- Can we understand the evolution of stars from their solar fusion cycle through supernovae explosions and collapse to neutron stars and black holes (directly from the Standard Model)?
- See Bronson Messer's talk just prior - we are hoping to start a new effort connecting our research
- Why does the universe contain more matter than anti-matter?
- ...

cosmic mass/energy budget



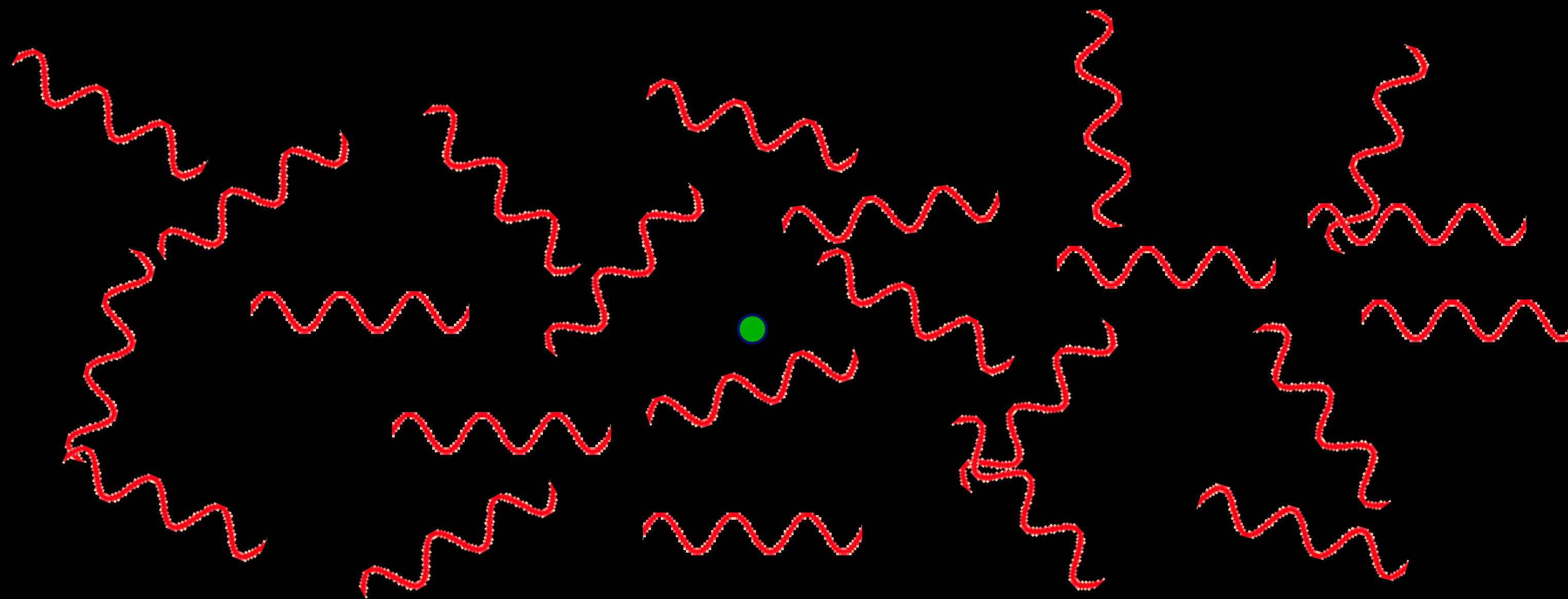
$$\Omega_{\text{mass+energy}} = 1 \text{ (or very close)}$$

cosmic mass/energy budget



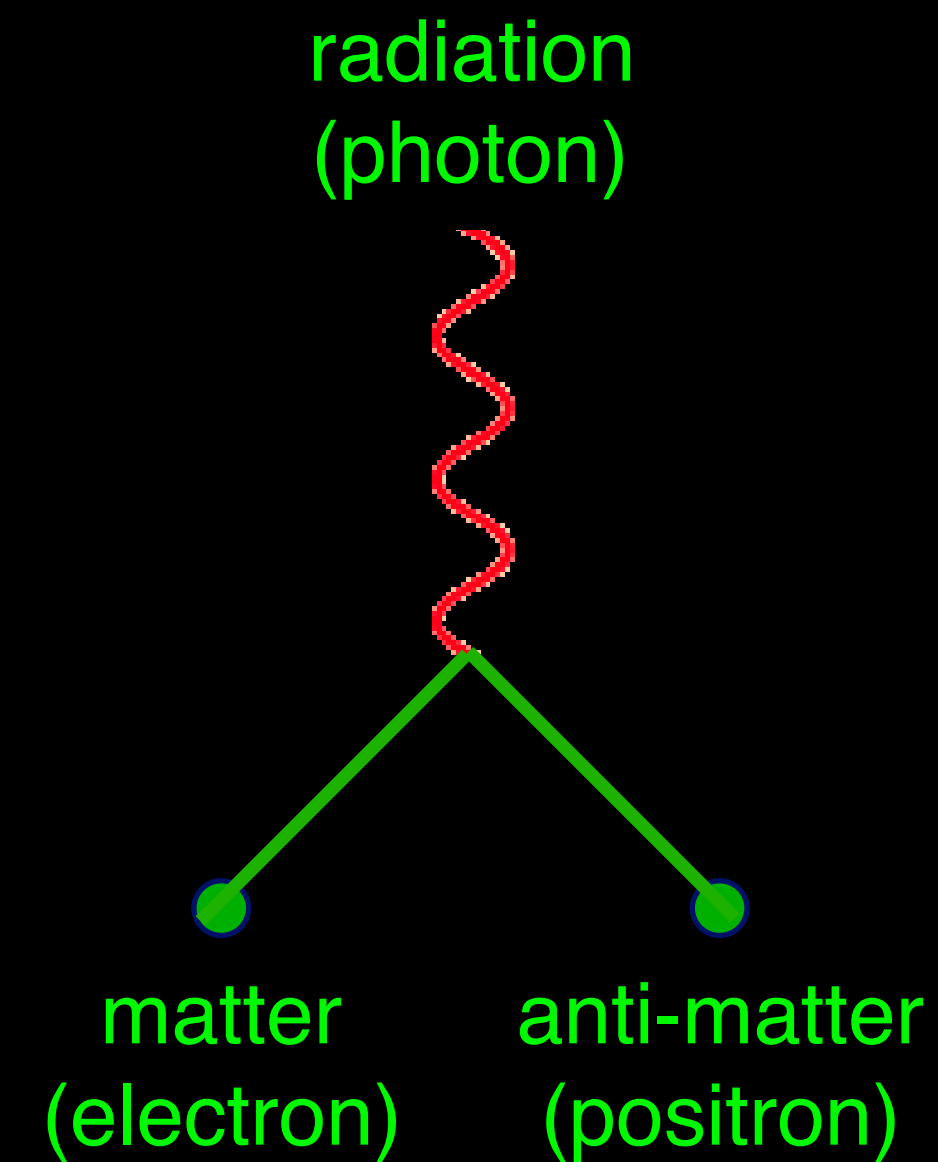
$$\Omega_{\text{mass+energy}} = 1 \text{ (or very close)}$$

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

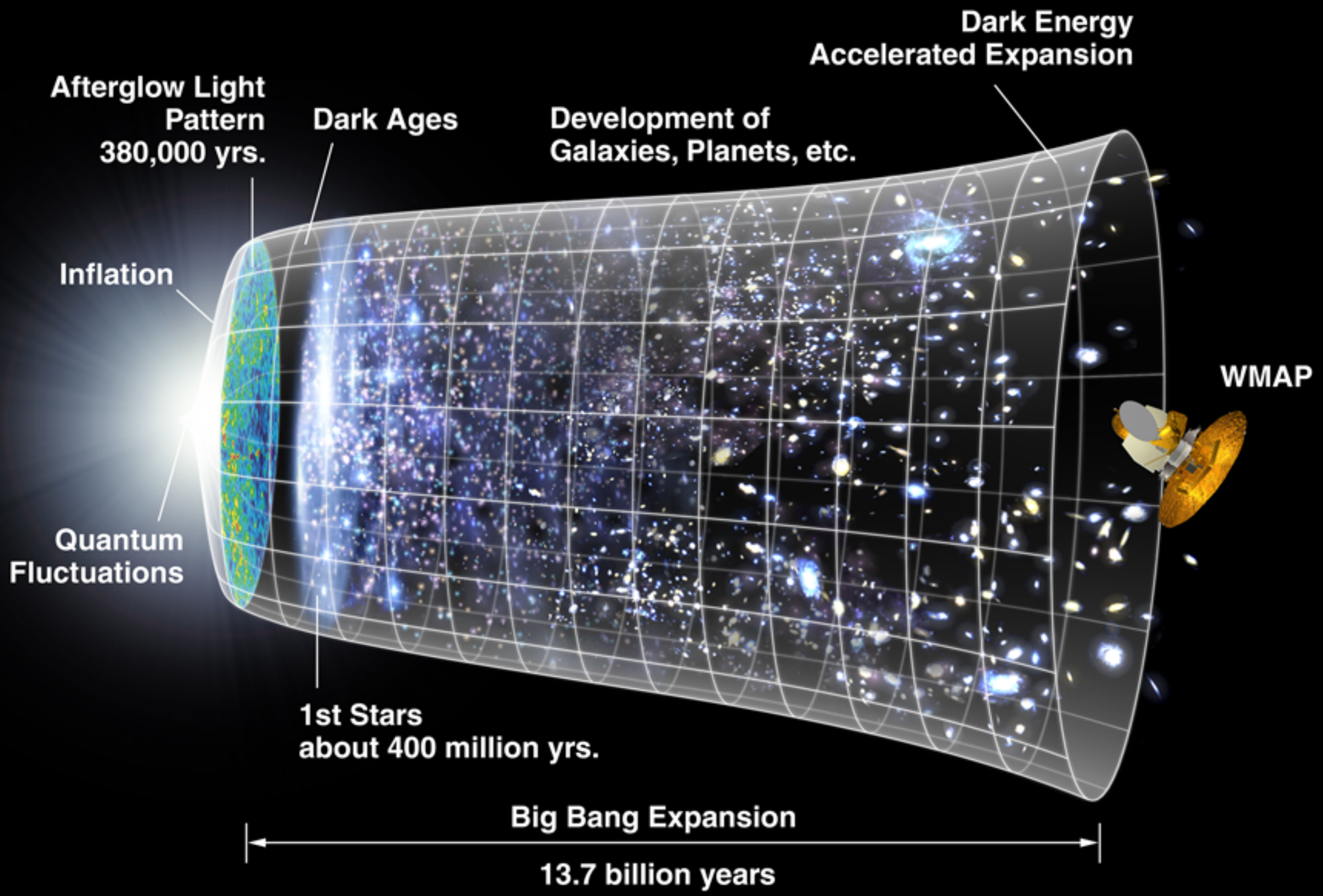


We observe there are more protons than anti-protons in the universe by an amount of roughly

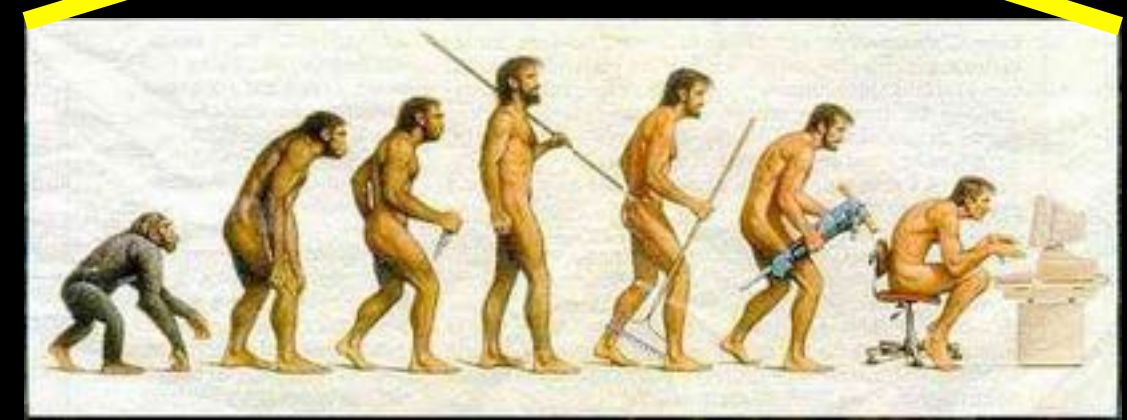
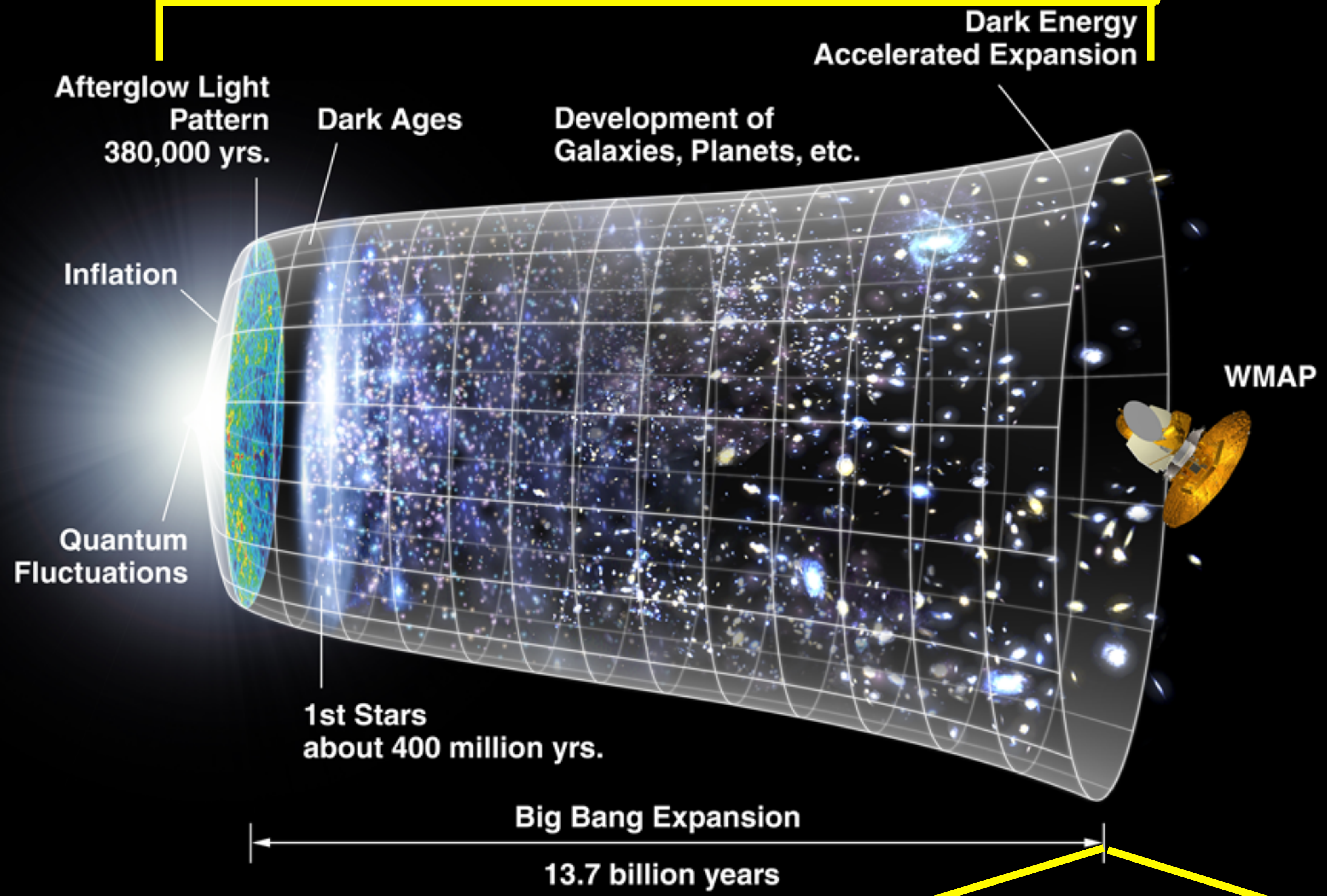
$$\frac{N_{proton} - N_{anti-proton}}{N_{photon}} \simeq 10^{-9}$$

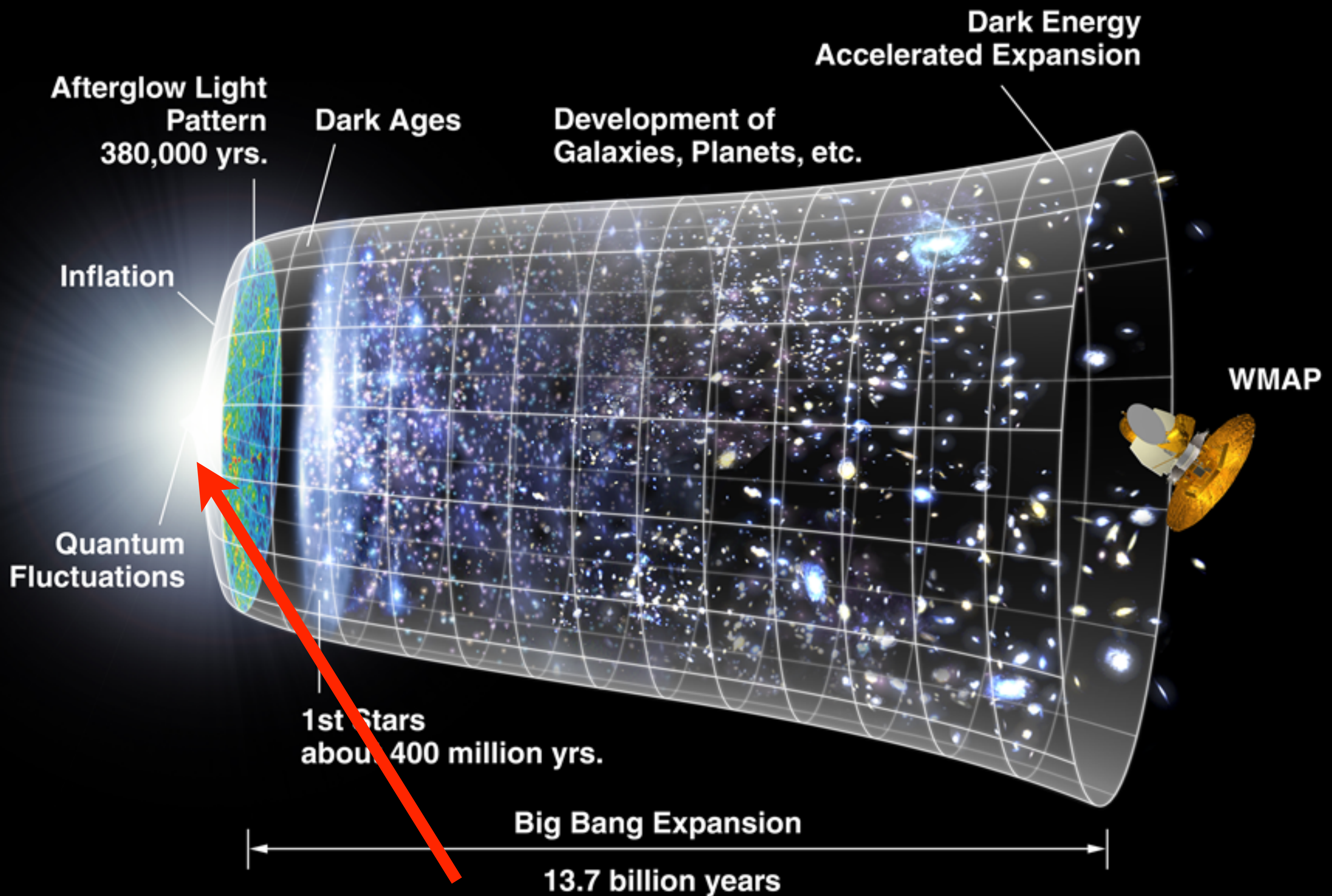


While tiny, this is still **10,000** times or more greater than we would predict with the Standard Model - why is there so much matter in the universe?

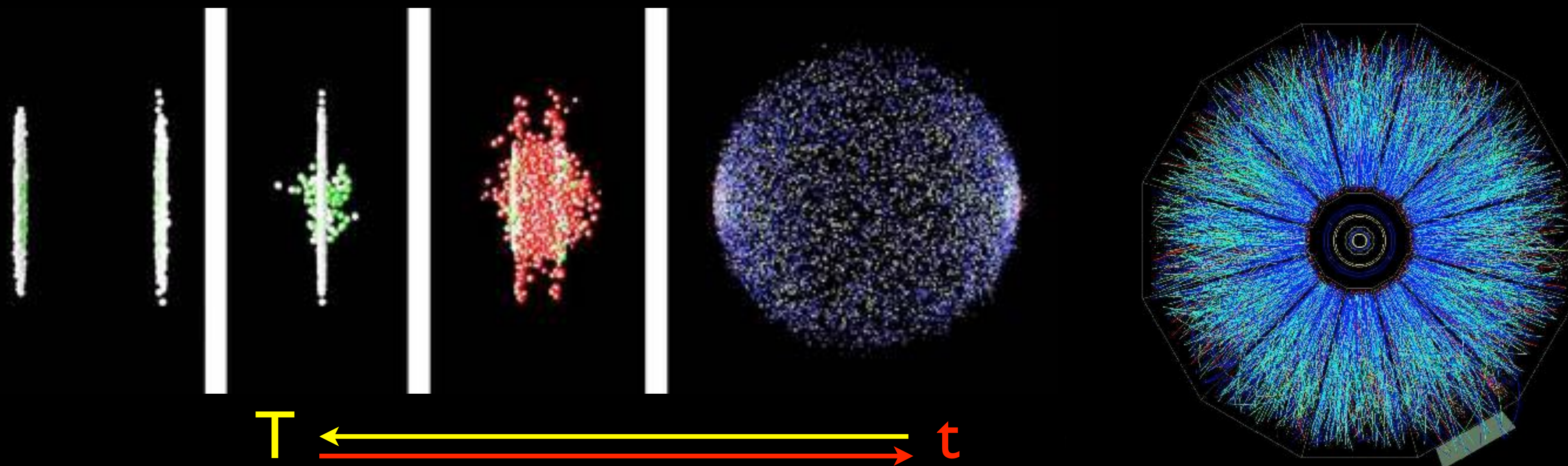


Standard Model of Particle Physics

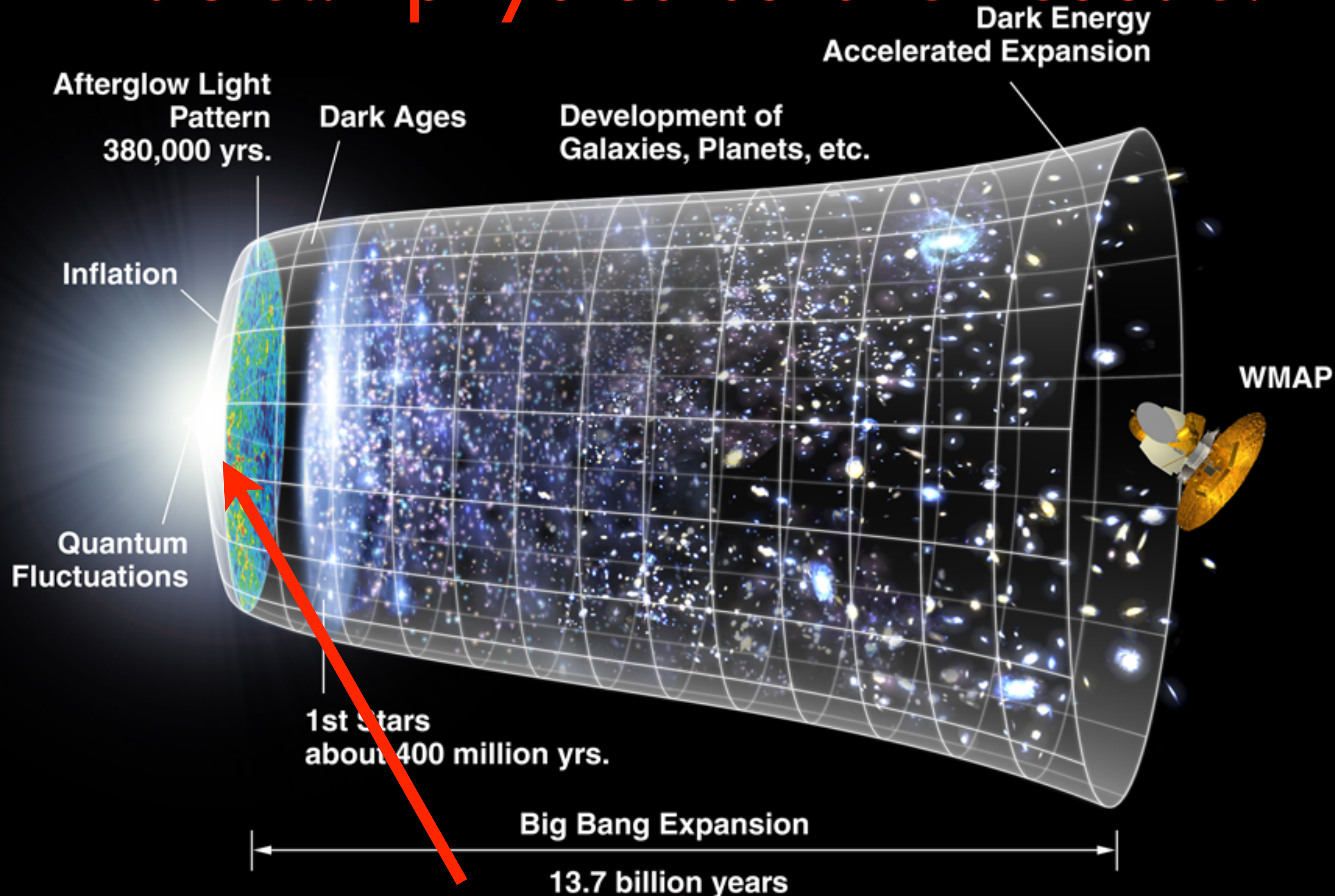




Formation of Matter
 $T \approx 1 \text{ trillion K } (10^{12} \text{ K})$
 $t \approx 30 \text{ micro seconds } (3 \times 10^{-5} \text{ s})$



Nuclear physics to the rescue!

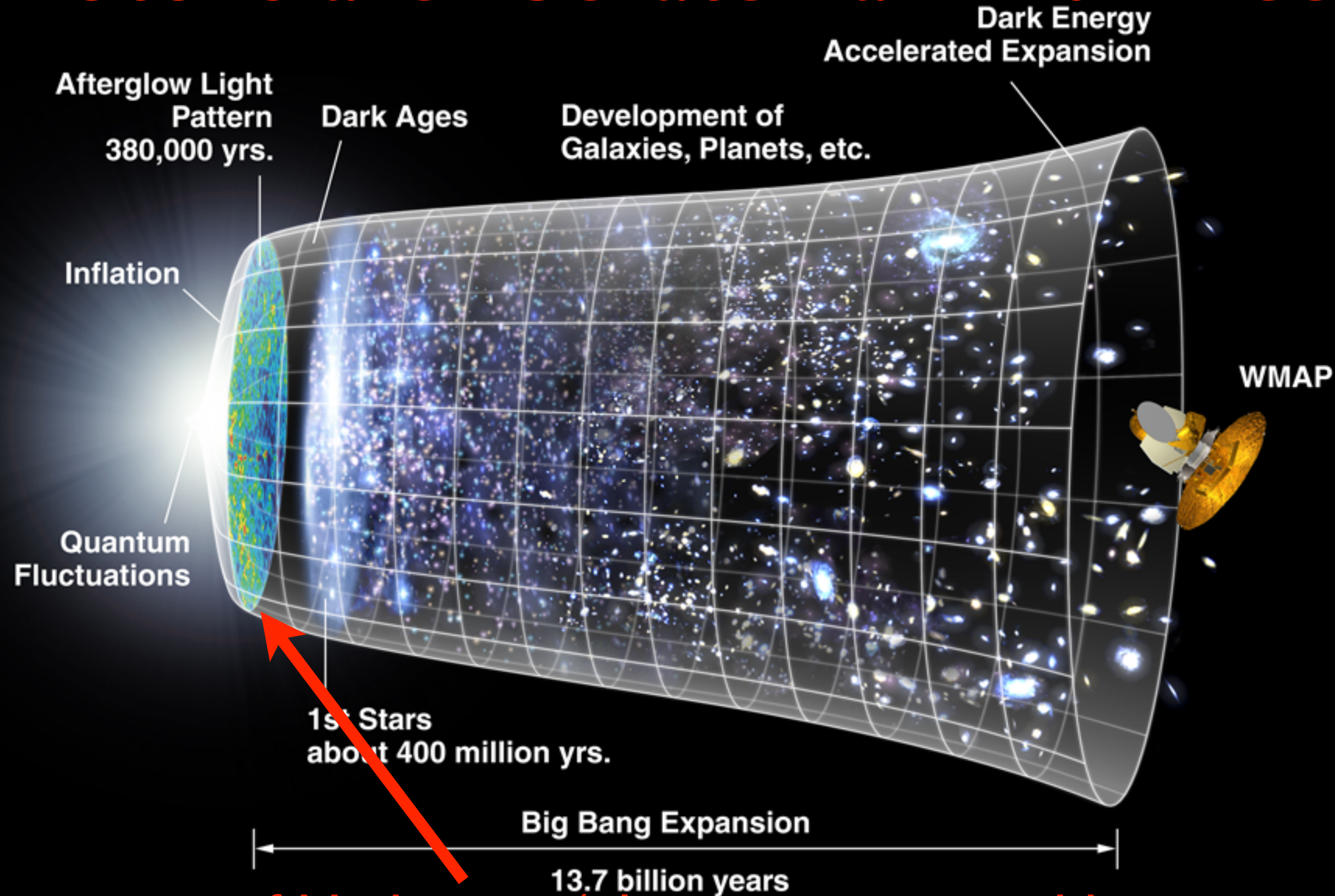


Formation of light nuclei

$T \approx 1 \text{ billion K } (10^9 \text{ K})$

$t \approx 3 \text{ minutes}$

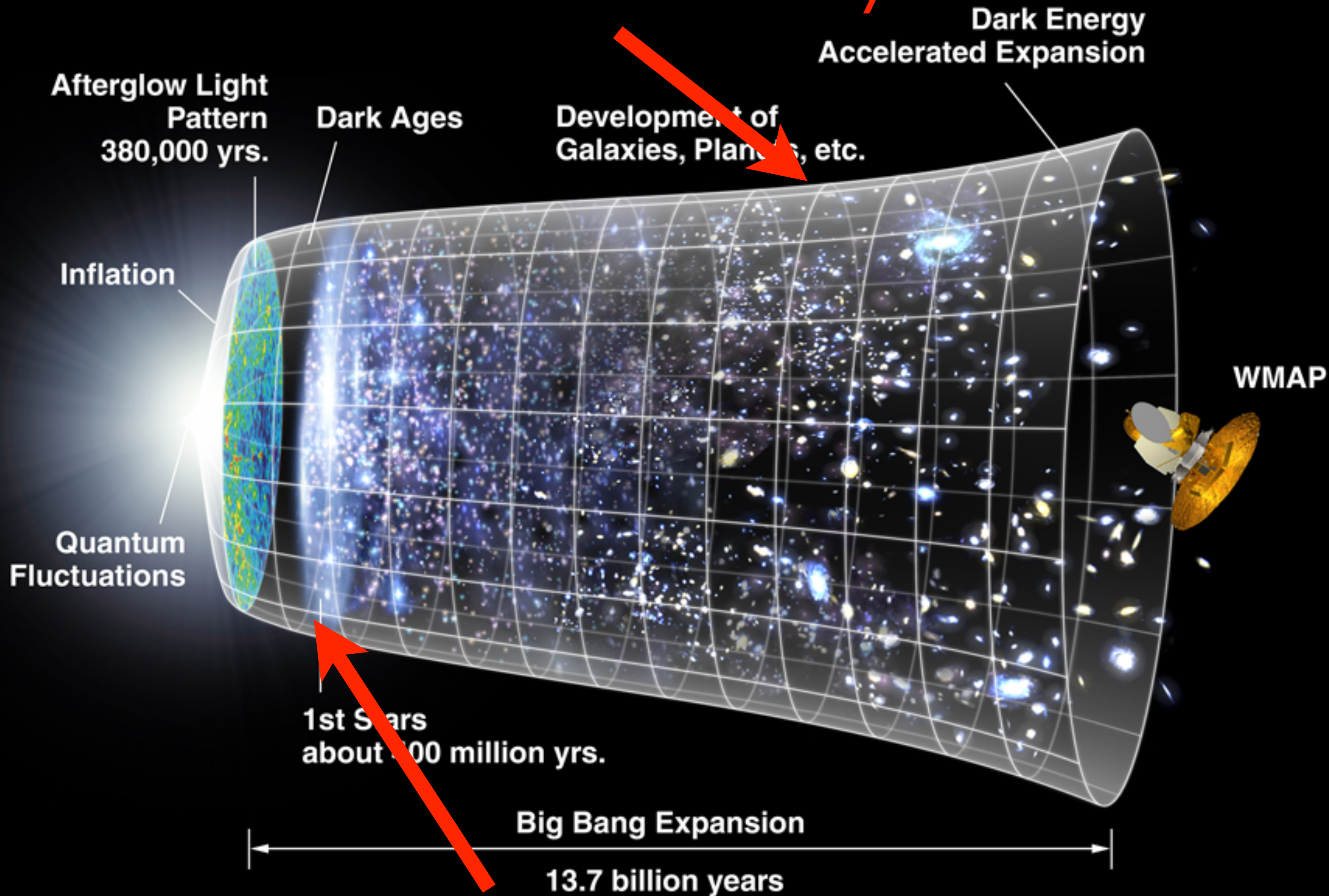
Photons are liberated and run free!



Formation of Hydrogen (electrons captured by protons)

$$T \approx 4,000 \text{ K}$$
$$t \approx 380,000 \text{ years}$$

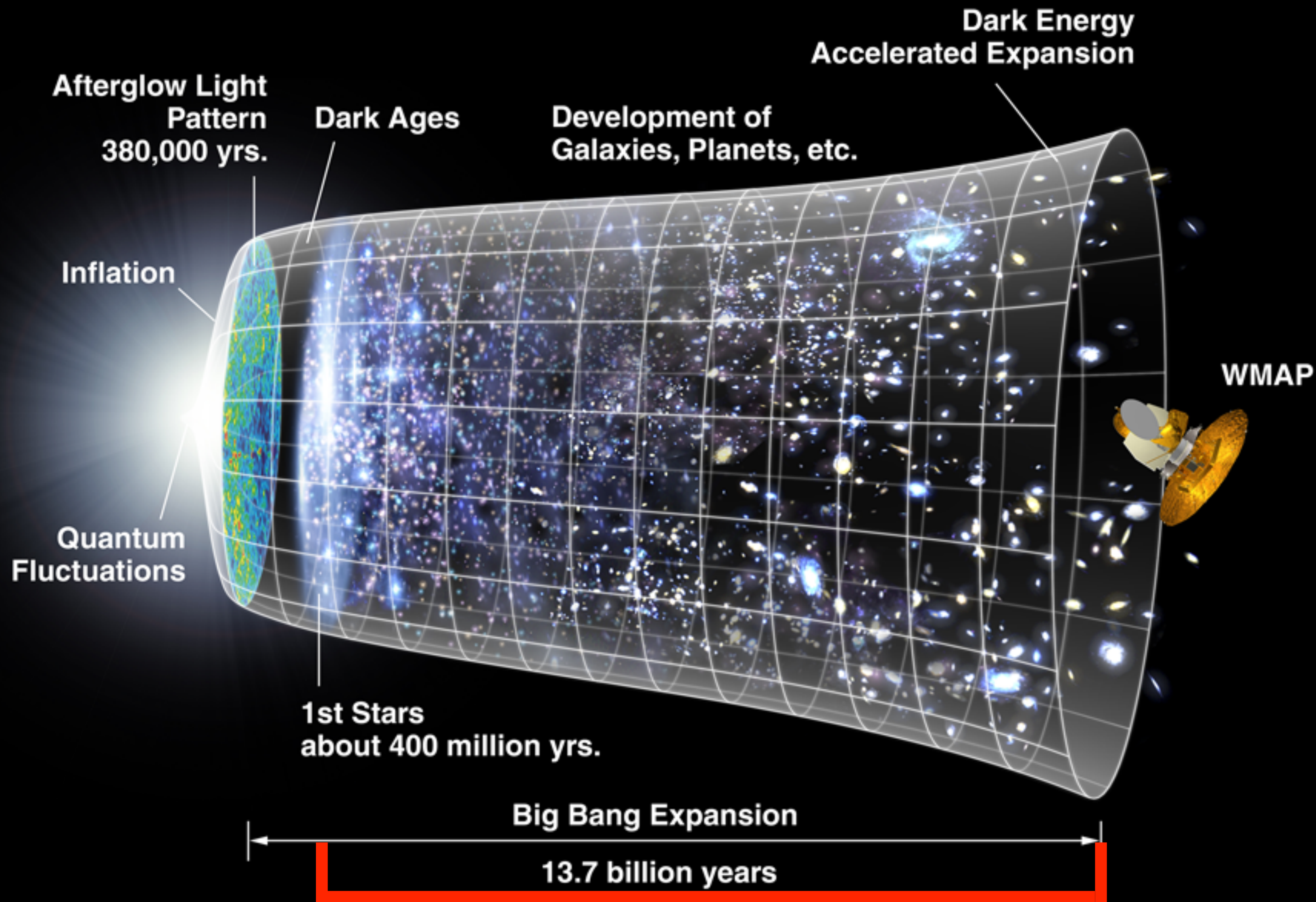
Formation of our solar system



Formation of first stars

$T \approx 20 \text{ K}$

$t \approx 200 \text{ Million years}$



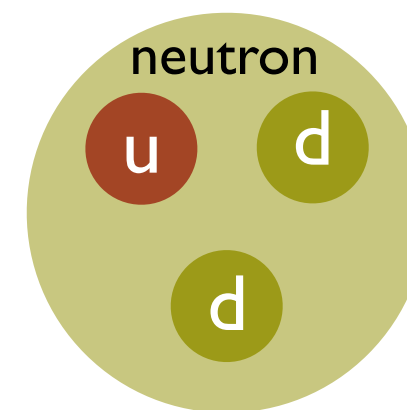
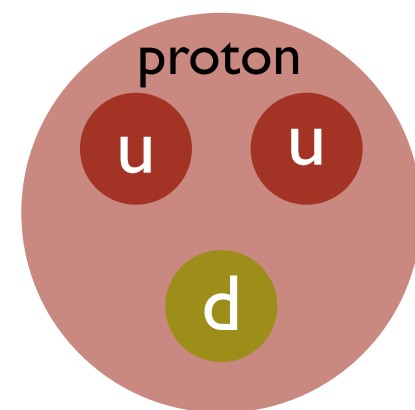
Death of stars, creation of heavy nuclei and *life*, creation of new, *ultradense* states of nuclear matter

From Quarks to Protons and Neutrons

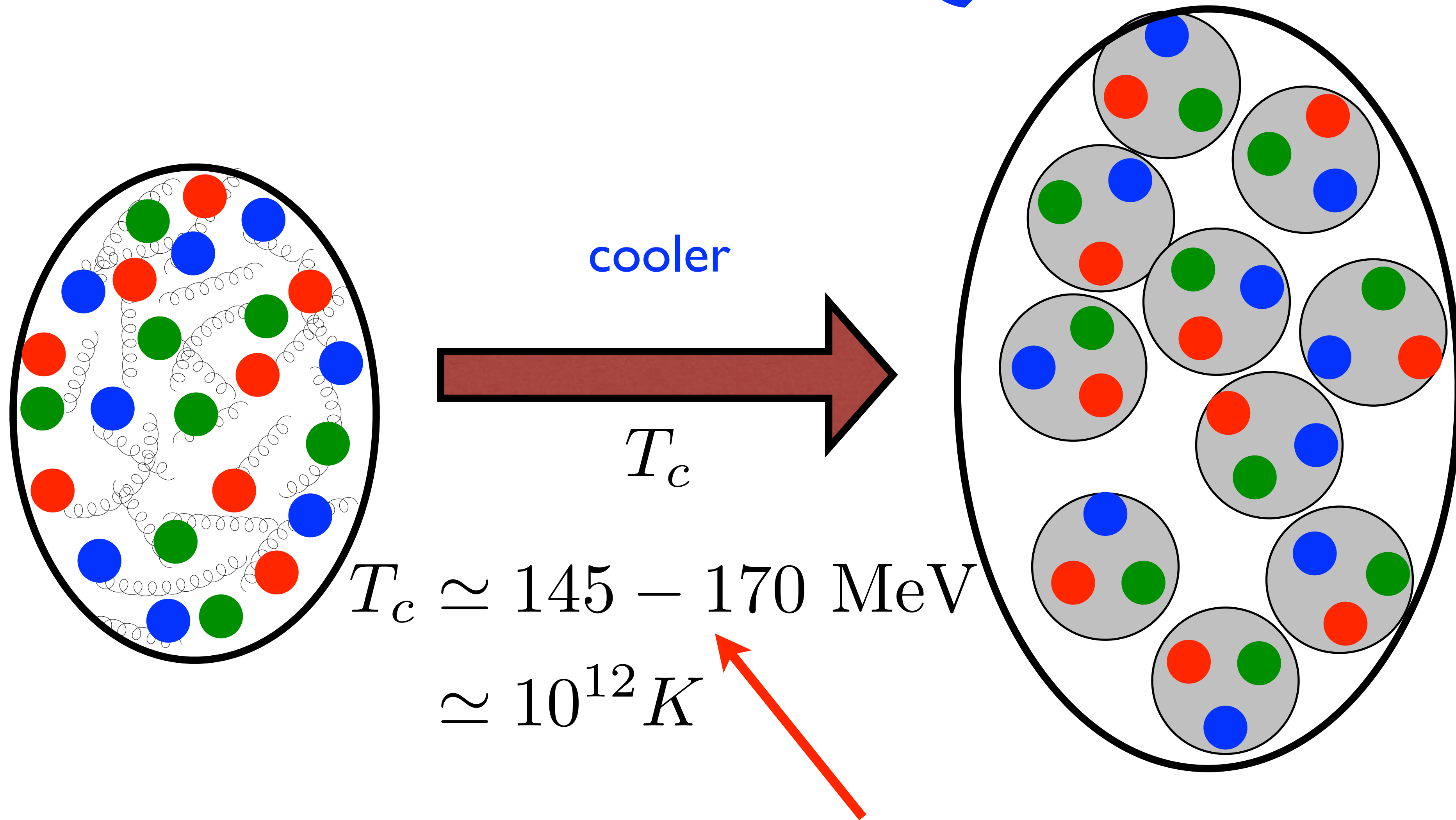
$$T \simeq 1 \text{ trillion K } (10^{12} \text{ K})$$

$$t \simeq 30 \text{ micro seconds } (3.0 \times 10^{-5} \text{ s})$$

- protons and neutrons are not fundamental - but they are composite states of *quarks* and *gluons*

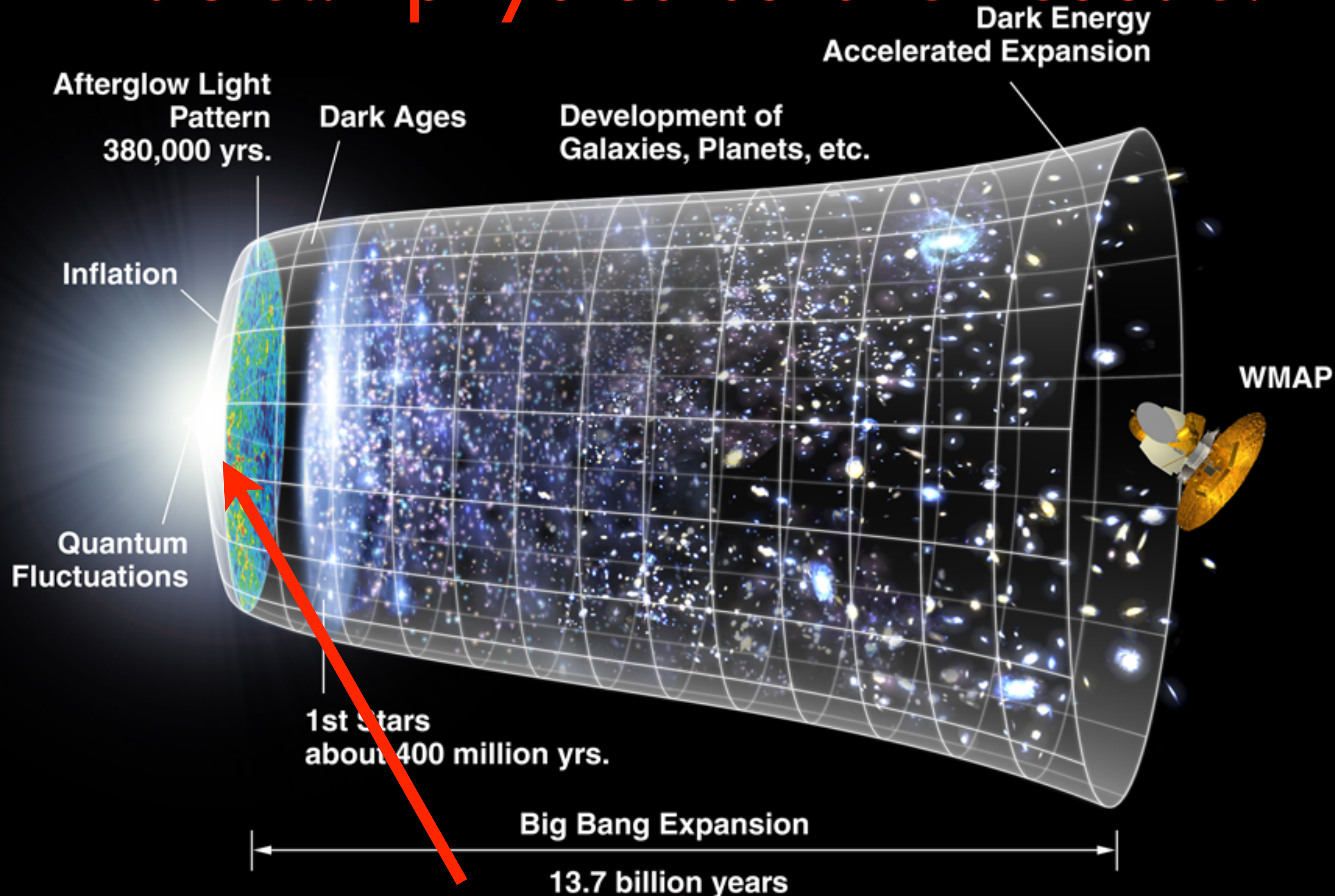


Confinement of Quarks



computed by hot-QCD and Budapest-Wuppertal Lattice Collaborations
with previous generation supercomputers

Nuclear physics to the rescue!



Formation of light nuclei

$T \approx 1 \text{ billion K } (10^9 \text{ K})$

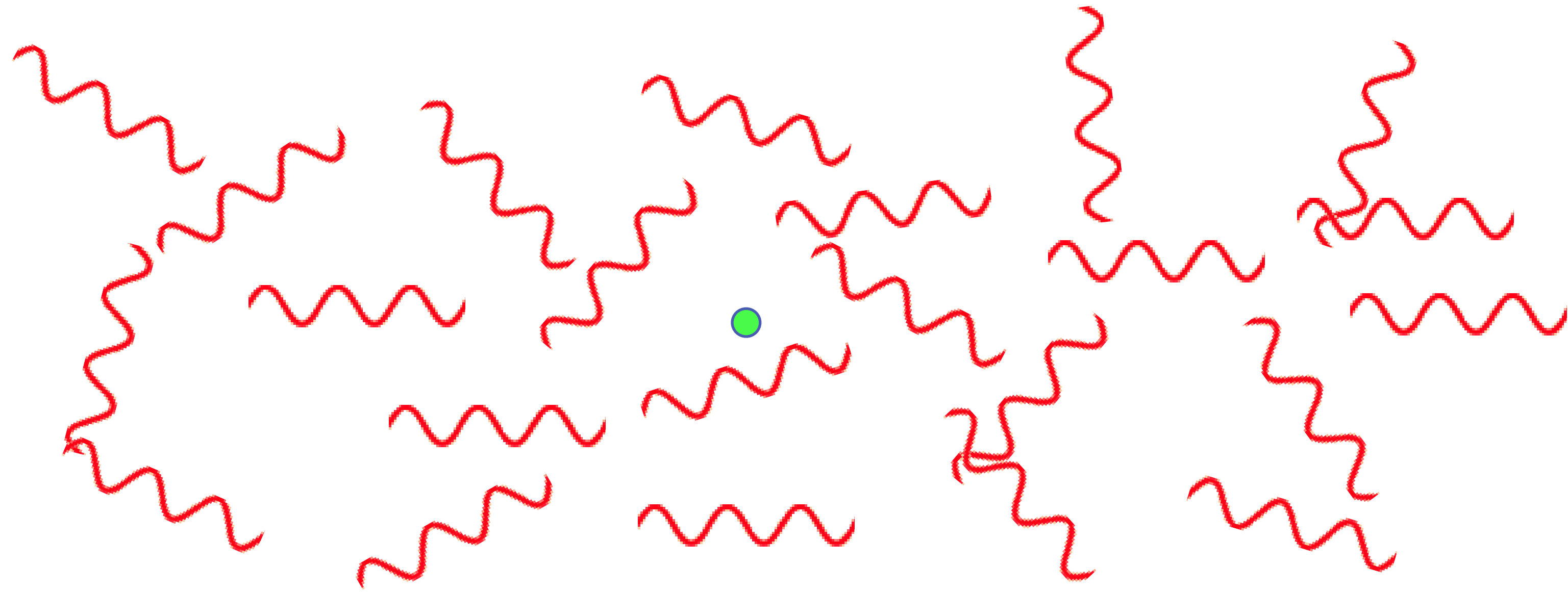
$t \approx 3 \text{ minutes}$

Big Bang Nucleosynthesis

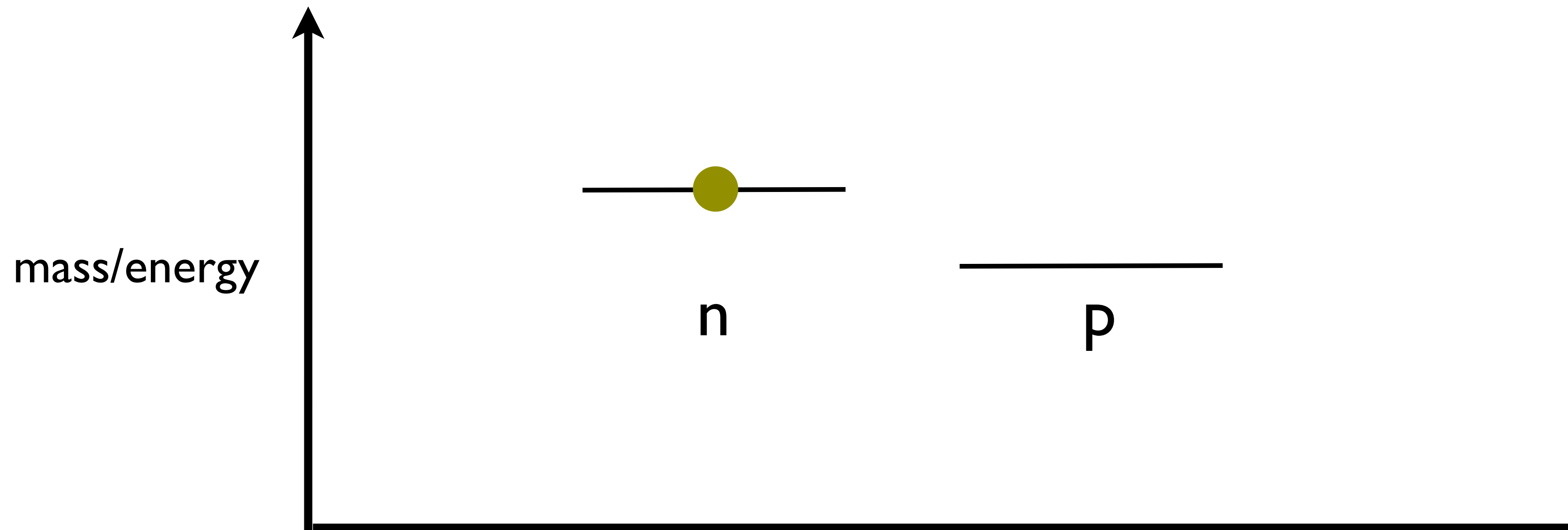
$T \simeq 1 \text{ trillion K} \rightarrow 1 \text{ billion K}$

$t \simeq 3 \times 10^{-5} \text{ s} \rightarrow 3 \text{ min}$

Our initial condition is a soup of radiation plus a small excess amount of matter, in the form of protons, neutrons, electrons and photons



when systems cool, they settle into the lowest energy state



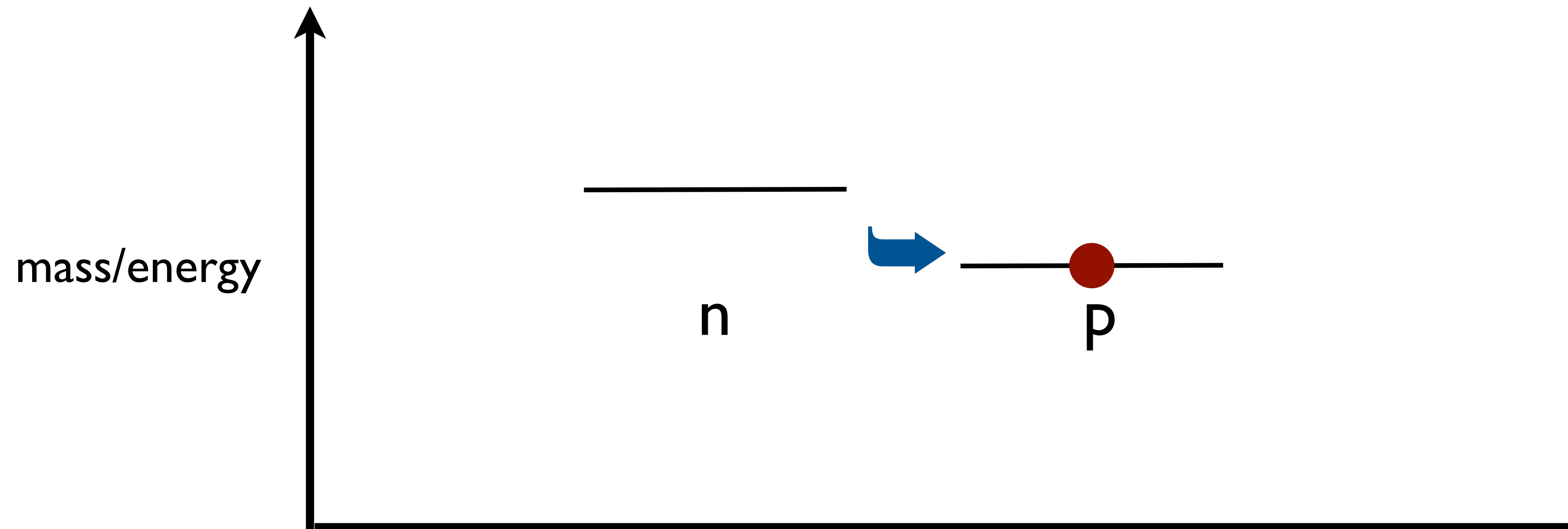
$$M_n - M_p = 1.29333217(42) \text{ MeV}$$

$$E_{\text{Hydrogen}} = 13.6 \text{ eV}$$

$$\frac{M_n + M_p}{2} = 938.9187473(58) \text{ MeV}$$

$$1 \text{ MeV} = 10^6 \text{ eV}$$

when systems cool, they settle into the lowest energy state

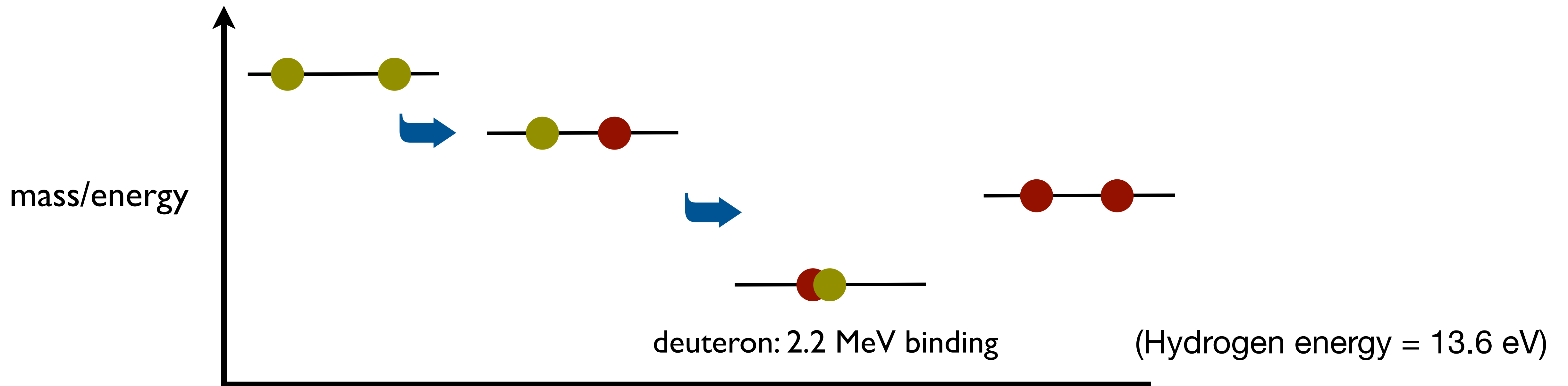


$$\tau_n \sim 15 \text{ min}$$

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

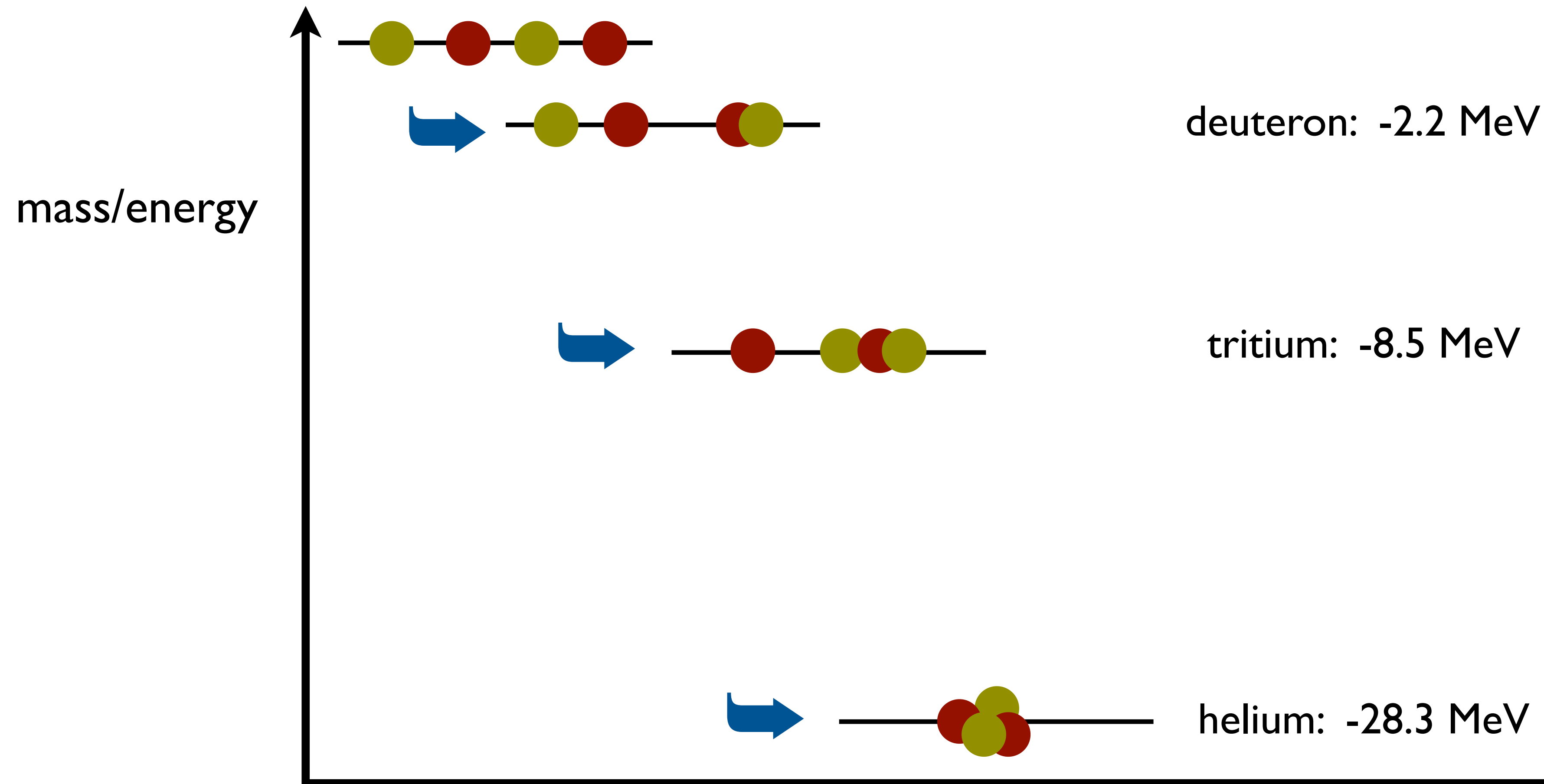
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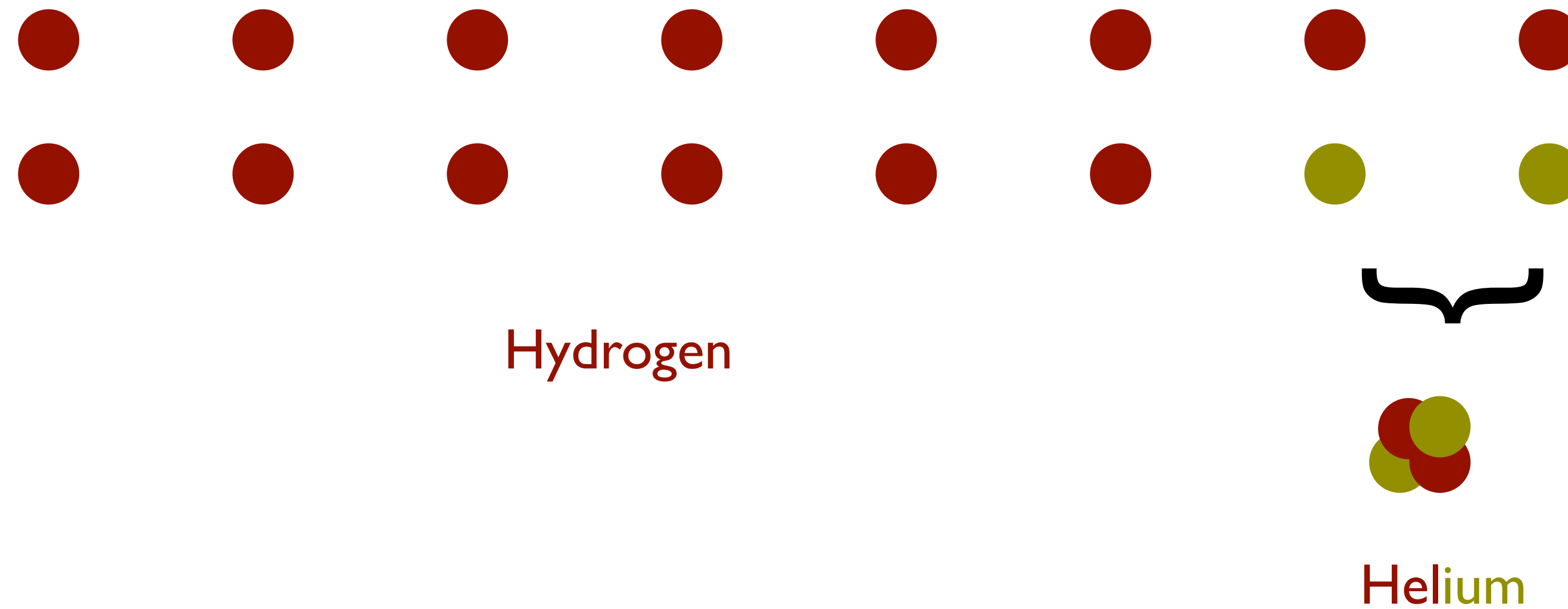
Answer: formation of nuclei

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**

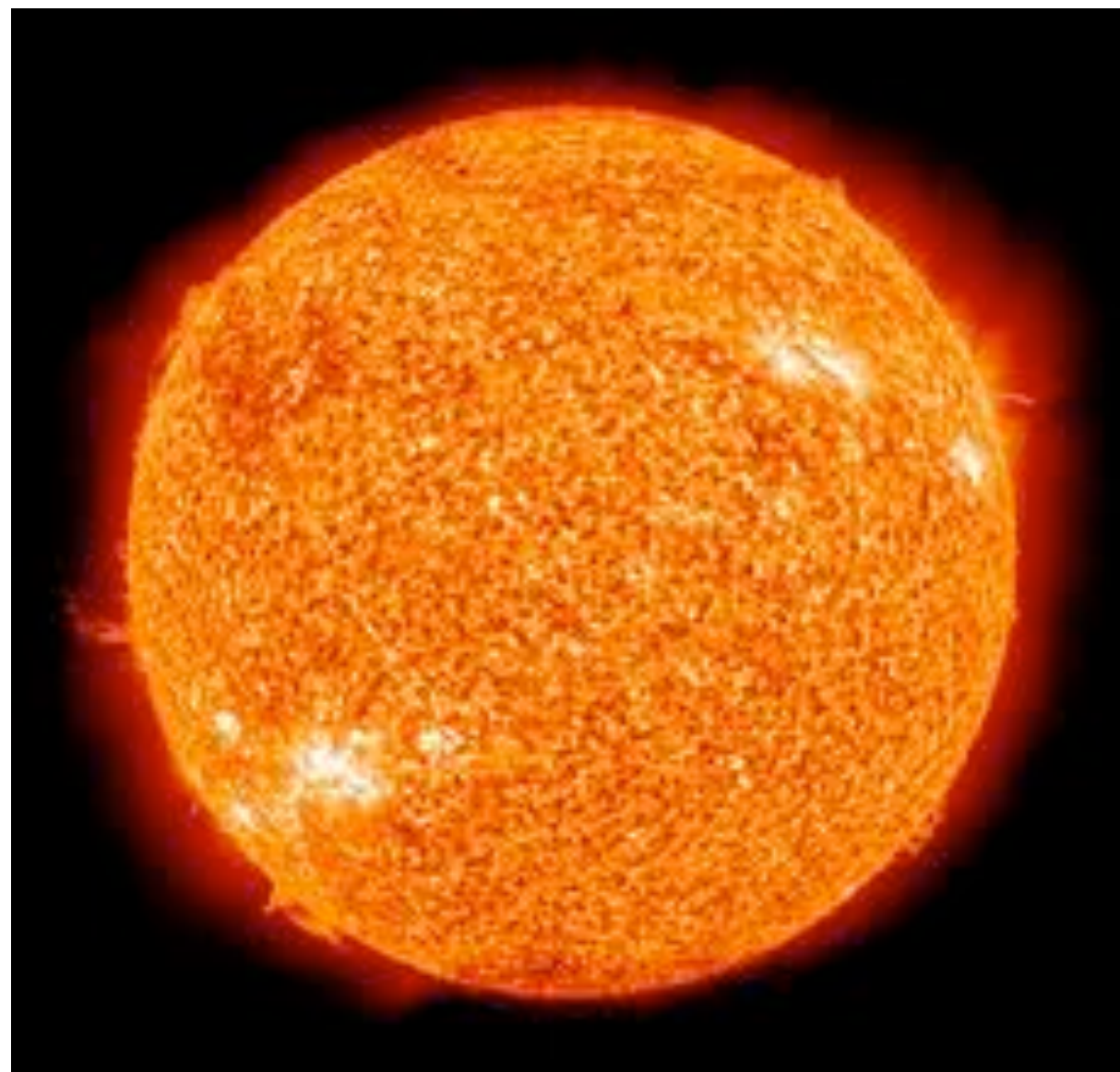
The deuterium “bottleneck” is broken, neutrons flow into He



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)



The evolution of the universe is very sensitive to

- what is the lifetime of a neutron?
- what is the excess of matter over anti-matter?

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

$$B_d = 2.22 \text{ MeV}$$

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!

Can we understand the emergence of B_d and how fine-tuned it is in terms of the fundamental theory?

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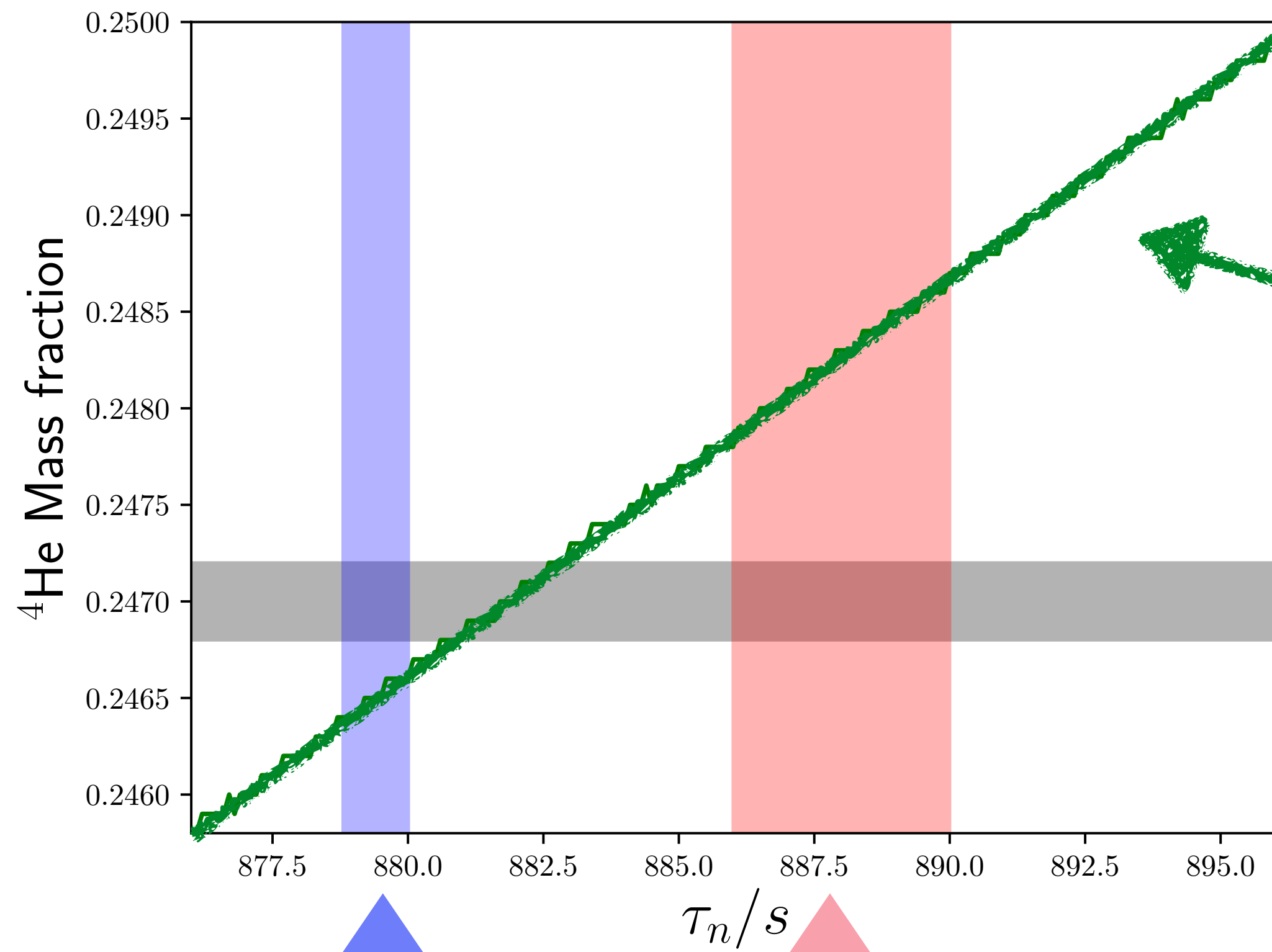
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Yes!
With  **summit!**

This picture is also very sensitive to the lifetime of the neutron



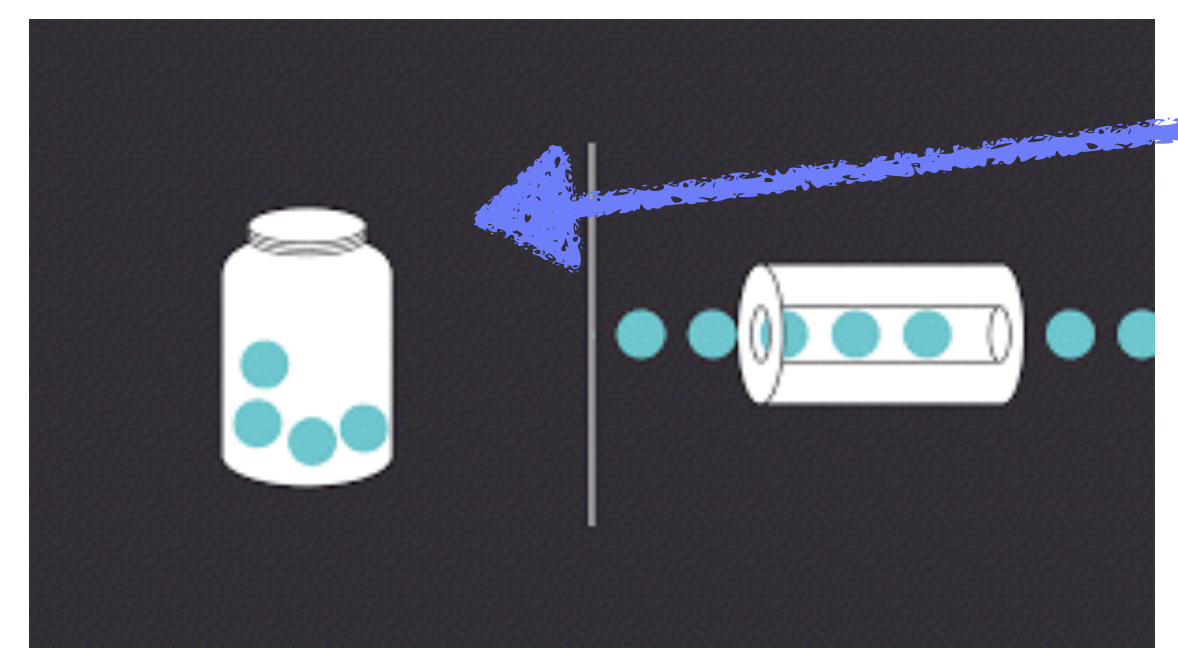
$$\tau_n = \frac{(5172.0 \pm 1.1) \text{ seconds}}{1 + 3g_A^2}$$

Czarnecki, Marciano, Sirlin

Predicted primordial ^4He mass fraction of the universe as a function of the neutron lifetime

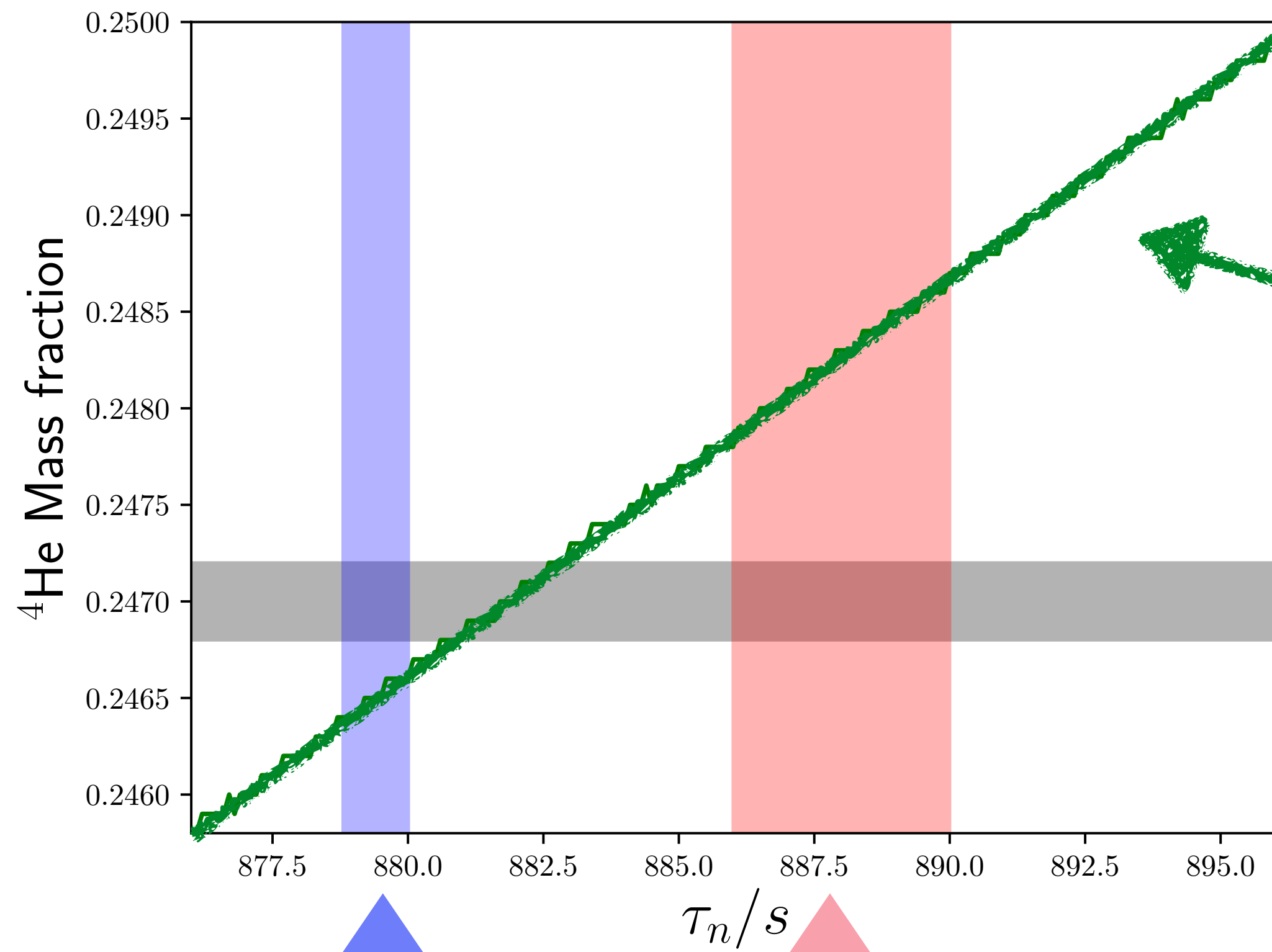
Observed primordial ^4He mass fraction of the universe

Two different methods of measuring the neutron lifetime disagree at the 99% level
bottle and beam



Is one of the experiments wrong? Or is there new physics hiding here?

This picture is also very sensitive to the lifetime of the neutron



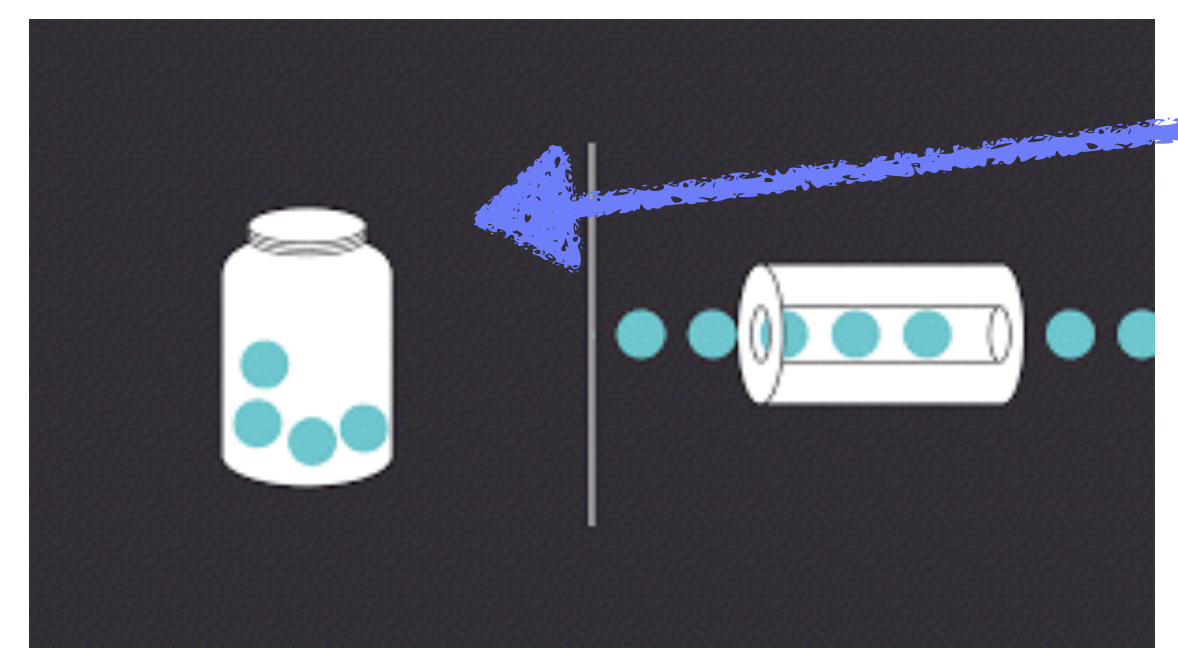
$$\tau_n = \frac{(5172.0 \pm 1.1) \text{ seconds}}{1 + 3g_A^2}$$

Czarnecki, Marciano, Sirlin

In order to predict this number, we need to use massive super-computers

Predicted primordial ^4He fraction of the universe of the neutron lifetime

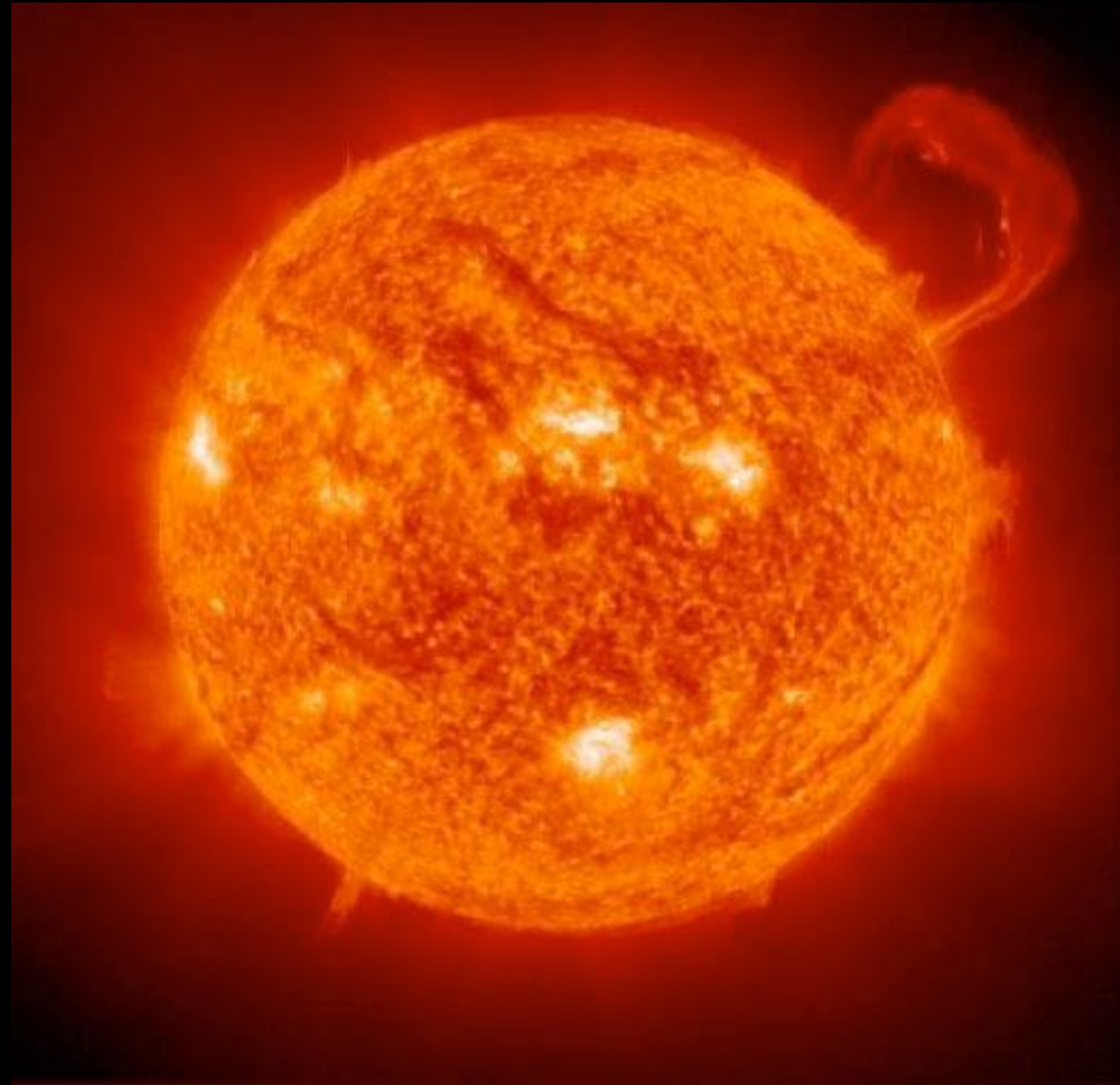
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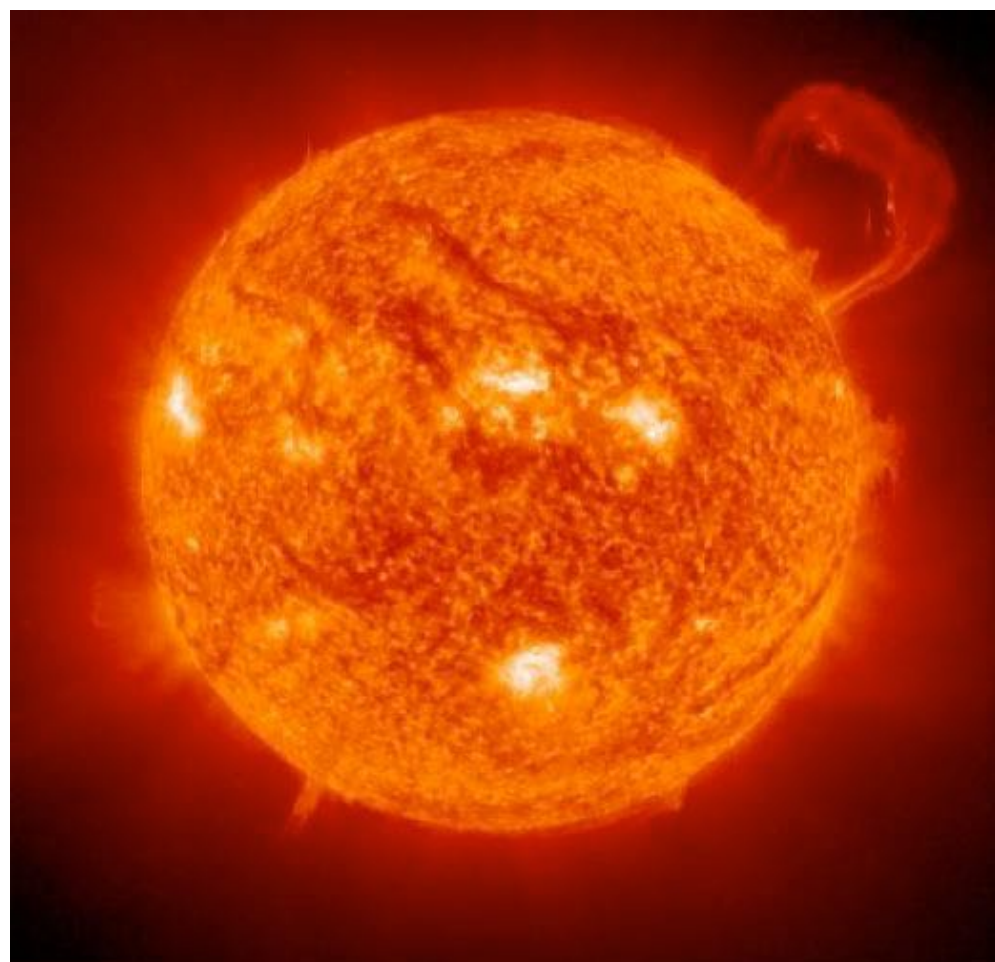
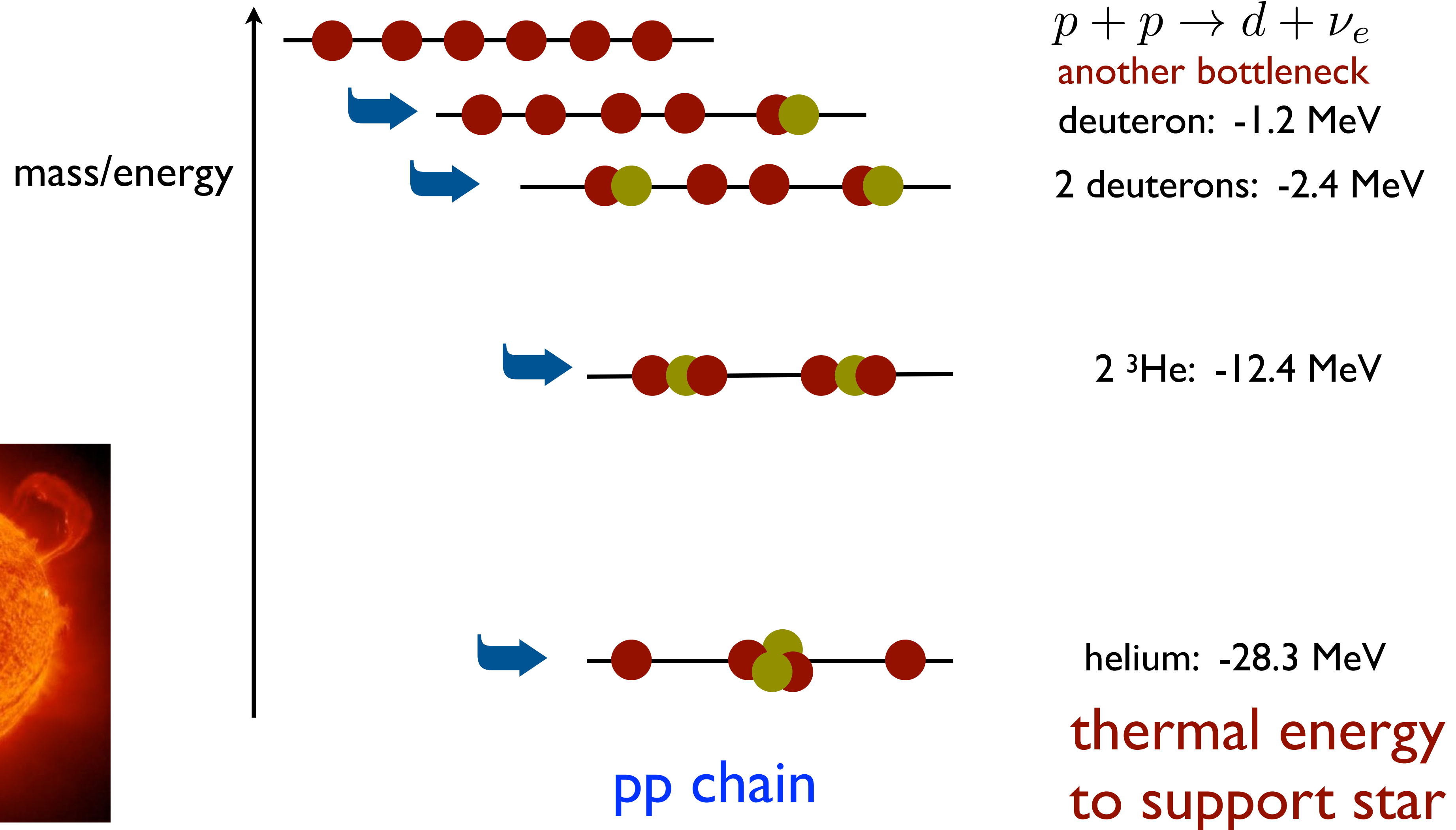
Solar Fusion



$T \simeq 20 \text{ K}$
 $t \simeq 200 \text{ Million years}$

One needs neutrons and protons to make new nuclei.

Small stars burn protons only, manufacturing the needed neutrons

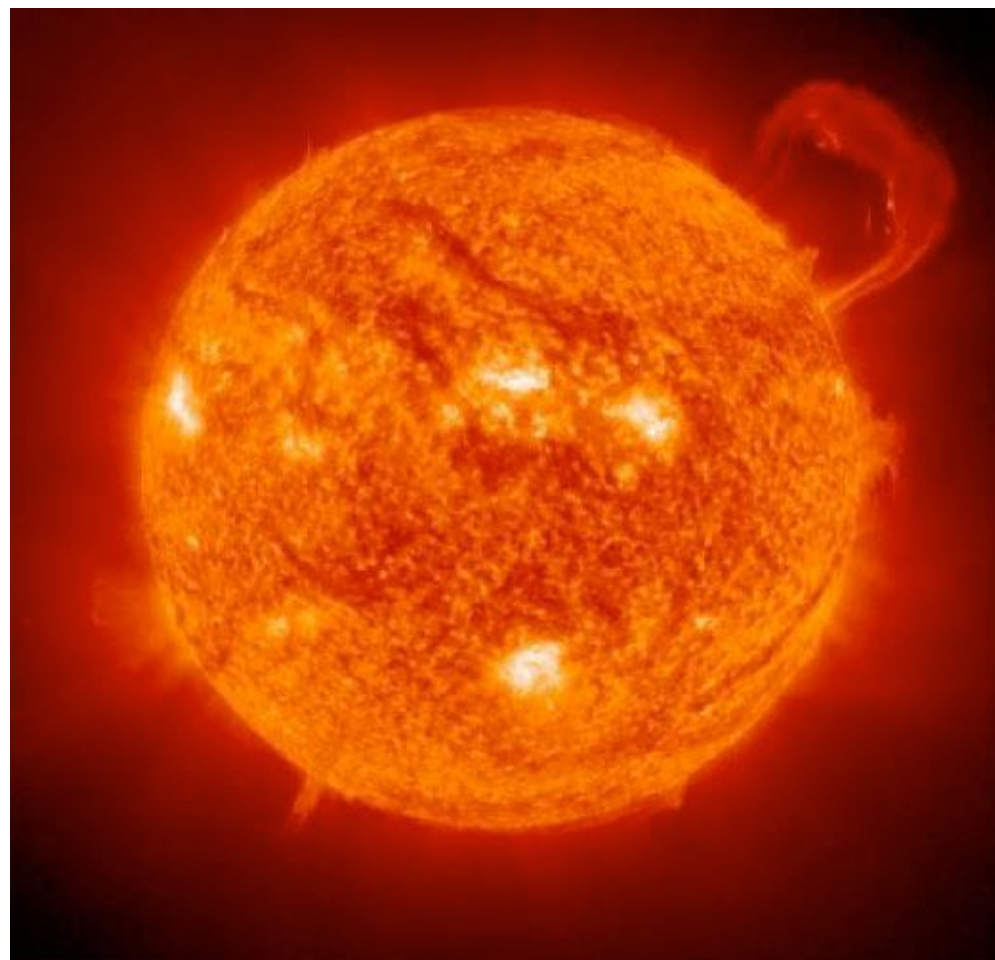


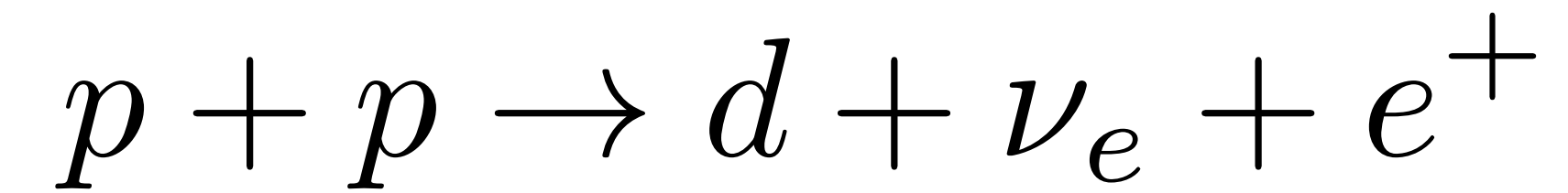
This is how our Sun generates its energy

80% of all stars generate their energy by hydrogen burning

At its very center the Sun generates 275 watts/m³ - similar to the energy generated by a **compost (garbage) heap (of the same size)!**

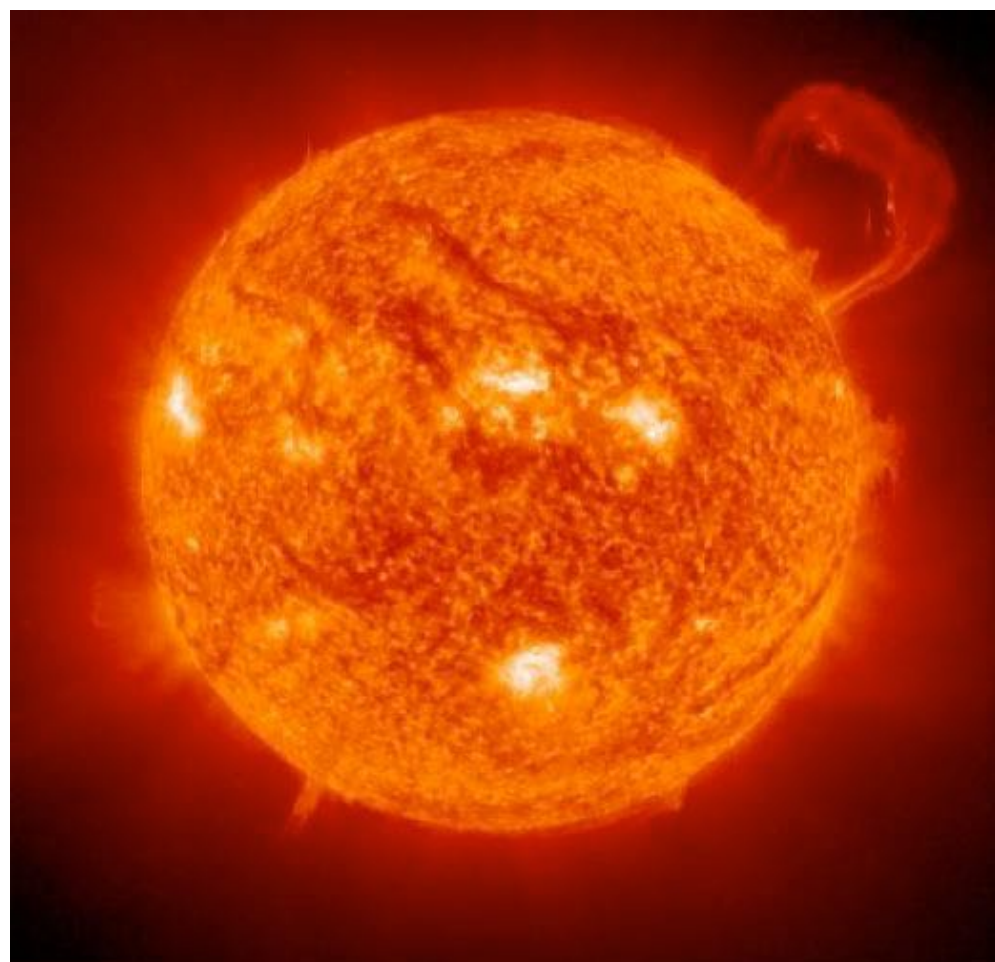
And this is why the Sun has burned for 4.6 b.y., and will burn for 5 b.y. more, fortunately -- a very big, very slow reactor

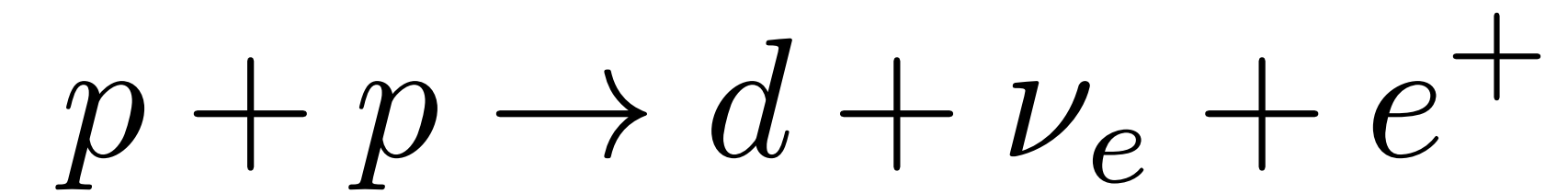




This fundamental reaction can not be measured!
(Coulomb Repulsion)

We believe we know the rate, but we have not been able to
predict it directly from the fundamental theory,
can we?

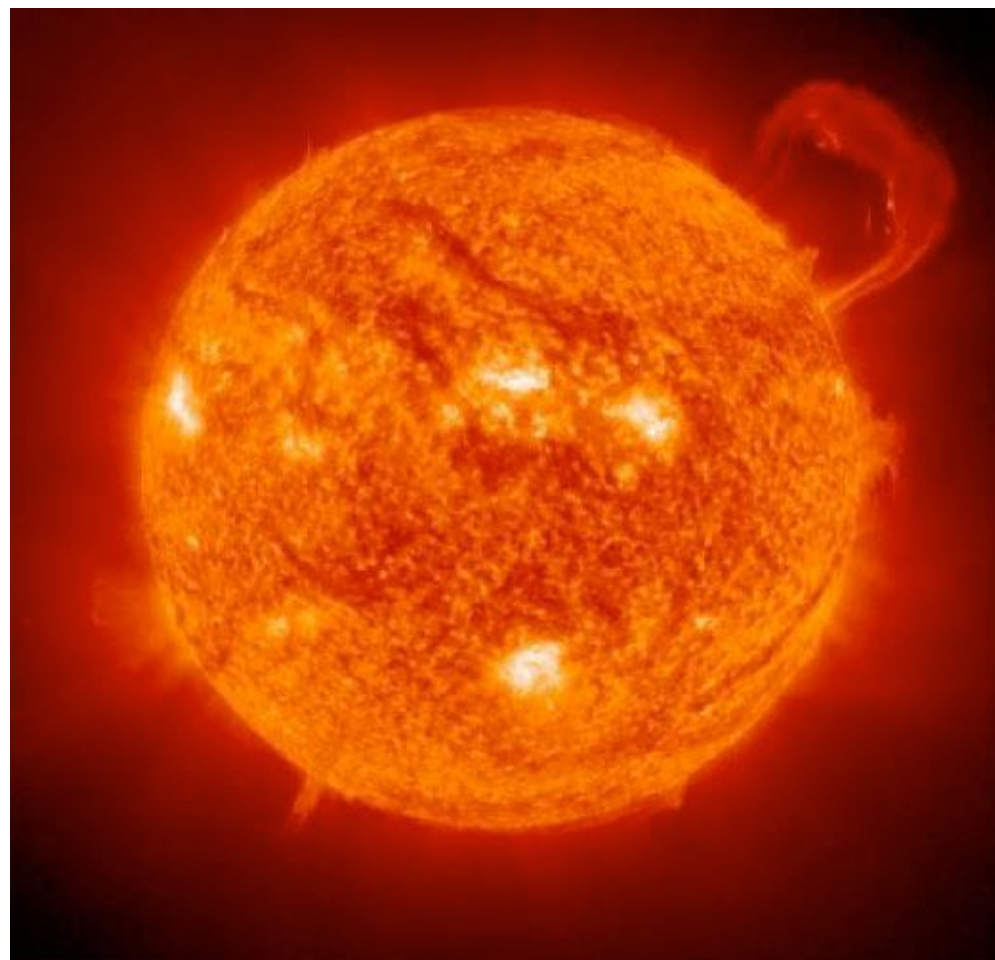




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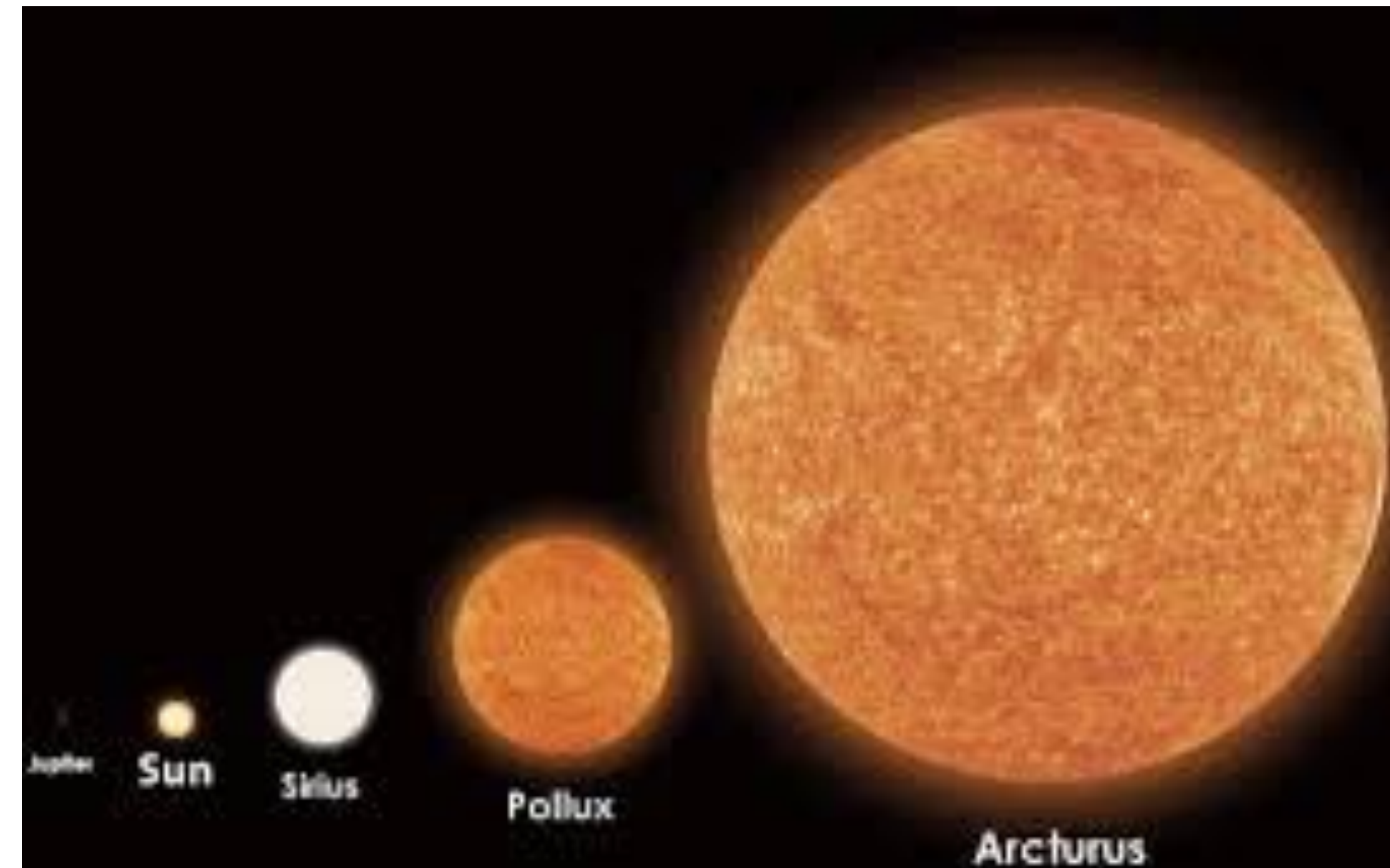
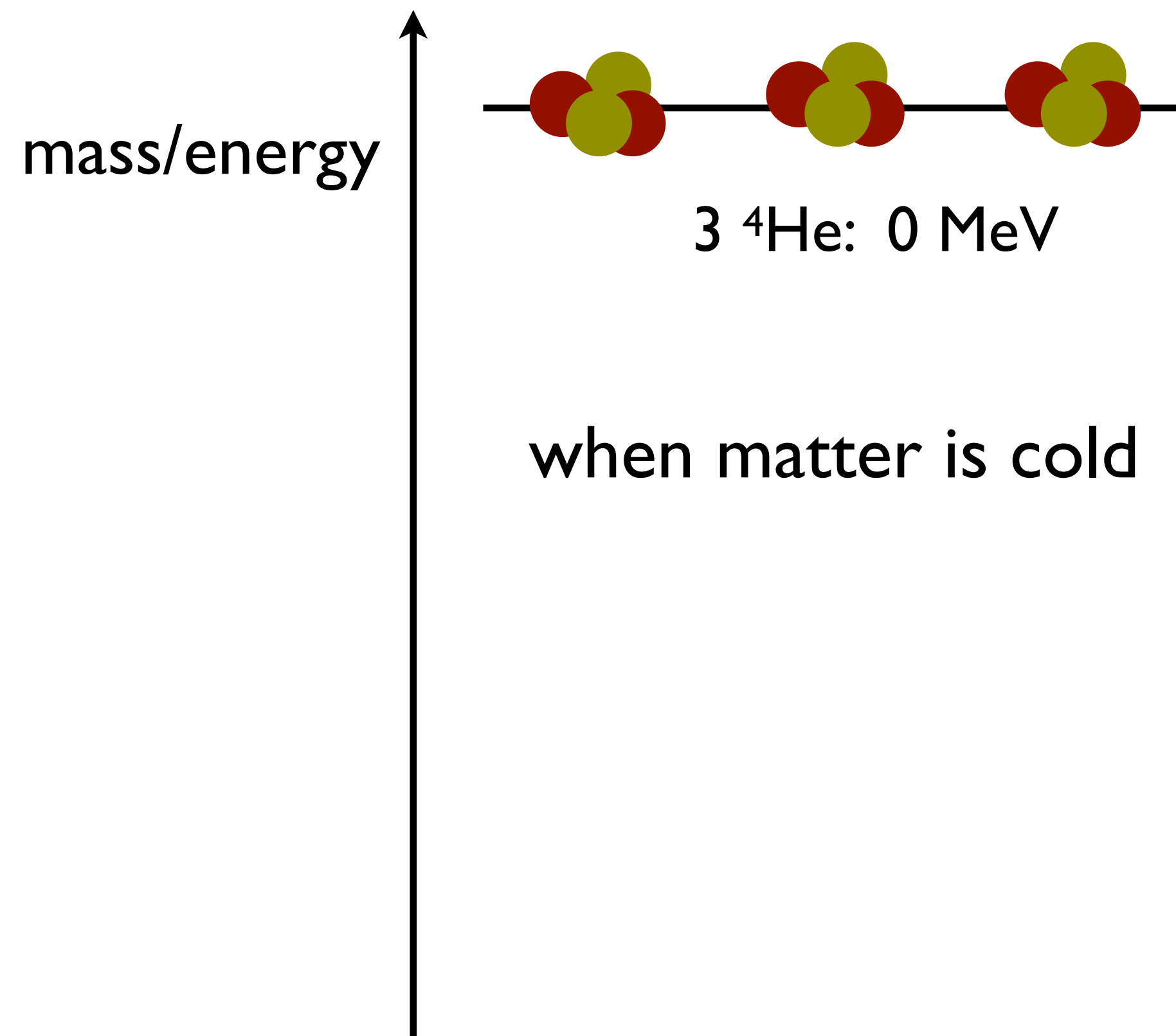
Yes!
With  **Summit!**



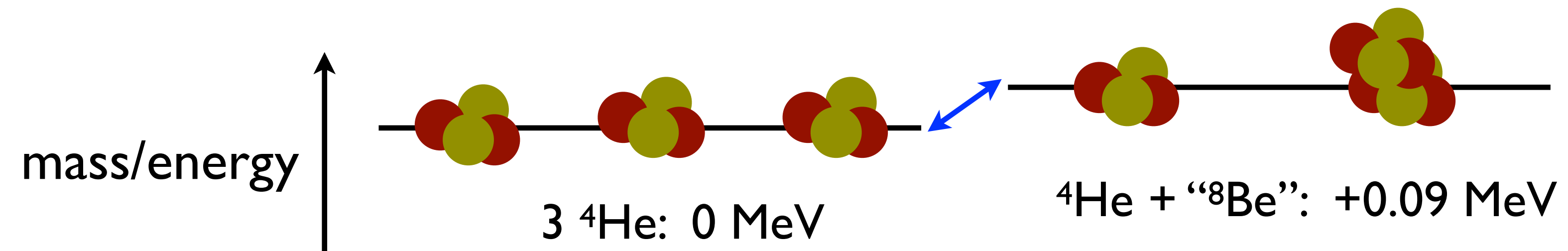
Large stars use He and neutrons to build new nuclei.

Higher temperatures and higher densities are needed.

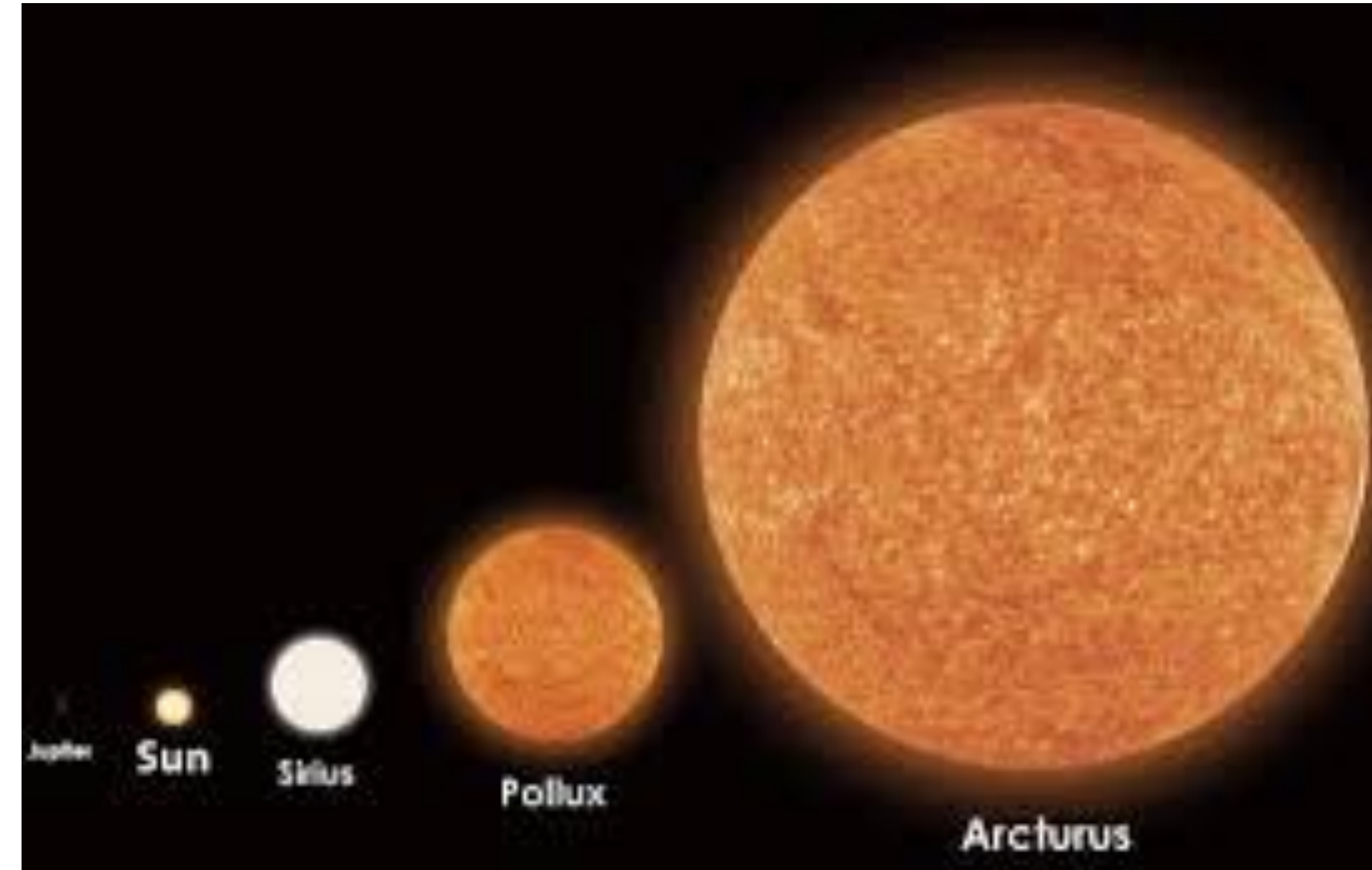
The Big Bang could not do this because the density was too low.



even more finely tuned

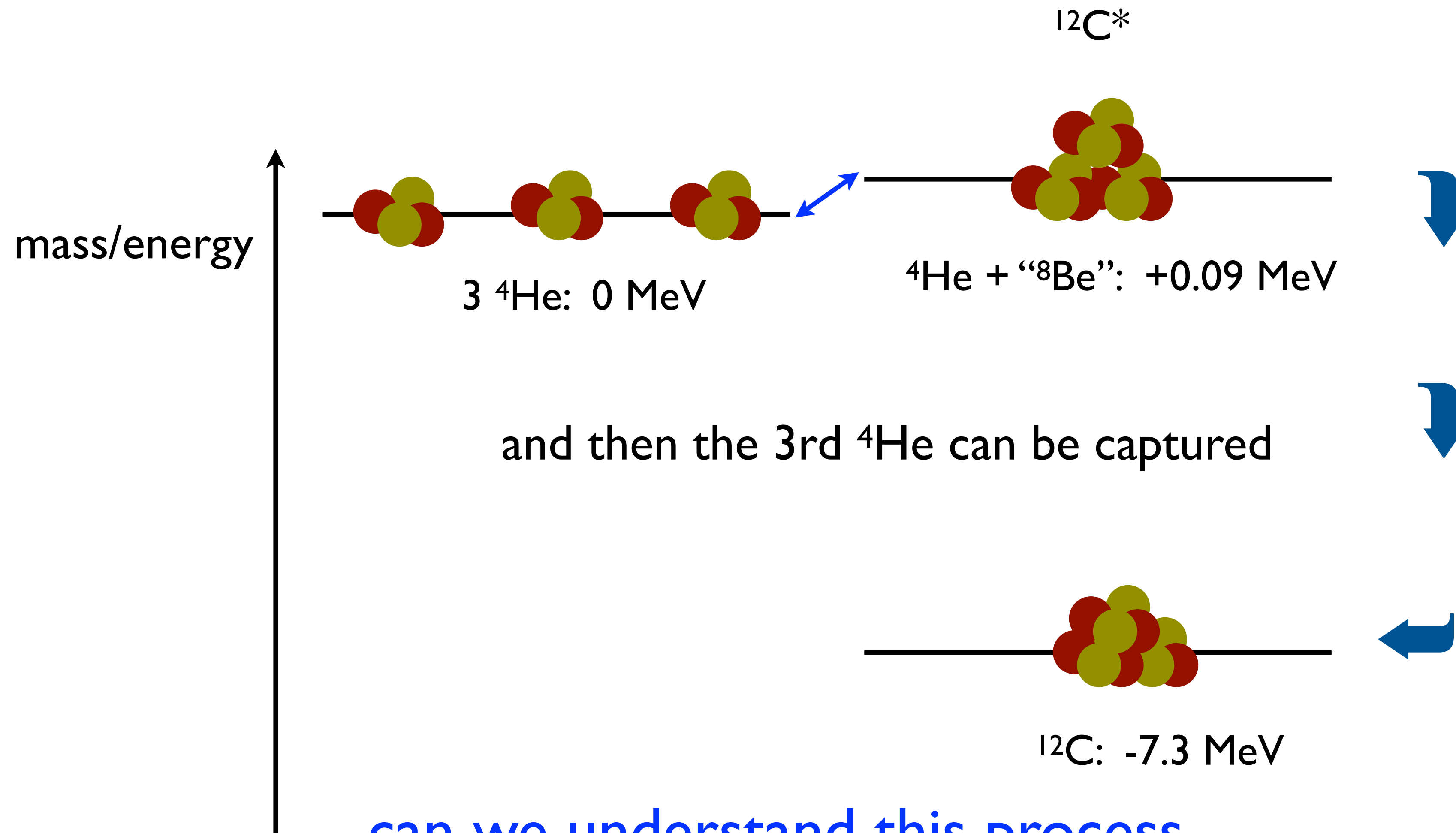


but when matter is hot, $T > 10^8$ K



even more finely tuned - source of complex life

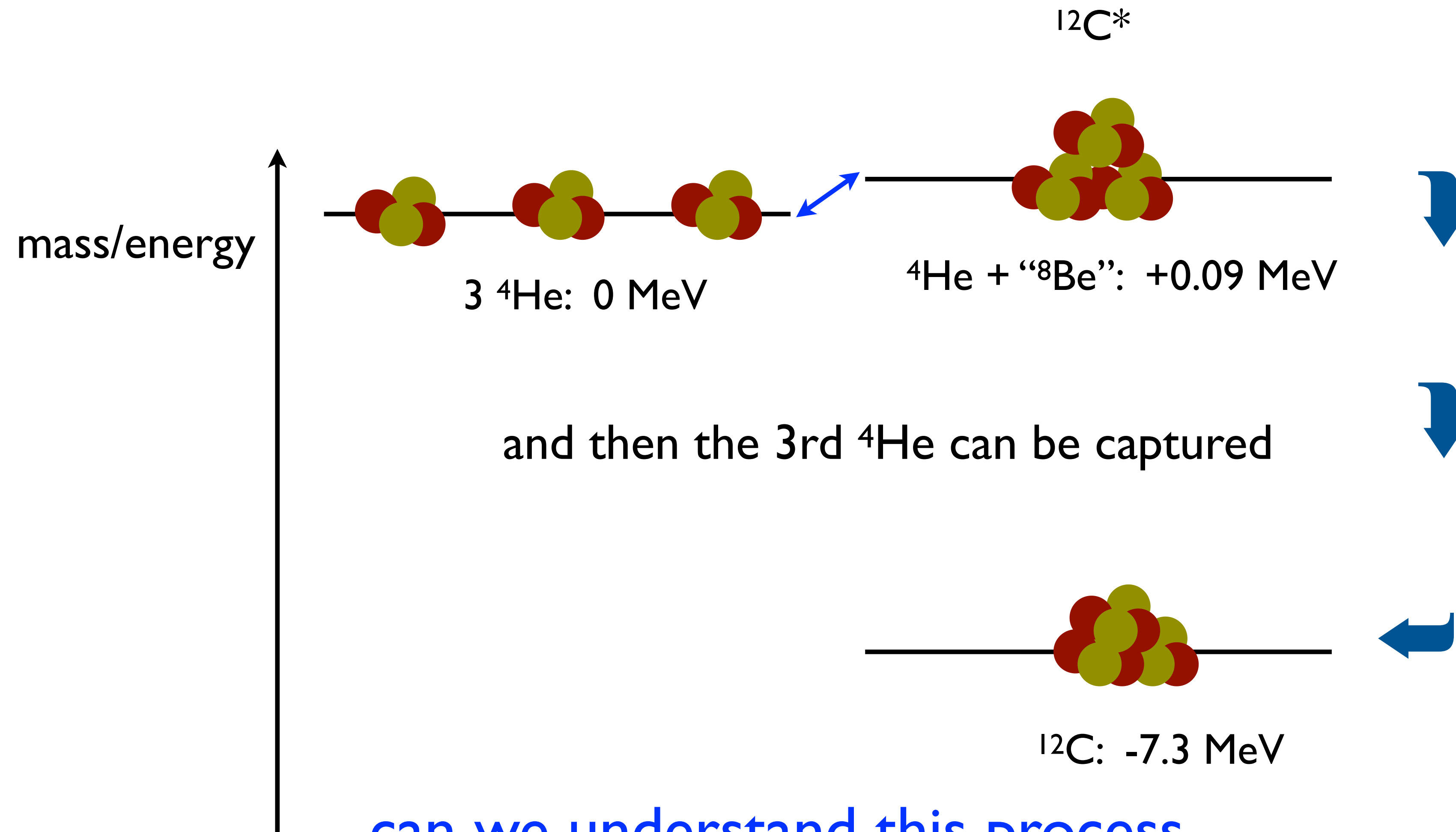
the triple- α process **Hoyle State**



can we understand this process
from the fundamental theory?

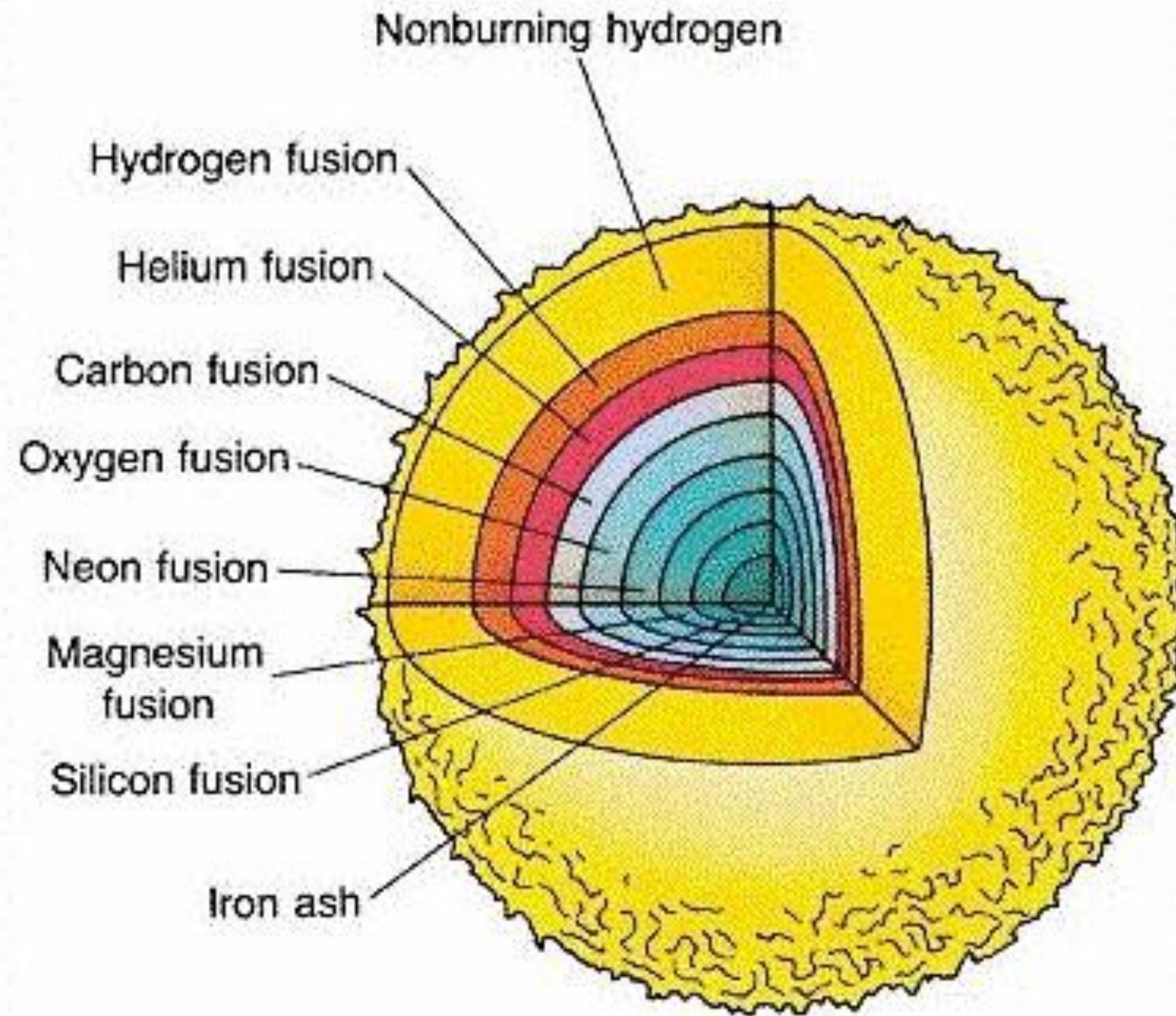
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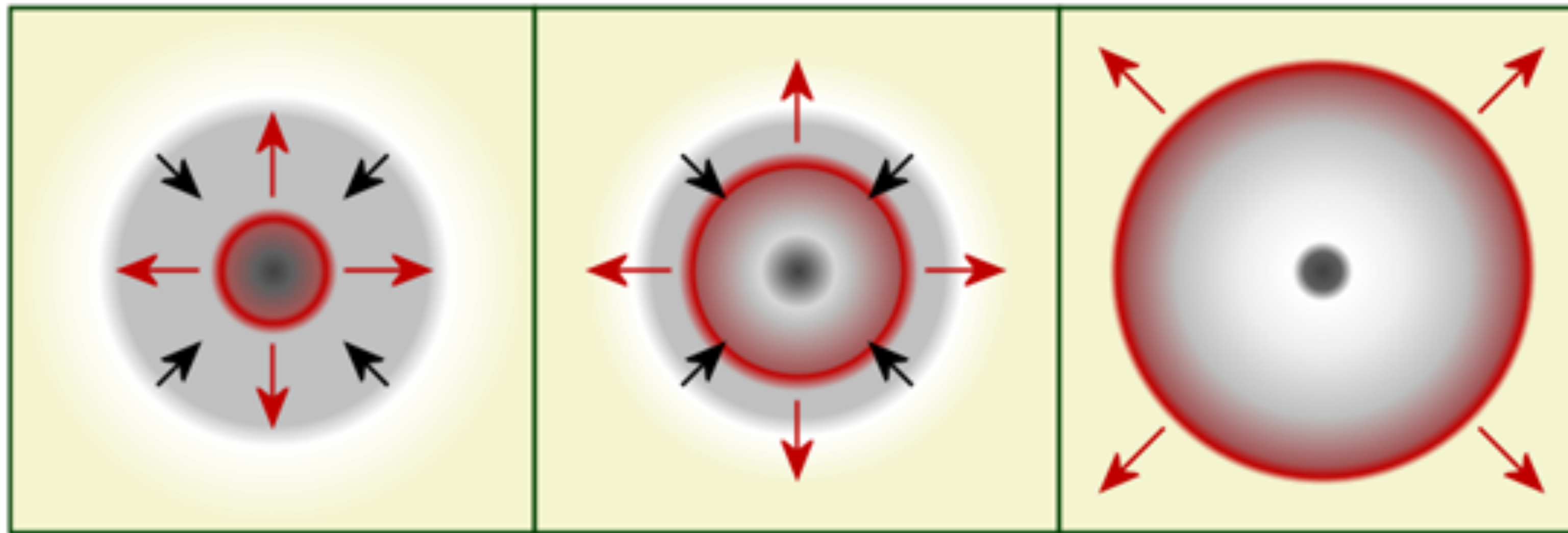
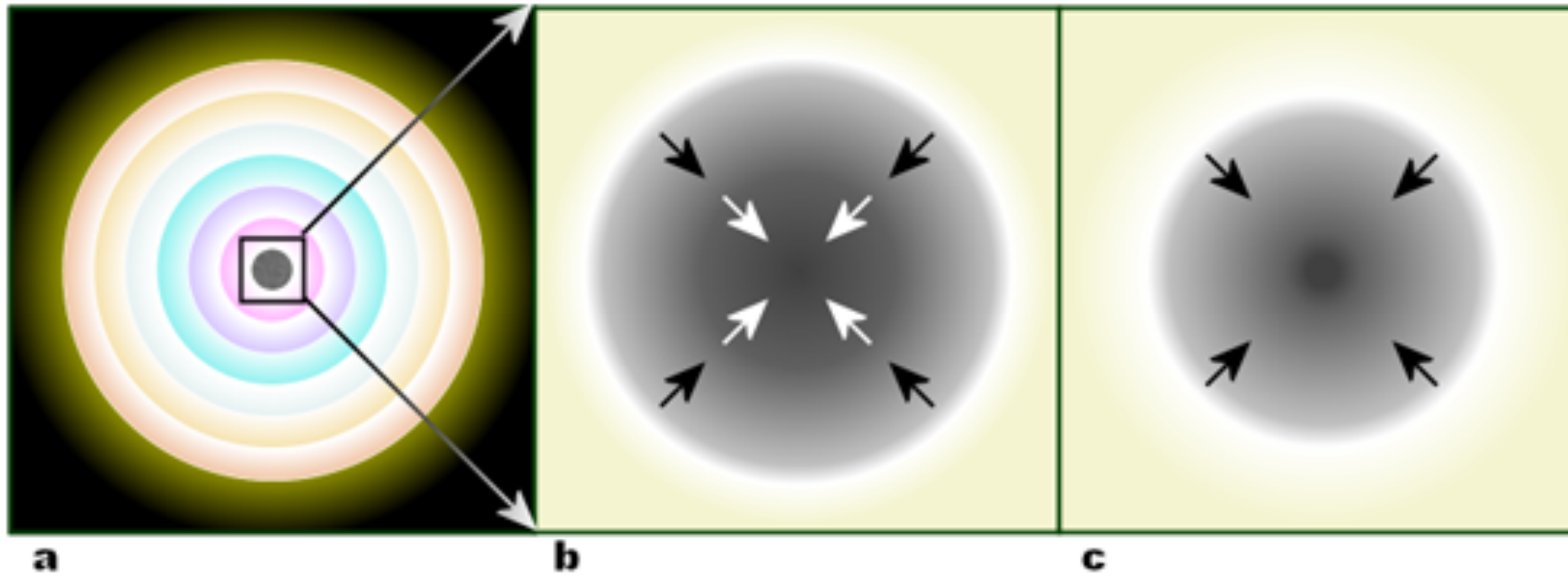


can we understand this process
from the fundamental theory?

Yes!
maybe with 



He, C, O, ... Si burning produces energy until Iron (Fe)



d core collapse **e** supernova, shock-wave-aided **f** ejection of mantle

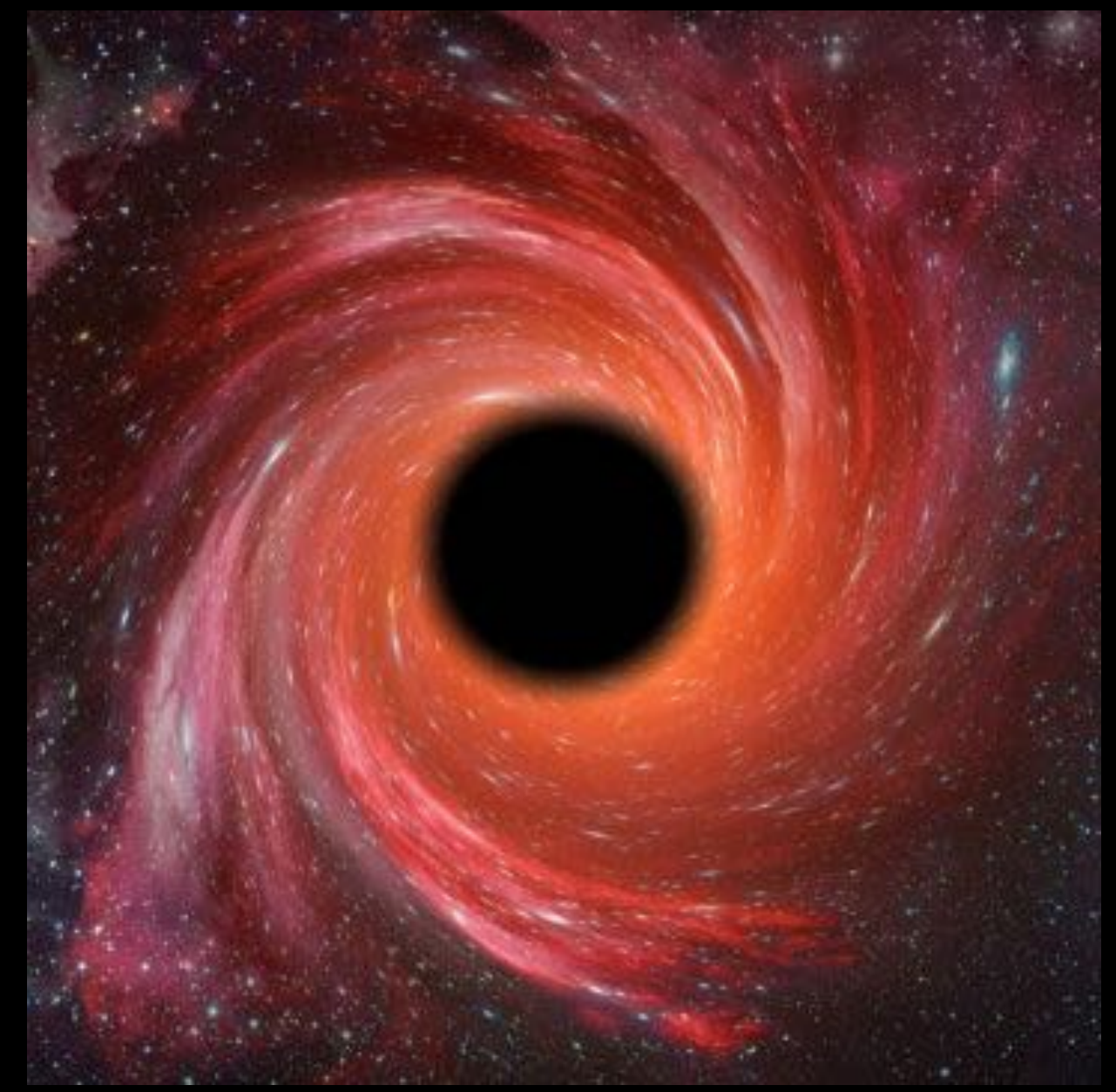
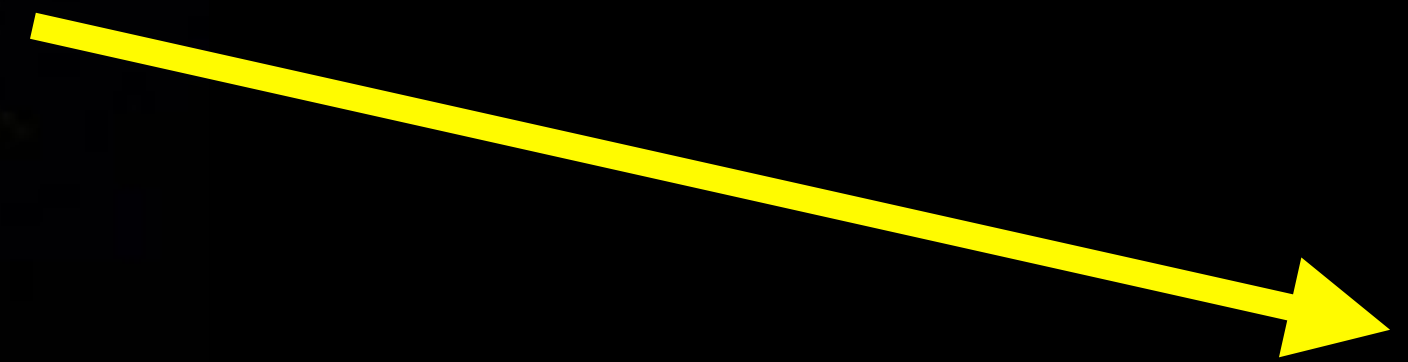
Supernova



neutron star



black hole



“We are all made of star stuff”

In Memoriam
Carl Sagan
1934-1996



much coming from the ejecta of supernova



Can we understand properties of neutron stars directly from the fundamental theory?



Can we understand properties of neutron stars directly from the fundamental theory?

Yes! With **FRONTIER**





Can we understand properties of neutron stars directly from the fundamental theory?

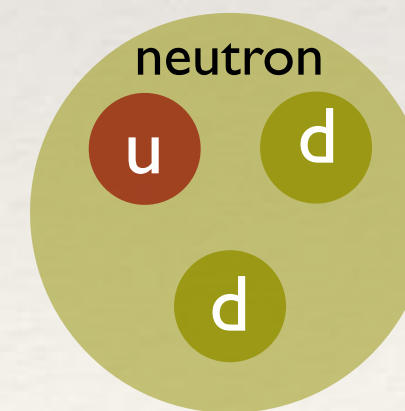
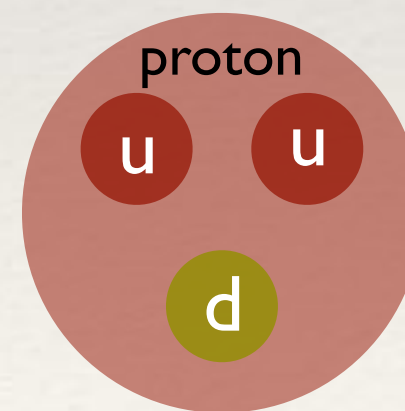
Yes! With

FRONTIER

Will it have GPUs?
I hope so!

Need for HPC

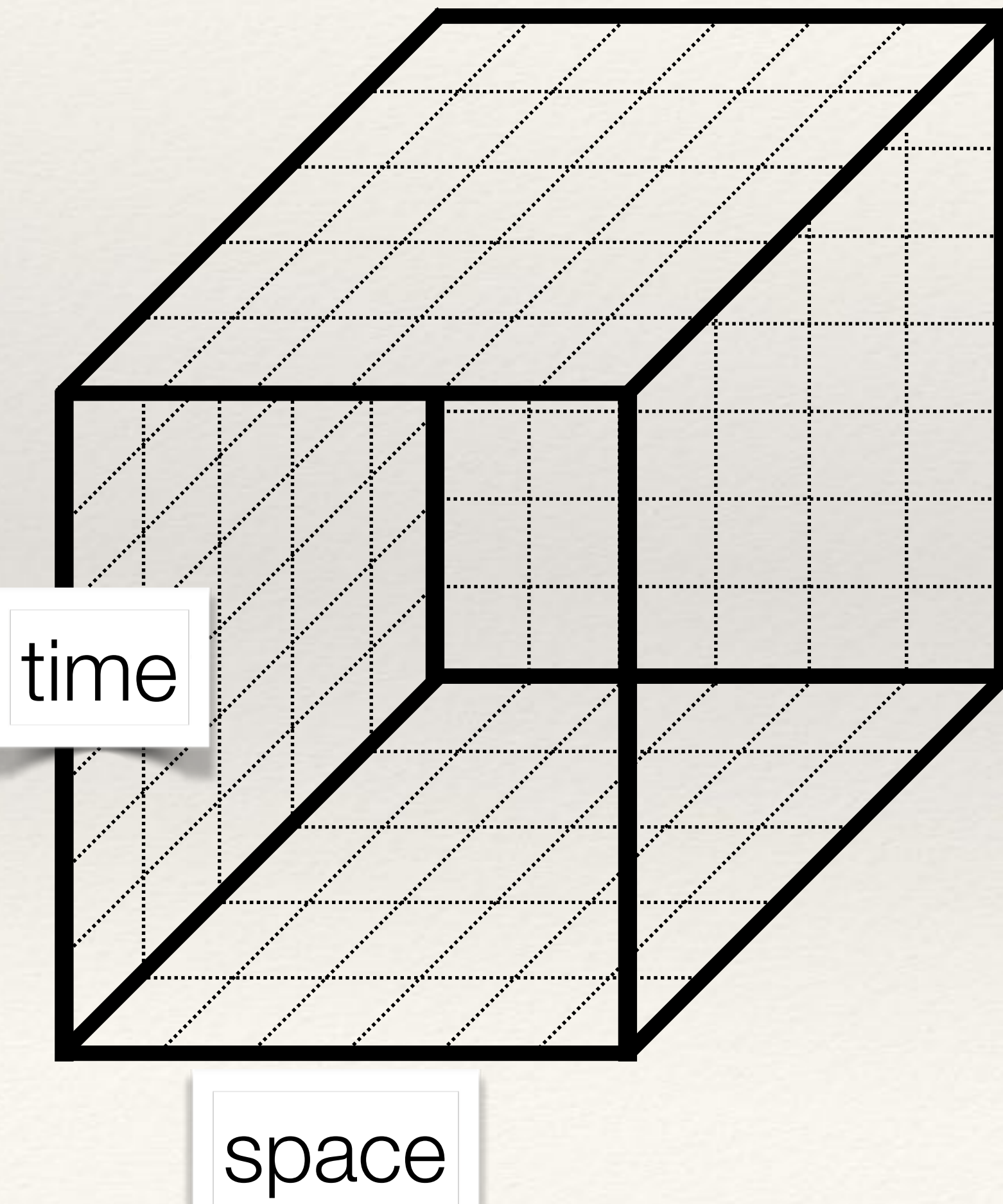
- The inherent challenge in understanding properties of matter (nuclear physics) directly from the fundamental theory, the Standard Model of Particle Physics - is that the nuclear interactions are very strong - so perturbative methods fail
 - Analogy: $1/(1-x) = 1 + x + x^2 + x^3 + \dots$
 - If $|x| < 1$, then each successive contribution is smaller.
 - If $|x| > 1$, then contributions grow.
- The fundamental theory of nuclear strong interactions is Quantum Chromodynamics
 - a relativistic, quantum mechanical theory of quarks and gluons
 - inherently a 4-dimensional theory



Need for HPC

- ultimately, we have to perform this integral of integrals

$$C(t) = \langle \hat{O}(t) \hat{O}^\dagger(0) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U \det(D + M) e^{-\int d^4x \mathcal{L}[U(t,x,y,z)]} O[U](t) O[U]^\dagger(0)$$

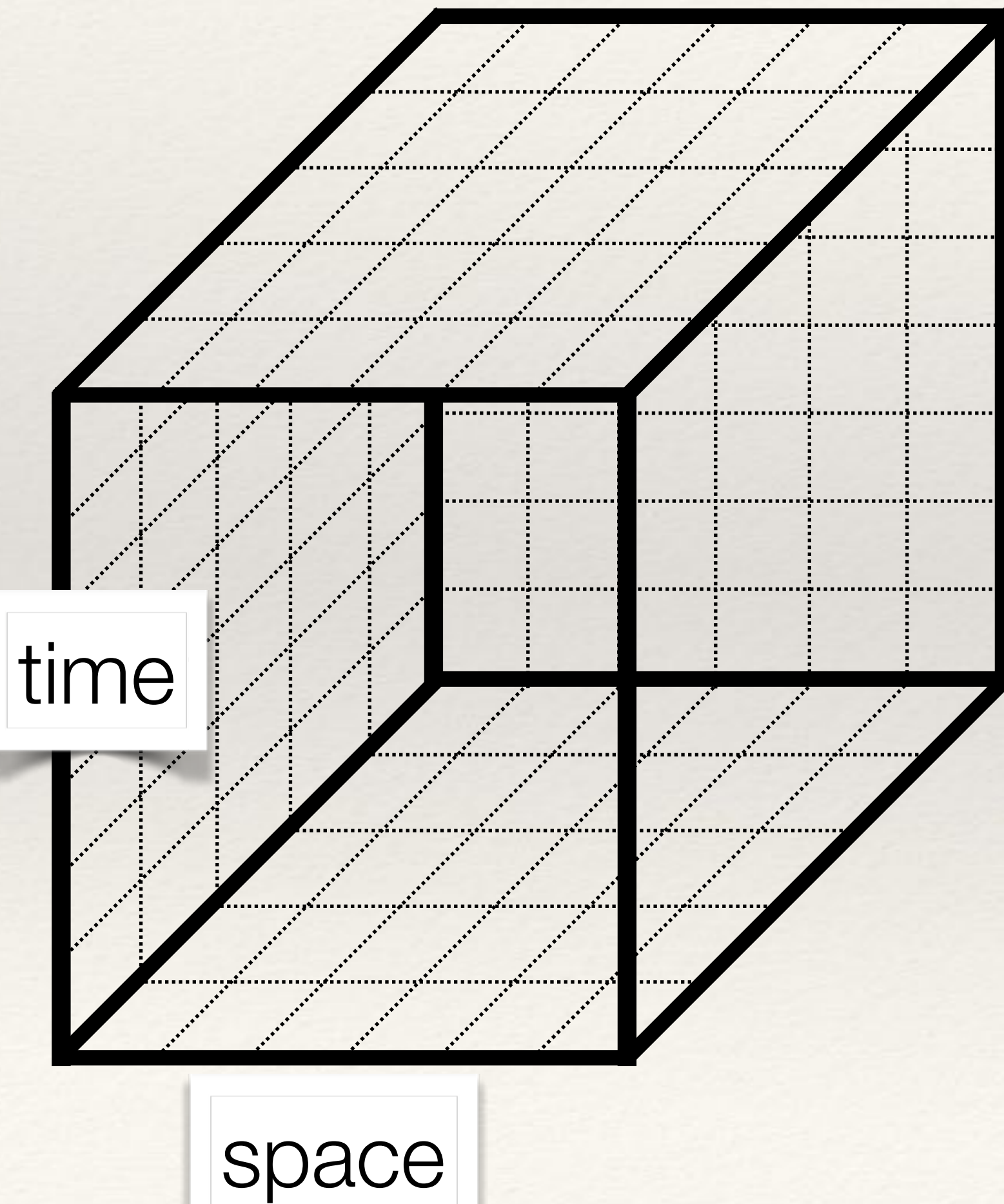


Need for HPC

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Probability



Need for HPC

- ultimately, we have to perform this integral of integrals

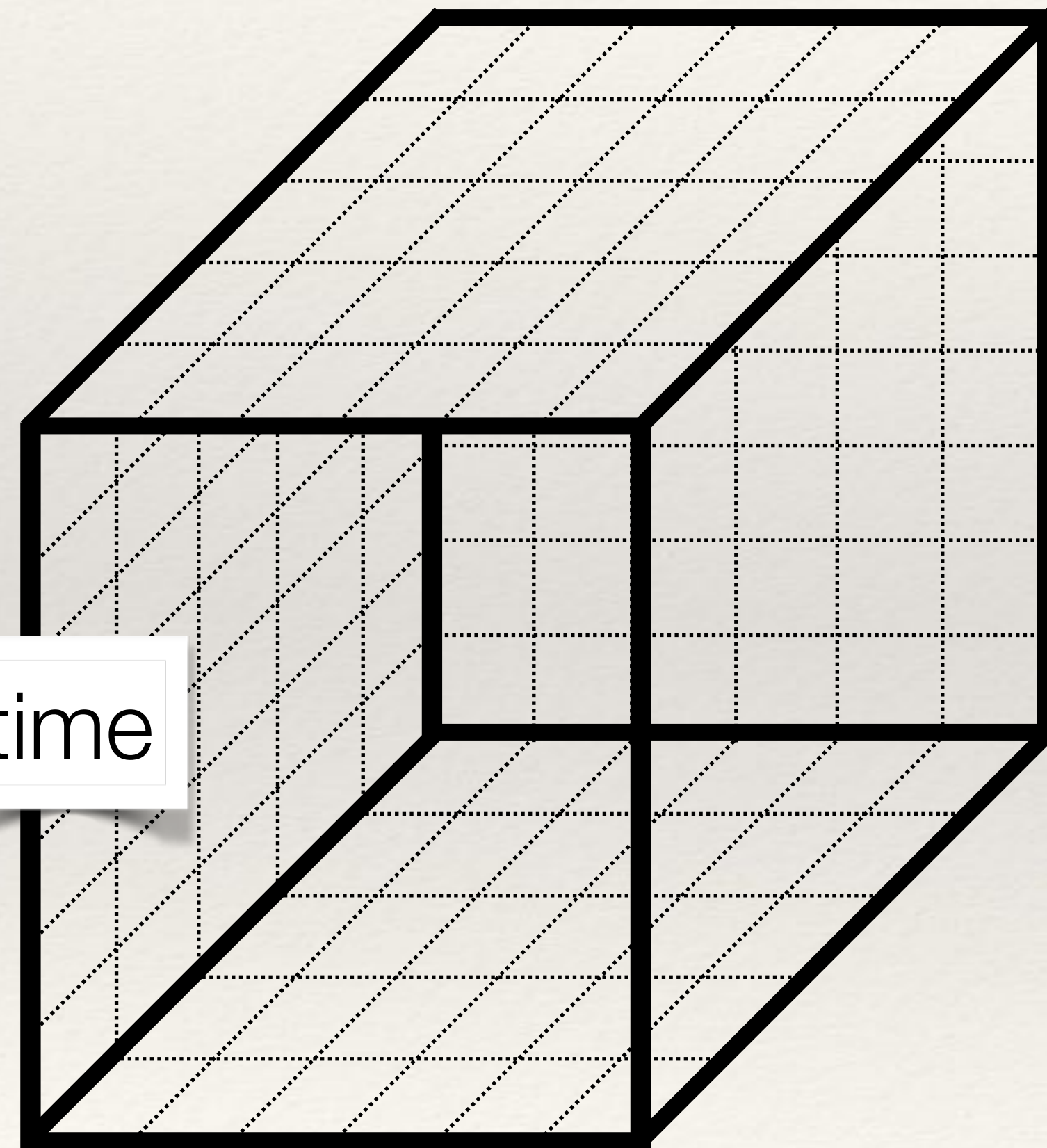
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Probability

$$\{U_1, U_2, U_3, \dots, U_N\}$$

Markov Chain Monte Carlo



time

space

Need for HPC

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$$C(t) = \langle \hat{O}(t) \hat{O}^\dagger(0) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U \det(D + M) e^{-\int d^4x \mathcal{L}[U(t,x,y,z)]} \mathcal{O}[U](t) \mathcal{O}[U]^\dagger(0)$$

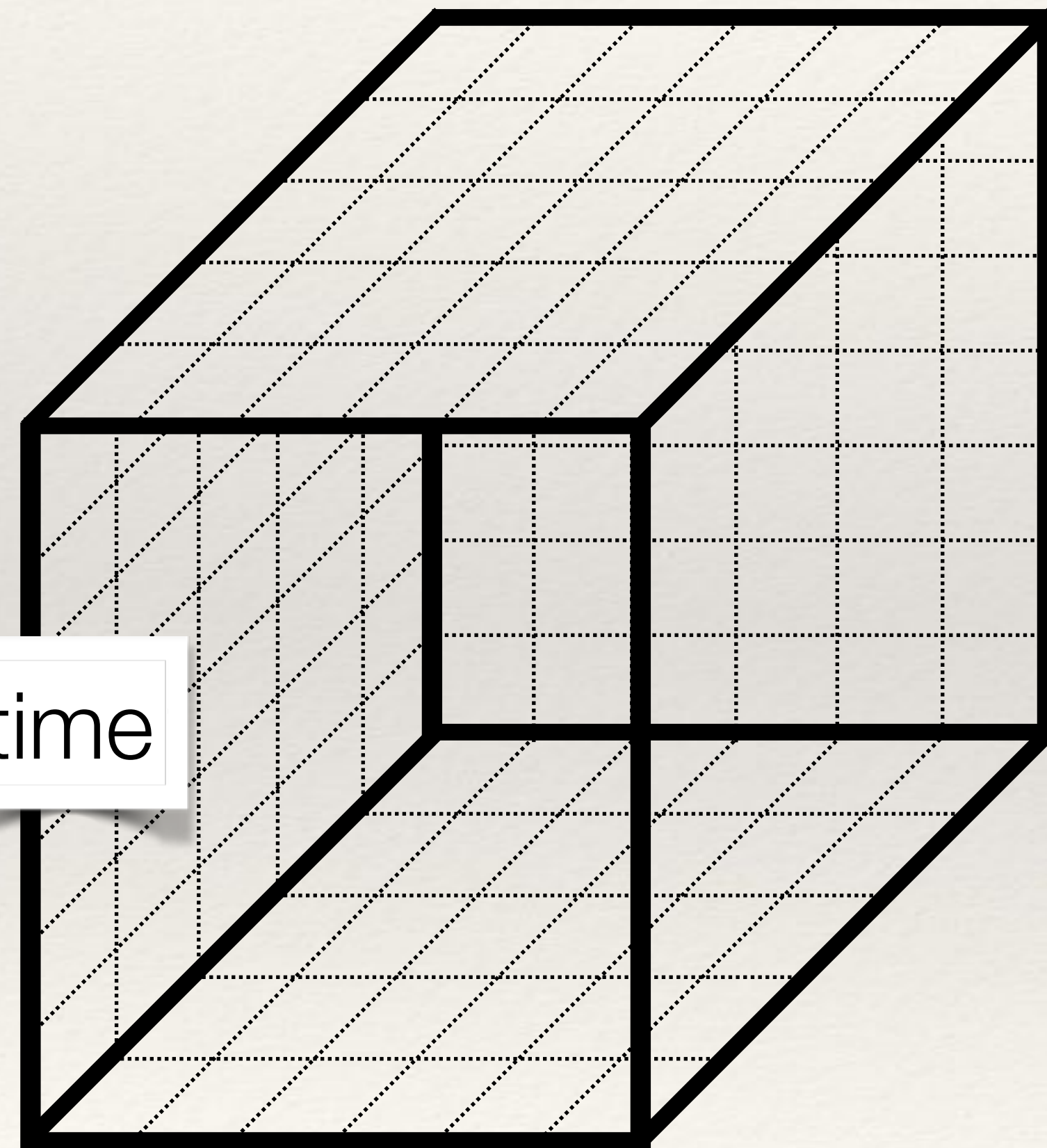


Probability

$$\{U_1, U_2, U_3, \dots, U_N\}$$

Markov Chain Monte Carlo

$$\approx \frac{1}{N} \sum_{i=1}^N \mathcal{O}(t) \mathcal{O}^\dagger(0)[U_i]$$



time

space

Need for HPC

- ultimately, we have to perform this integral of integrals

$$C(t) = \langle \hat{O}(t) \hat{O}^\dagger(0) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U \det(D + M) e^{-\int d^4x \mathcal{L}[U(t,x,y,z)]} O[U](t) O[U]^\dagger(0)$$

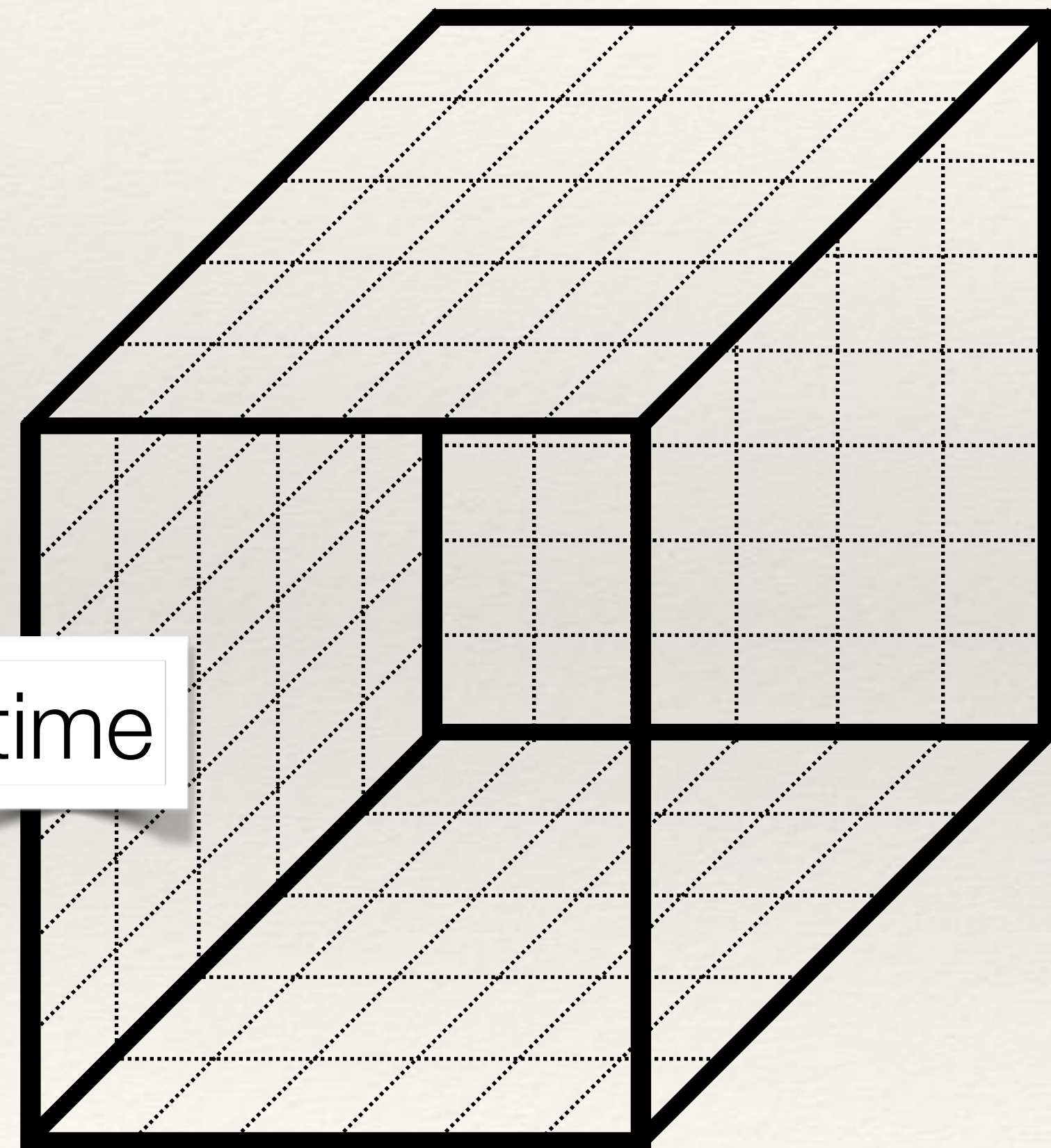


Probability

$$\{U_1, U_2, U_3, \dots, U_N\}$$

Markov Chain Monte Carlo

$$\approx \frac{1}{N} \sum_{i=1}^N O(t) O^\dagger(0)[U_i] + O\left(\frac{1}{\sqrt{N}}\right)$$



time

space

Need for HPC

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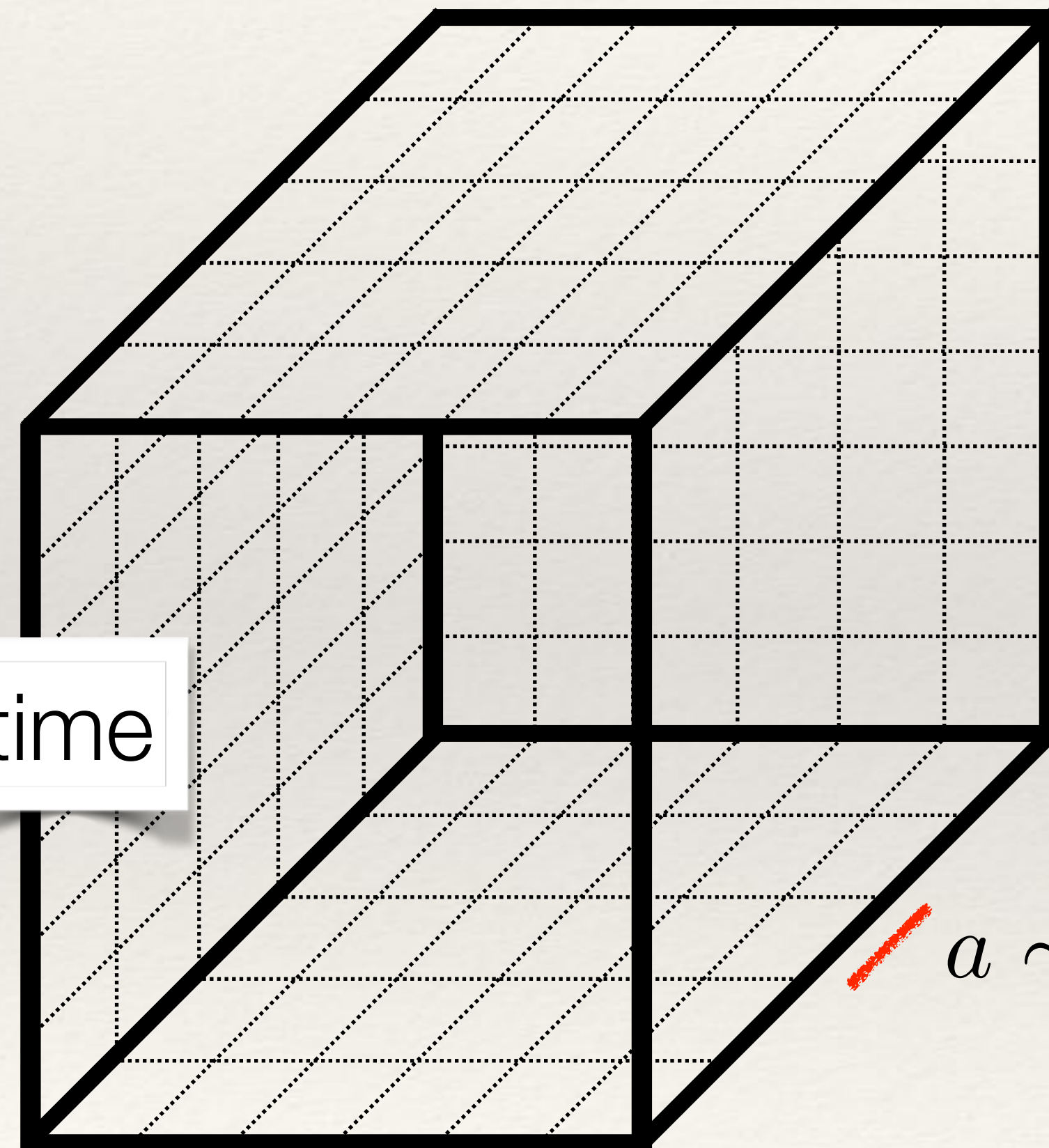


Probability

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$$\approx \frac{1}{N} \sum_{i=1}^N O(t) O^\dagger(0)[U_i] + O\left(\frac{1}{\sqrt{N}}\right)$$



$$a \sim 10^{-16} \text{ meters} \sim \frac{1}{10} \text{ size proton}$$

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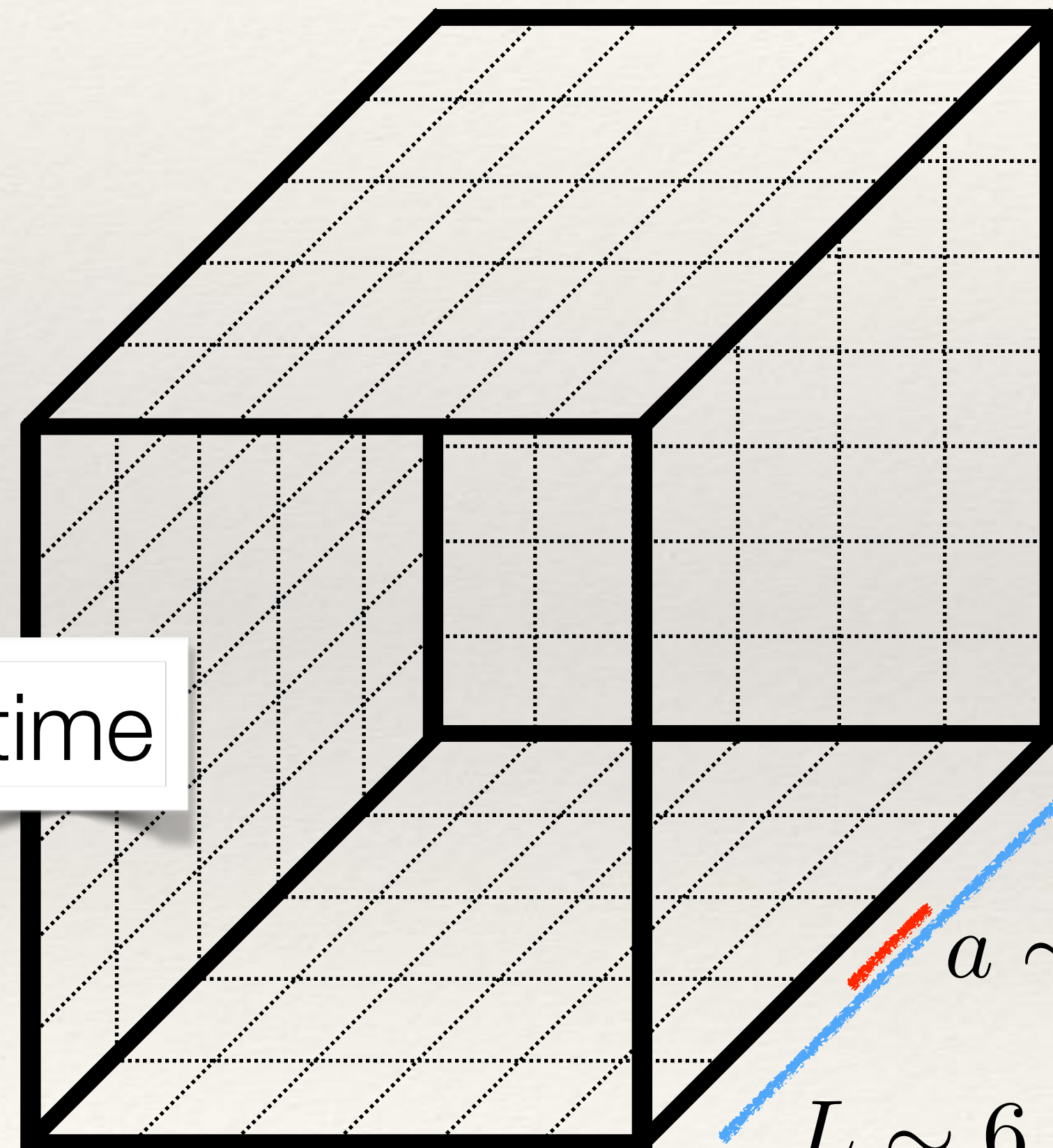


Probability

$$\{U_1, U_2, U_3, \dots, U_N\}$$

Markov Chain Monte Carlo

$$\approx \frac{1}{N} \sum_{i=1}^N O(t) O^\dagger(0)[U_i] + O\left(\frac{1}{\sqrt{N}}\right)$$



$$a \sim 10^{-16} \text{ meters} \sim \frac{1}{10} \text{ size proton}$$

$$L \sim 6 \times 10^{-15} \text{ meters} \sim 6 \times \text{size proton}$$

space

Need for HPC

- ultimately, we have to perform this integral of integrals

$$C(t) = \langle \hat{O}(t) \hat{O}^\dagger(0) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U \det(D + M) e^{-\int d^4x \mathcal{L}[U(t,x,y,z)]} O[U](t) O[U]^\dagger(0)$$

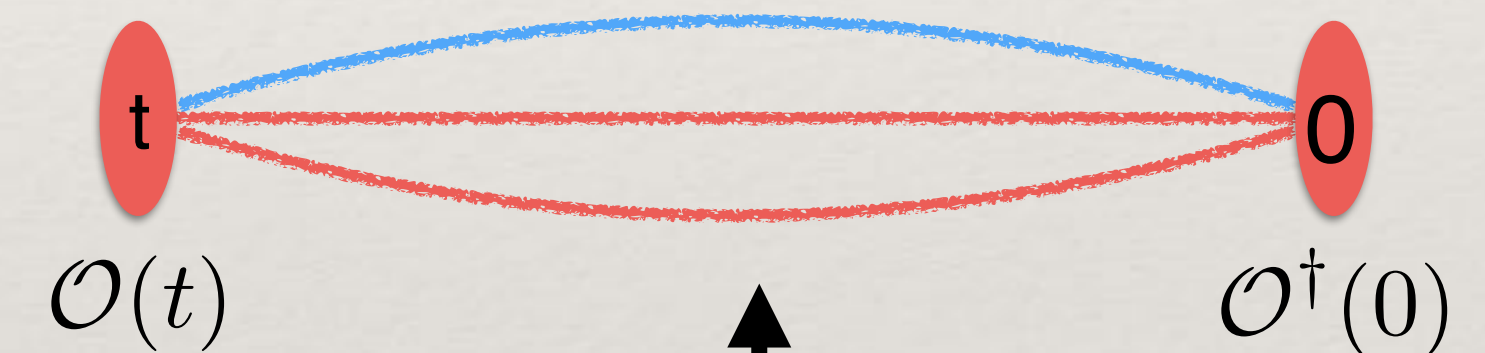
Probability

$$\{U_1, U_2, U_3, \dots, U_N\}$$

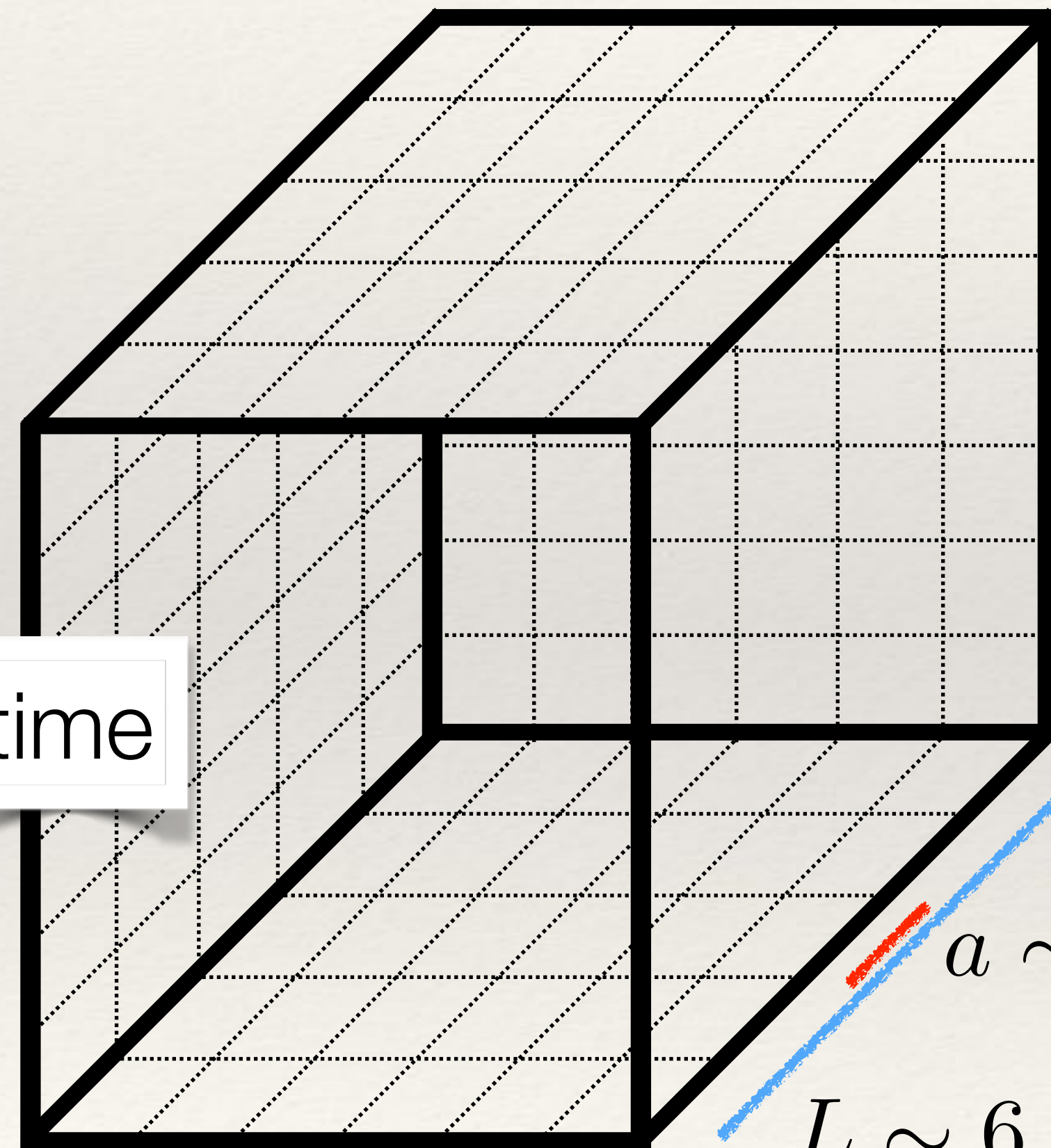
Markov Chain Monte Carlo

$$\approx \frac{1}{N} \sum_{i=1}^N O(t) O^\dagger(0) [U_i] + O\left(\frac{1}{\sqrt{N}}\right)$$

Suppose $O^\dagger(0)$ is an initial proton and $O(t)$ is a final state proton



These objects are *quark propagators*



$$a \sim 10^{-16} \text{ meters} \sim \frac{1}{10} \text{ size proton}$$

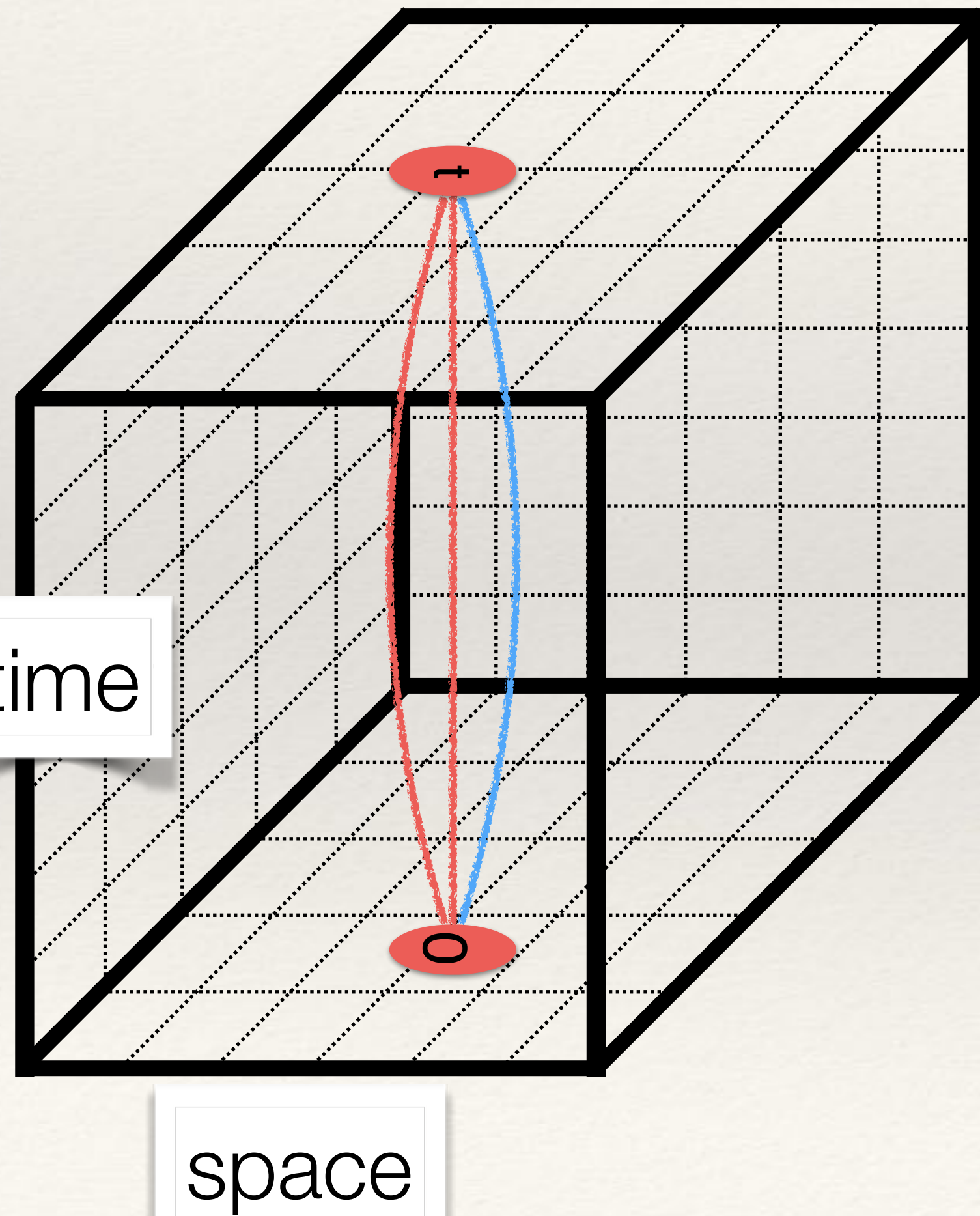
$$L \sim 6 \times 10^{-15} \text{ meters} \sim 6 \times \text{ size proton}$$

space

Need for HPC

- This integral describes the probability of finding the final state proton given the initial proton

$$C(t) = \langle \hat{O}(t) \hat{O}^\dagger(0) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}U \det(D + M) e^{-\int d^4x \mathcal{L}[U(t,x,y,z)]} O[U](t) O[U]^\dagger(0)$$



“ $S_Q(t,0)$ = Quark Propagator”

$$[D + M]_{y,z} S_{z,x} = \delta_{y,x} = \begin{cases} \text{if } x = y & 1 \\ \text{else} & 0 \end{cases}$$

Known Matrix

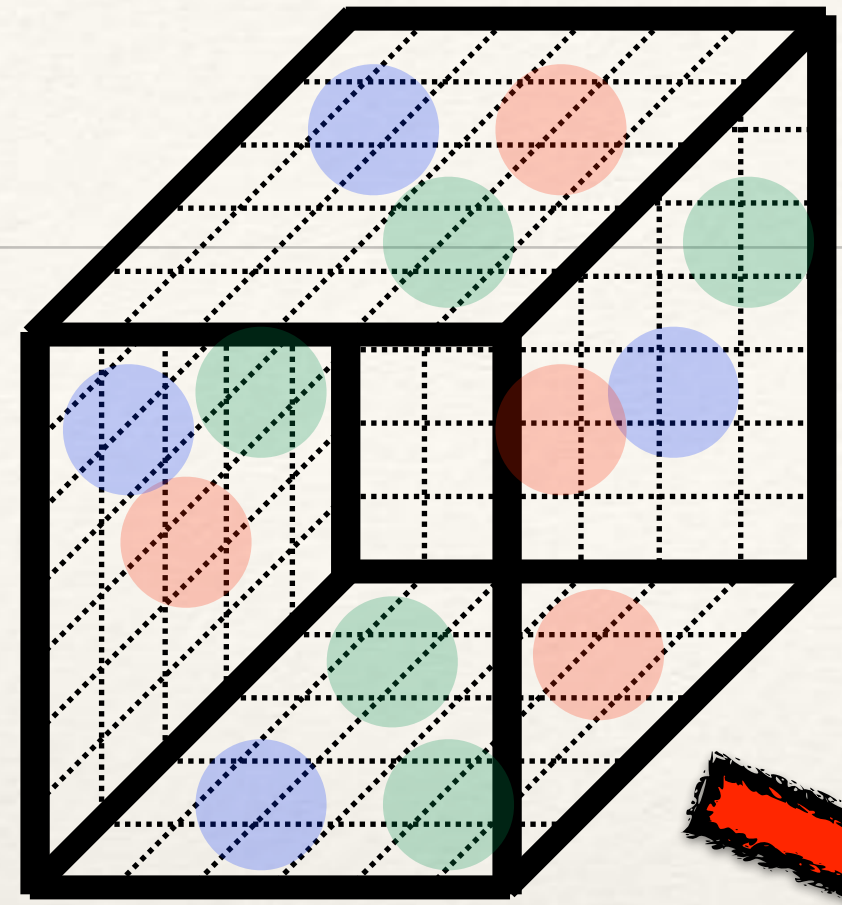
Sparse, Large :

$\sim 400,000,000$

Solve the Quark Propagators with Conjugate Gradient

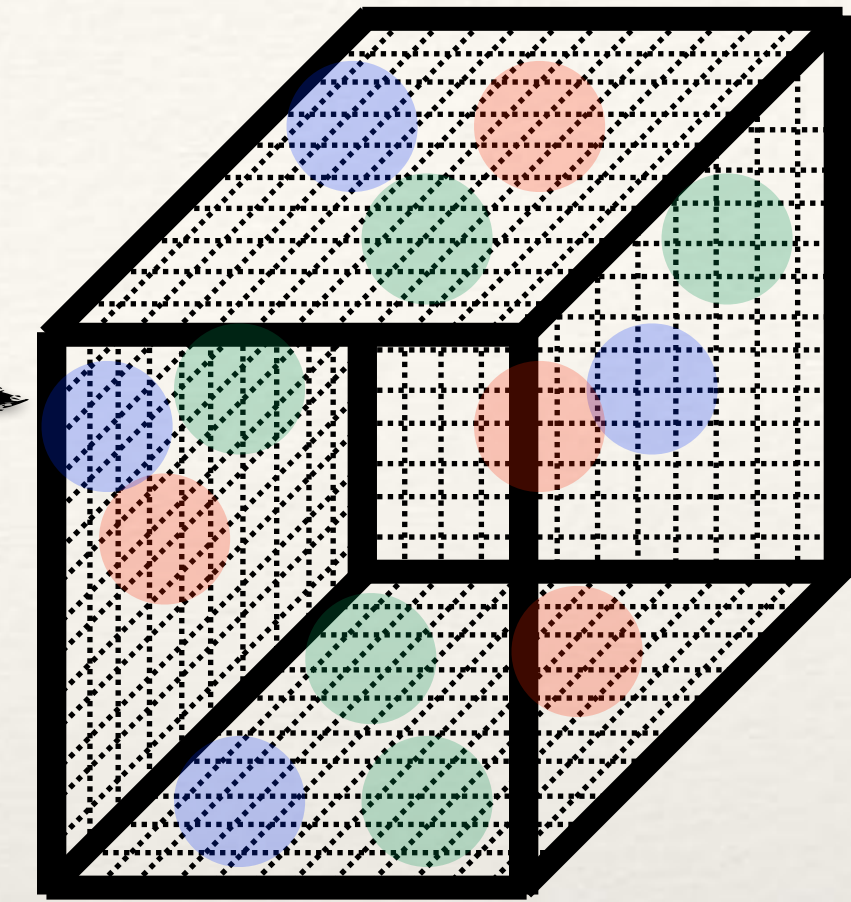
- **sparse Matrix-vector**
- GPUs are what allow us to do the calculations very efficiently
 - lots of memory bandwidth
 - memory access patterns are structured and predictable

Need for HPC



continuum limit
need 3 or more
lattice spacings

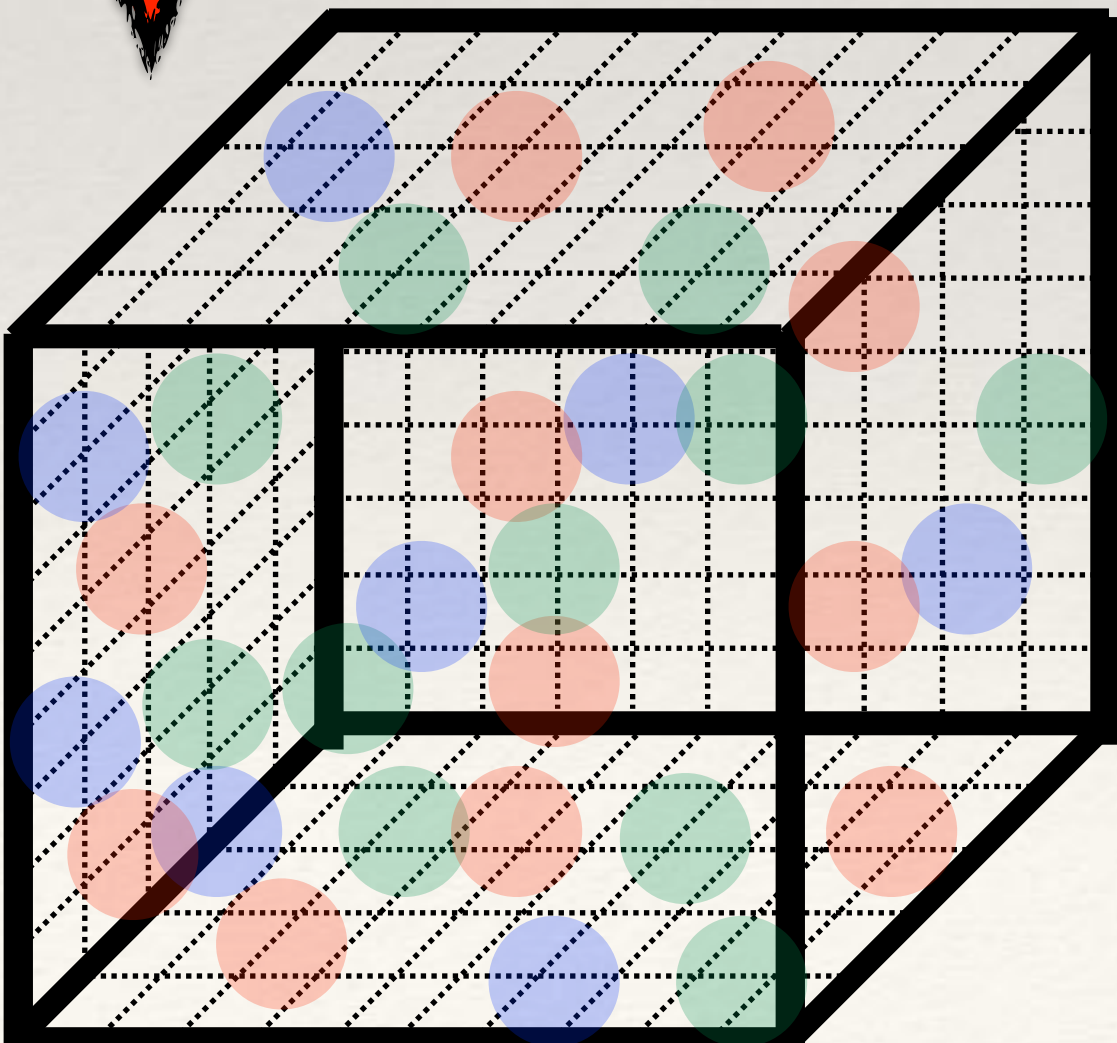
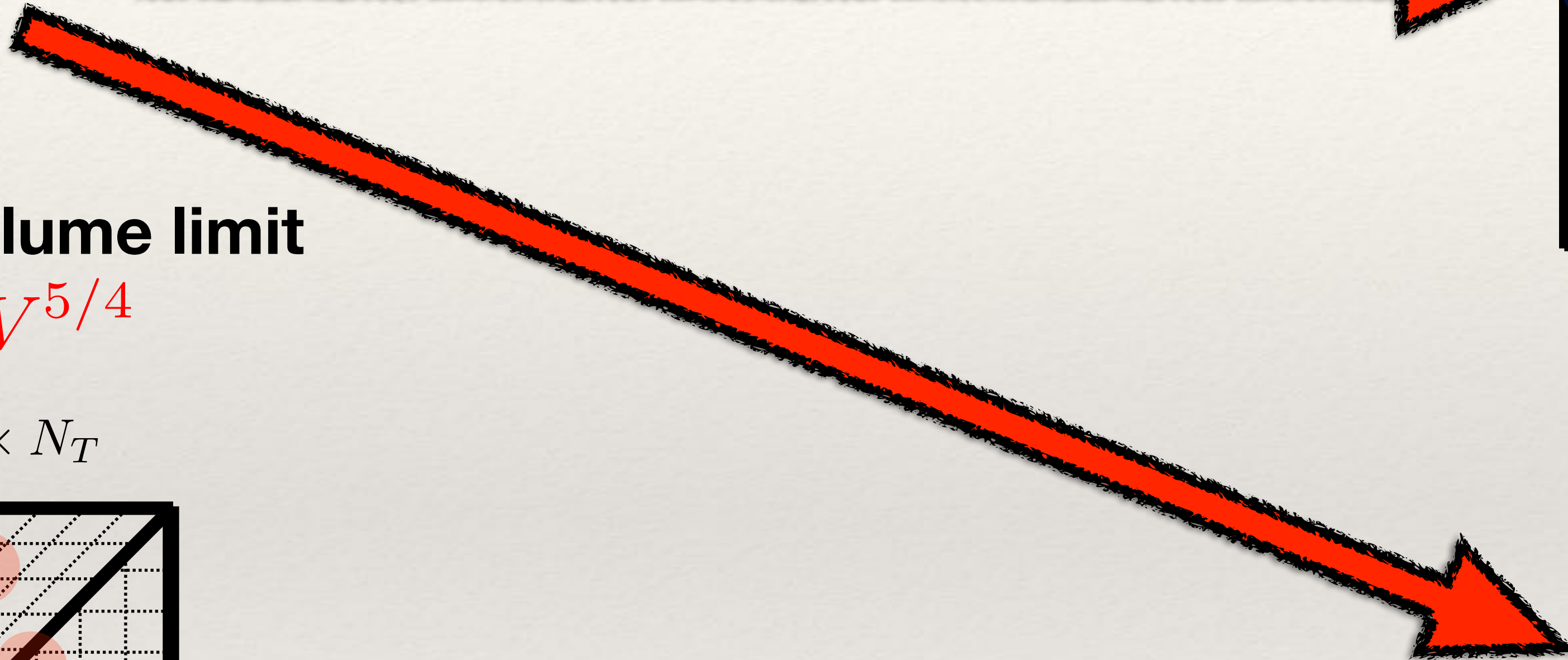
$$t_{comp} \propto \frac{1}{a^6}$$



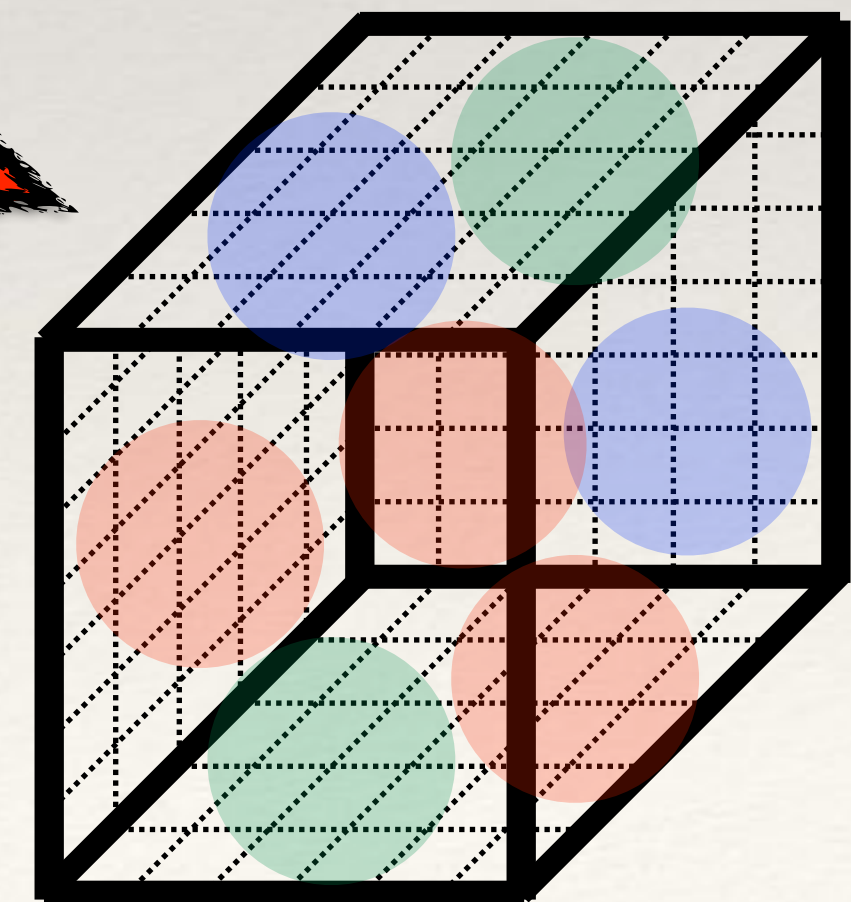
infinite volume limit

$$t_{comp} \propto V^{5/4}$$

$$V = N_L^3 \times N_T$$



physical pion masses
exponentially bad
signal-to-noise problem



Efficient Use of Sierra



Summit



Efficient Use of Sierra/Summit



#1 on Top 500 list

O(\$200M) machine

Important to get as much science per flop as possible

Nodes	: 4608
Processor	: IBM Power9 (2/node)
GPUs	: 27,648 NVIDIA V100 (6/node)
Node Performance:	42 TeraFlops
Memory/node	: 512GB DDR4 + 96GB HBM2
NV-LINK Memory	: 1600GB/node
Interconnect	: Mellanox 100G InfiniBand, Non-blocking Fat Tree
Peak Power	: 13 MegaWatts

Efficient Use of Sierra/Summit



#1 on Top 500 list

O(\$200M) machine

Important to get as much science per flop as possible

- Need optimized use of NVIDIA GPUs
- Need scalability (communication avoiding algorithms)
- Need to take advantage of the heterogeneous architecture
- Need to efficiently manage hundreds of thousands of tasks

TEN YEARS OF QUDA

in use as GPU backend for BQCD, Chroma, CPS, MILC, TIFR, etc.

Solvers for all major fermionic discretizations

Routines needed for gauge-field generation

Maximize performance

Exploit symmetries to minimize memory traffic

Mixed-precision methods (16 bit / 8 bit)

Domain-decomposed (Schwarz) preconditioners for strong scaling

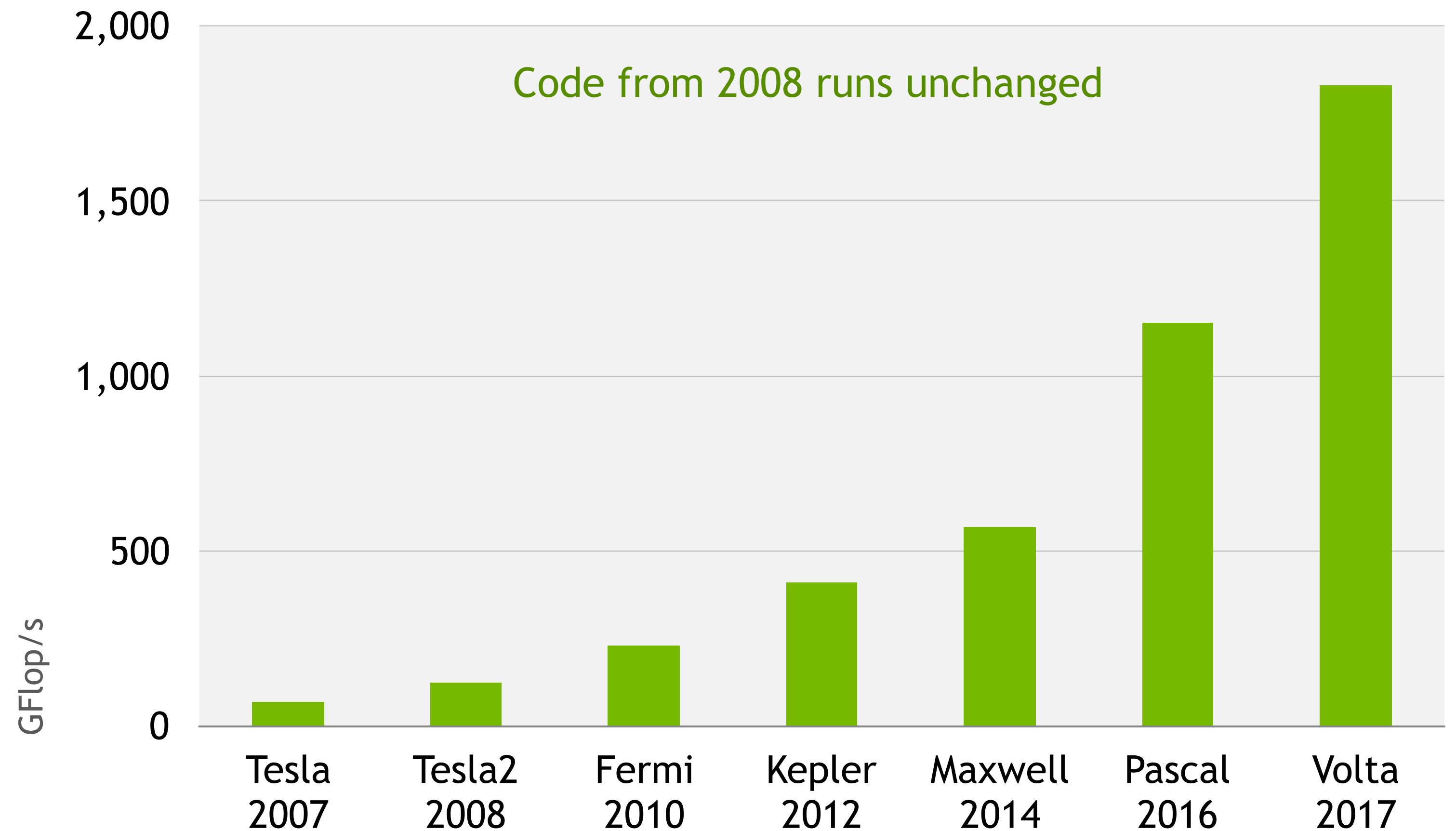
Eigenvector and deflated solvers (Lanczos, EigCG, GMRES-DR)

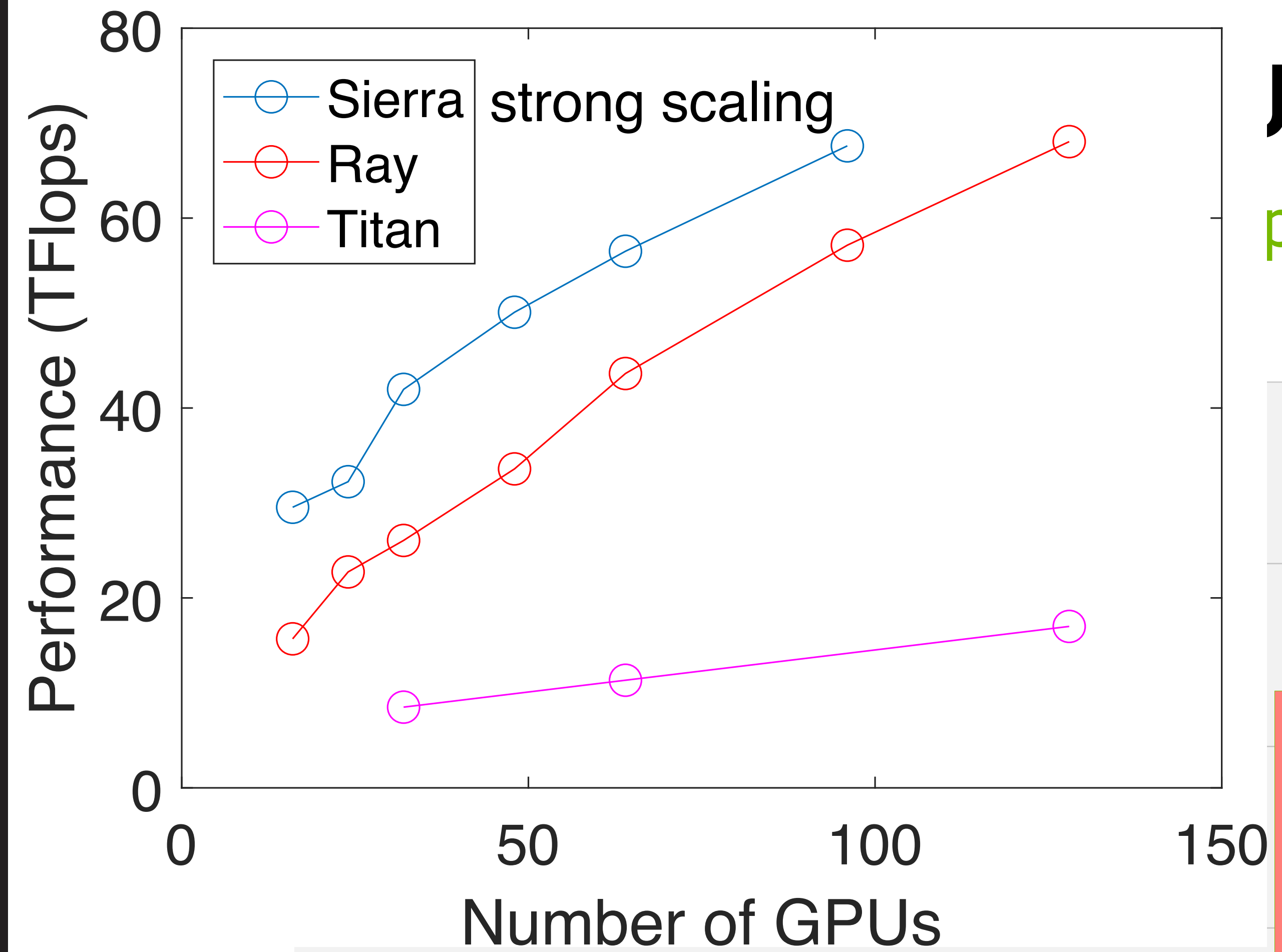
Multi-source solvers

Multigrid solvers for optimal convergence

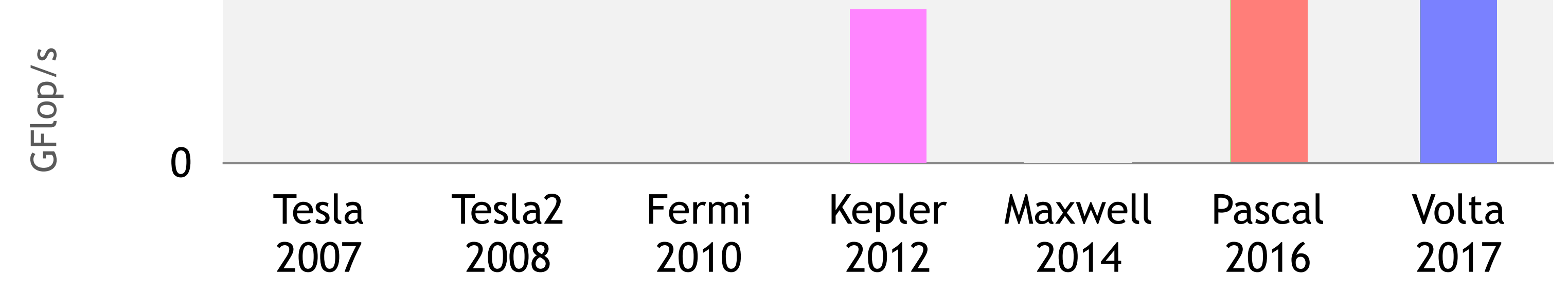
RECOMPILE AND RUN

Autotuning provides performance portability





JN
portability





VOLTA



PASCAL



MAXWELL



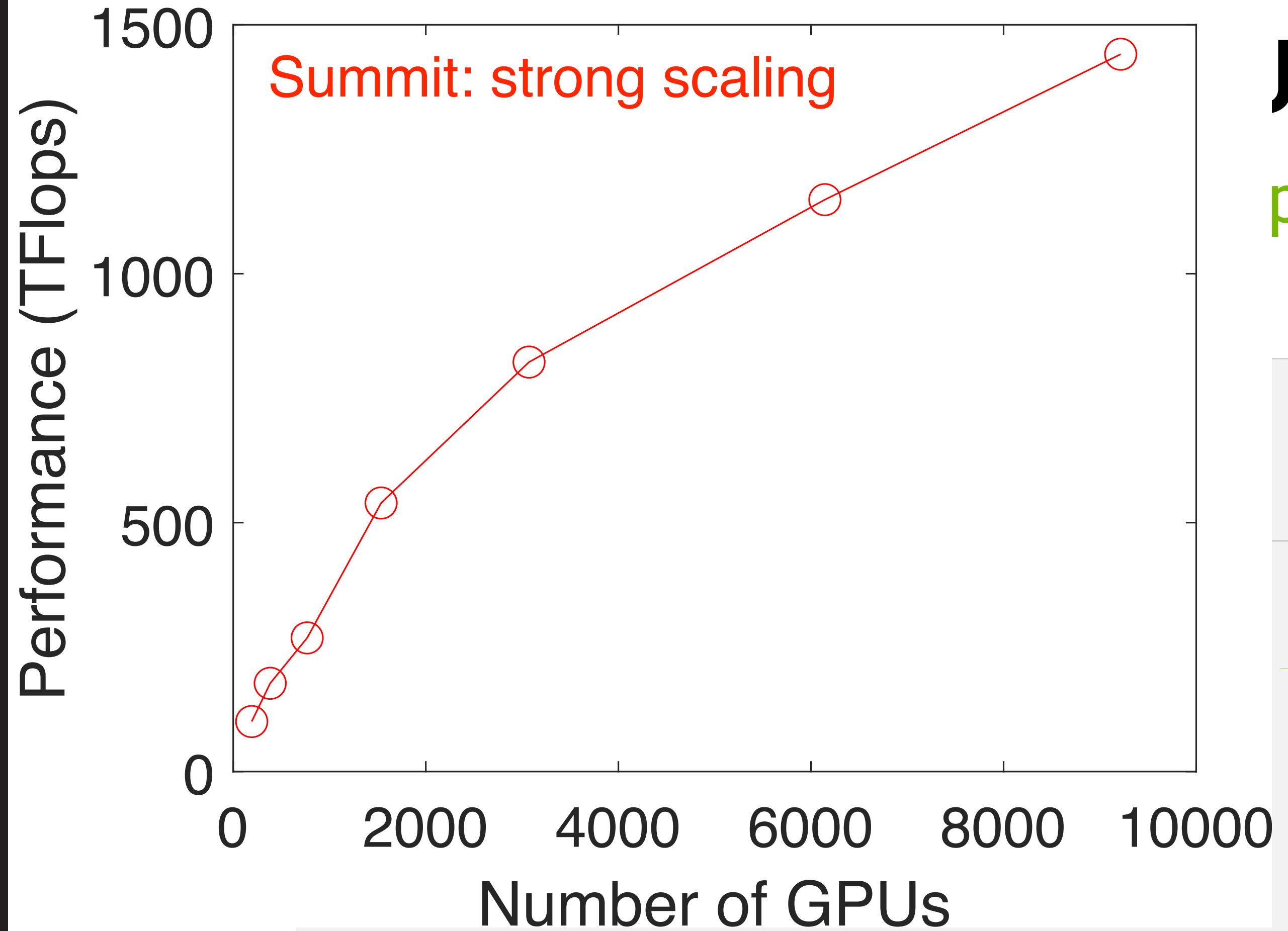
TESLA



KEPLER



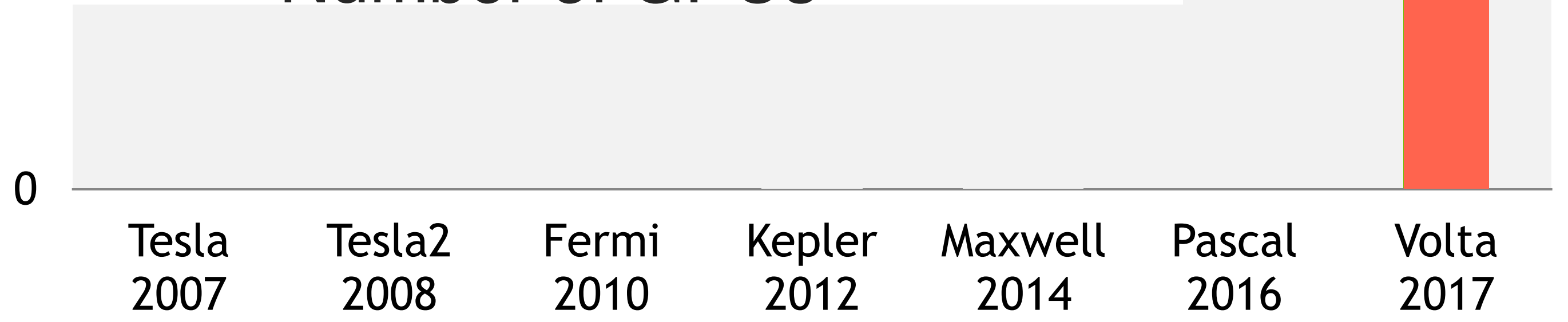
FERMI



JN

portability

GFlop/s



Efficient Use of Sierra/Summit

- ❑ For our research problems of today, the majority of computing requirements reside in the large, sparse, linear system solves (quark propagators)
- ❑ We use the QUDA library, which is highly optimized for NVIDIA GPUs, written using CUDA C++ - large open BSD developed code
<https://github.com/lattice/quda>
- ❑ See the talks

S9708 - Strong Scaling HPC Applications: Best Practices with a Lattice QCD case study
Kate Clark (one of our collaborators) and Mathias Wagner
Thursday, 11am

S9330 - Lattice QCD with Tensor Cores
Jiqun Tu
Thursday, 10am

for a detailed discussion of QUDA and new uses of the tensor cores, respectively

Our work flow: managing millions of tasks

TASK	RESOURCE NEEDS
GPU or CPU Create a “snapshots” of the QCD vacuum via Monte-Carlo sampling	0(6 - 100) Summit nodes serial walk through Monte-Carlo ~1000 snapshots per “ensemble”
Prepare source for linear solve	~1-8 Summit nodes for ~1 minute ~8-32 sources per snapshot ~1000 snapshots ~20 ensembles
Perform linear system solve	for each: 1-8 Summit nodes for 5min - 2 hours depending on the ensemble for all sources/snapshots/ensembles
Dense Matrix multiplication with solve subsequent solves based on first solve	for each: 1-8 Summit nodes for 5min - 30 min; 1-8 Summit nodes for 5min - 2 hours, ~100 subsequent solves for each solve
Dense Matrix multiplication with solve and secondary solve	for each: 1-8 Summit nodes for 5min - 30 min;

Our work flow: managing millions of tasks

TASK

GPU or CPU

Create a “snapshots” of the QCD

RESOURCE NEEDS

O(6 - 100) Summit nodes

- ❑ We need to run hundreds of thousands to millions of independent, small node tasks
- ❑ Running each job separately taxes the launch nodes on these supercomputers
- ❑ If we stack GPU tasks after CPU and so on, much of the wall-clock time will be wasted in the sense that the GPUs will not be in use - and the CPU wall-clock time is approaching a significant fraction of the GPU wall-clock time
- ❑ Job bundling wastes significant amounts of wall-clock time as performance of each task can vary substantially if nodes are close together or far apart
- ❑ We need a light-weight task manager capable of efficiently using all node resources and scheduling the tasks

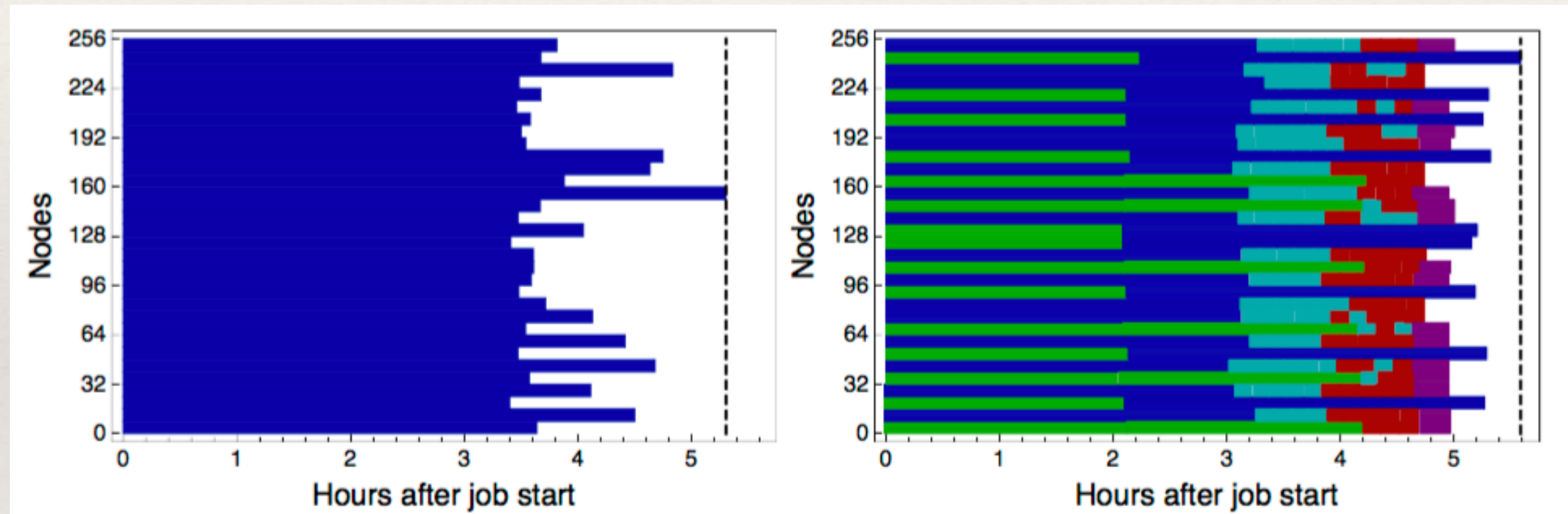
Dense Matrix multiplication with solve and secondary solve

for each: 1-8 Summit nodes for 5min - 30 min;

First Generation: MetaQ

- Bash script system to improve efficiency of running many jobs in a single large allocation
<https://github.com/evanberkowitz/metaq>

example from Titan



arXiv:1702.06122

- Naïve system resulted in waste of $\sim 30\%$ of time.
- MetaQ backfills tasks, reducing wasted (idle) cycles to about 5%

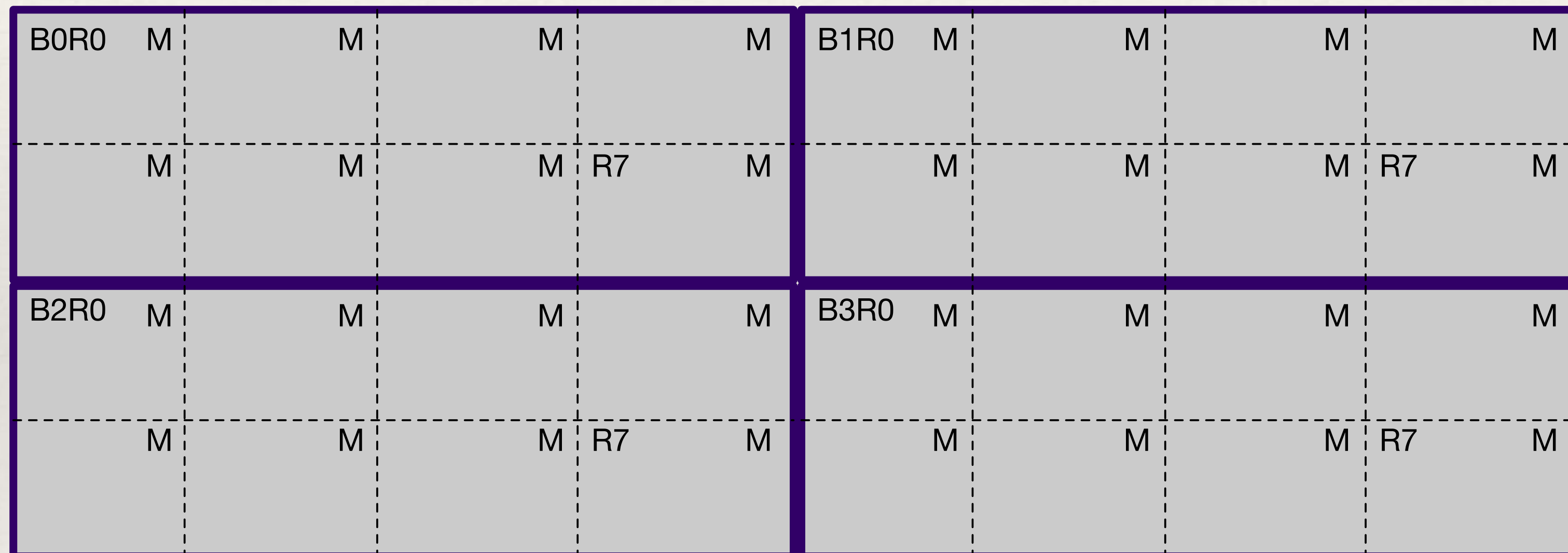
MPI_JM: MPI Job Manager

- ❑ Efficiently run a large set of tasks of bounded size in a large allocation of nodes.
- ❑ Low overhead on service node.
- ❑ Guarantee that communications are always physically local.
- ❑ Support overlay of jobs using distinct resources on the same nodes, i.e. GPU vs CPU jobs.
- ❑ Customizable collection/generation of workload with python based front-end.
 - ❑ Support pre and post actions that can be used to chain computations.
- ❑ Fault tolerance for startup on new super computers.

MPI_JM: https://github.com/kenmcelvain/mmpi_jm (temporarily private)

Start by placing jm_master on each node in allocation.

```
mpirun -n 32 -map-by node jm_master jobs
```



Block sizes, memory, and slot description come from a configuration file. Each block gets a sub-communicator.

MPI_JM

Controlling Interconnect Performance

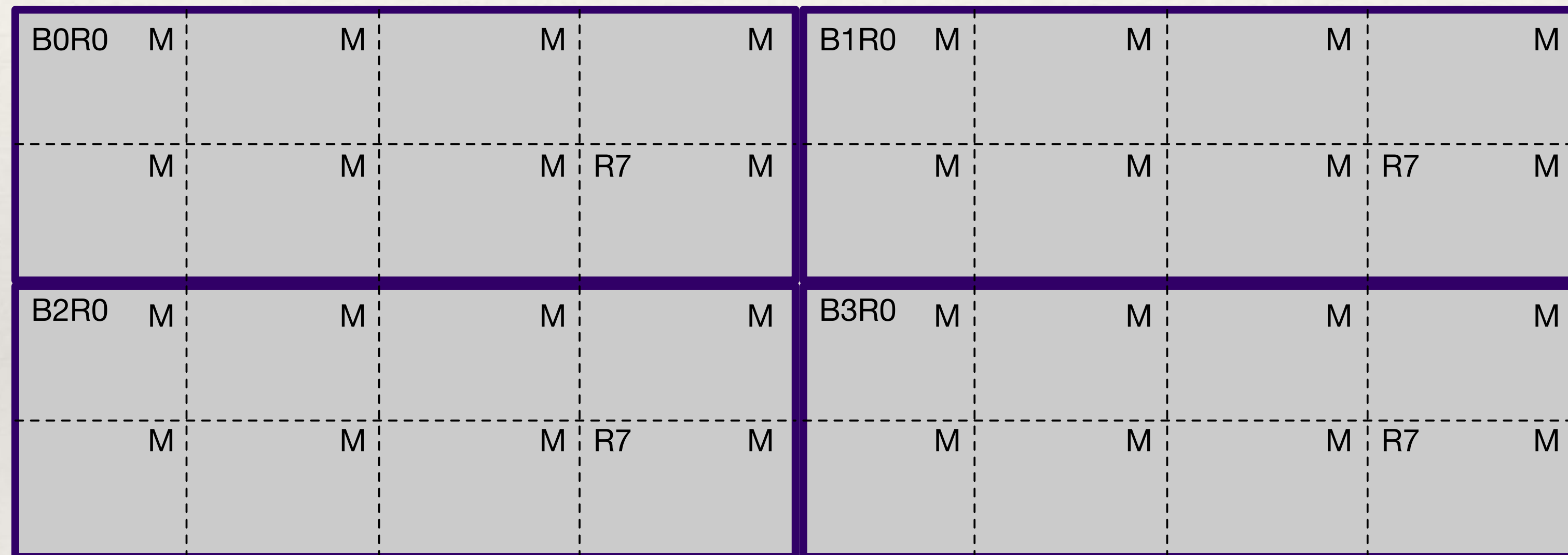
Maximize blocks with node numbers in sequence.

B0R0 M	M	M	M	B1R0 M	M	M	M
807	1130	2101	3355	1122	1123	1124	1125
M	M	M	R7 M	M	M	M	R7 M
3356	3516	3517	3518	1126	1127	1128	1129
B2R0 M	M	M	M	B3R0 M	M	M	M
3340	3341	3342	3343	3348	3349	3349	3350
M	M	M	R7 M	M	M	M	R7 M
3344	3345	3346	3347	3351	3352	3353	3354

As tasks finish and new ones are started, they will get consistent interconnect performance. We rely on individual tasks having bounded size.

MPI_JM

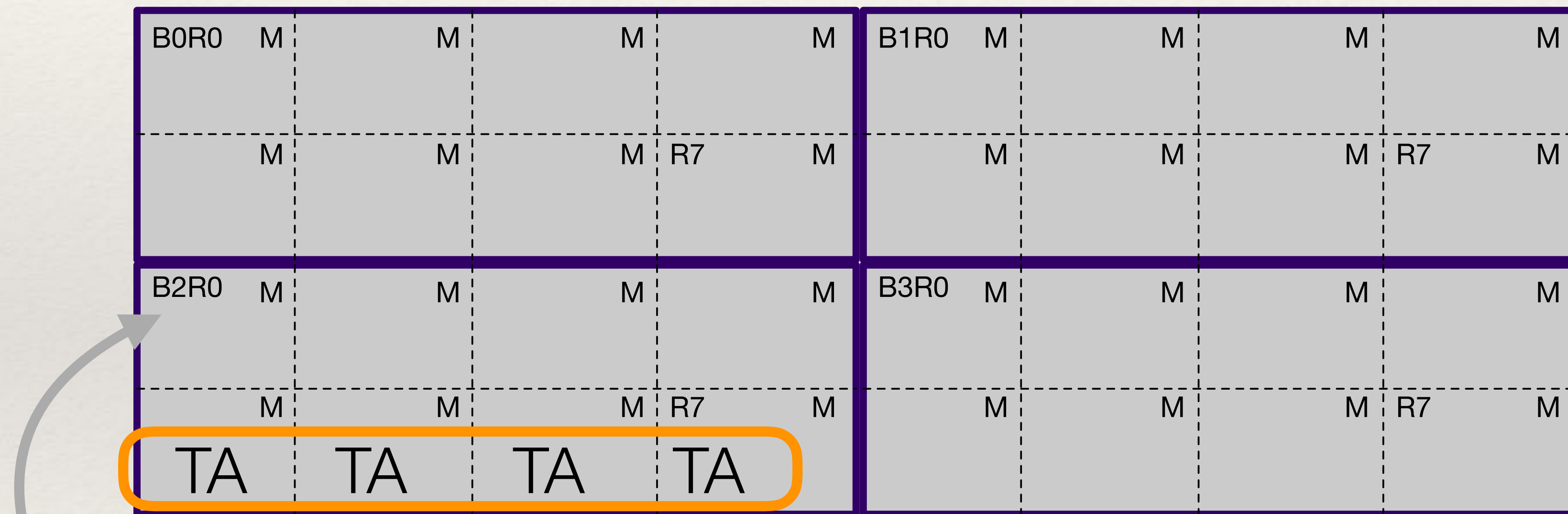
- The scheduler matches a task to block resources and sends task parameters to rank 0 of a block.
- The task “disconnects” until it completes.



Task TA: src, 4x16 CPU only
Task TB: solve, 8x1 CPU/GPU
Task TC: contract, 8x14 CPU only

MPI_JM

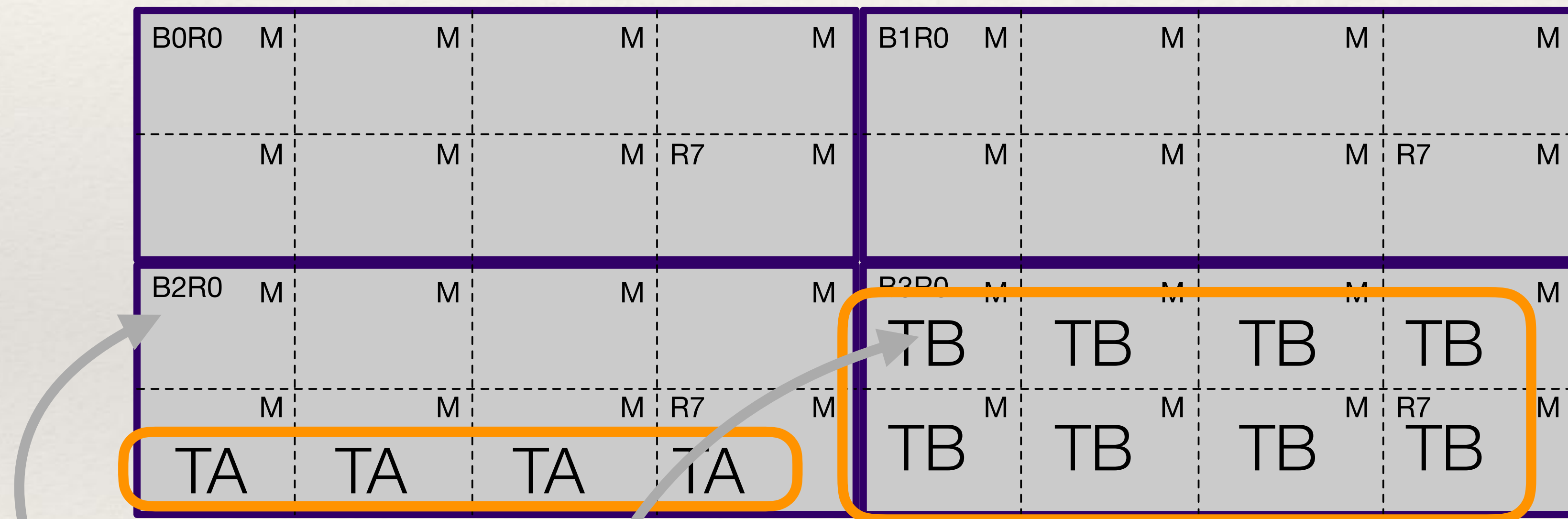
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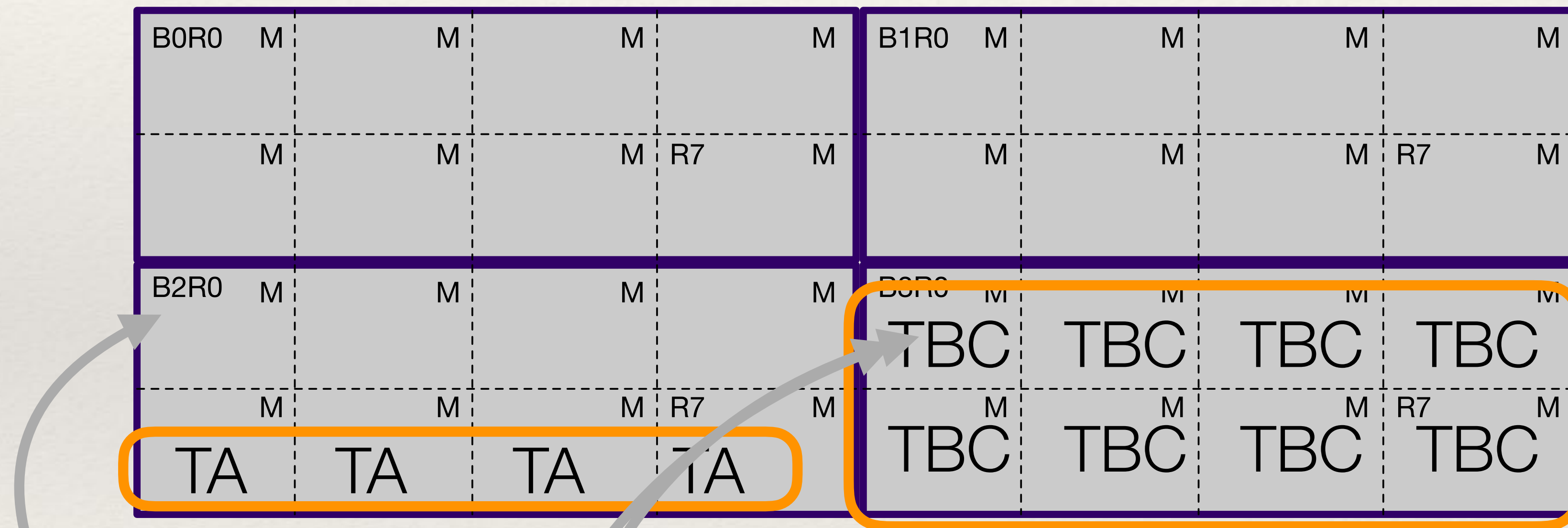
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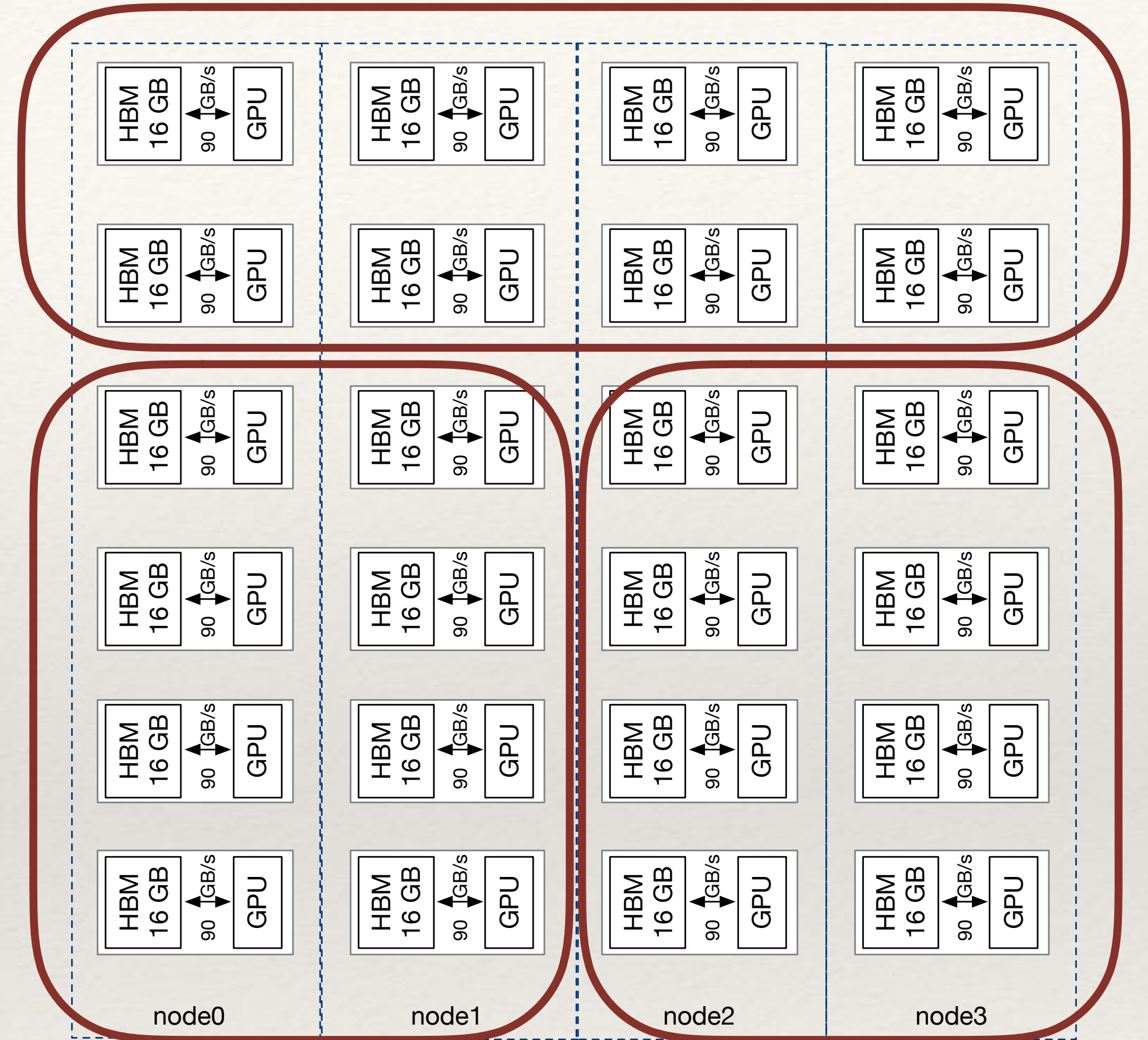
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MPI_JM

Not all problems have factors of 3 in them (Summit nodes have 6 GPUs/node)

MPI_JM provides micro-control of rank placement

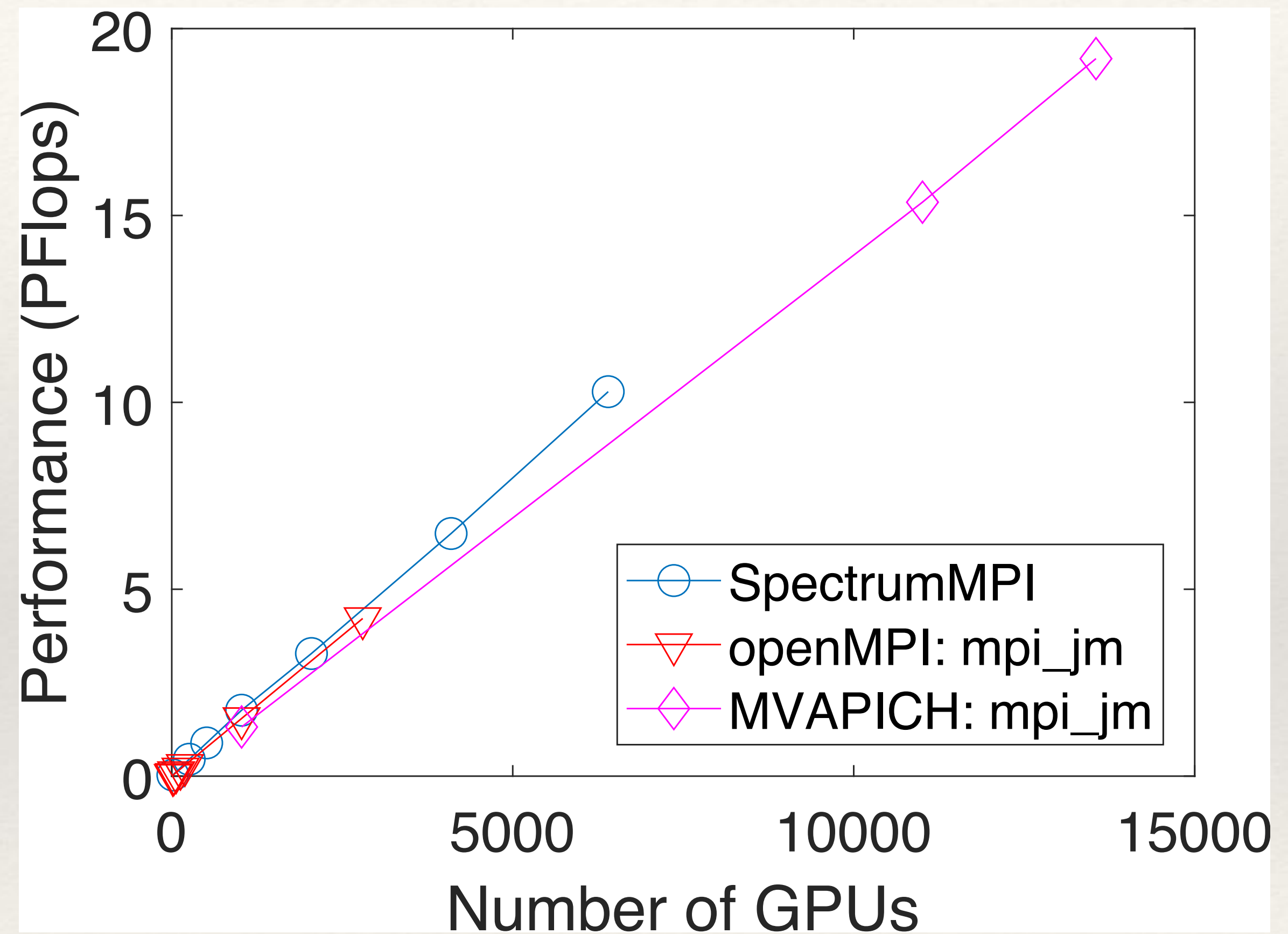
- ❑ Three 8 GPU jobs distributed over 4 Summit nodes.
- ❑ QUDA Autotuner configures the top job differently because interconnect is different.
- ❑ Most CPU cores remain open for CPU only jobs.
- ❑ Try to keep all parts of nodes doing productive work!



MPI_JM: Scaling in Sierra

- ❑ The SpectrumMPI run was done with 400 separate jobs.
- ❑ MPI_JM on OpenMPI was run with 7 independent jobs of 100 nodes due to reliability issues.
- ❑ Under **MVAPICH** full DPM support was available and separate lumps of nodes were started independently. Successful lumps connect afterwards and are managed together! ~4 min startup for all 4000 nodes!
- ❑ The combination of GPU performance and our management software got us selected as a 2018 Gordon Bell Finalist

MVAPICH runs done with single job



MPI_JM: Scaling in Sierra

- ❑ Compared to other applications, our peak performance does not seem impressive
- ❑ Machine-to-machine, compared to Titan @ ORNL (Titan is 18,688 nodes 16-core AMD + 1 K20/node)

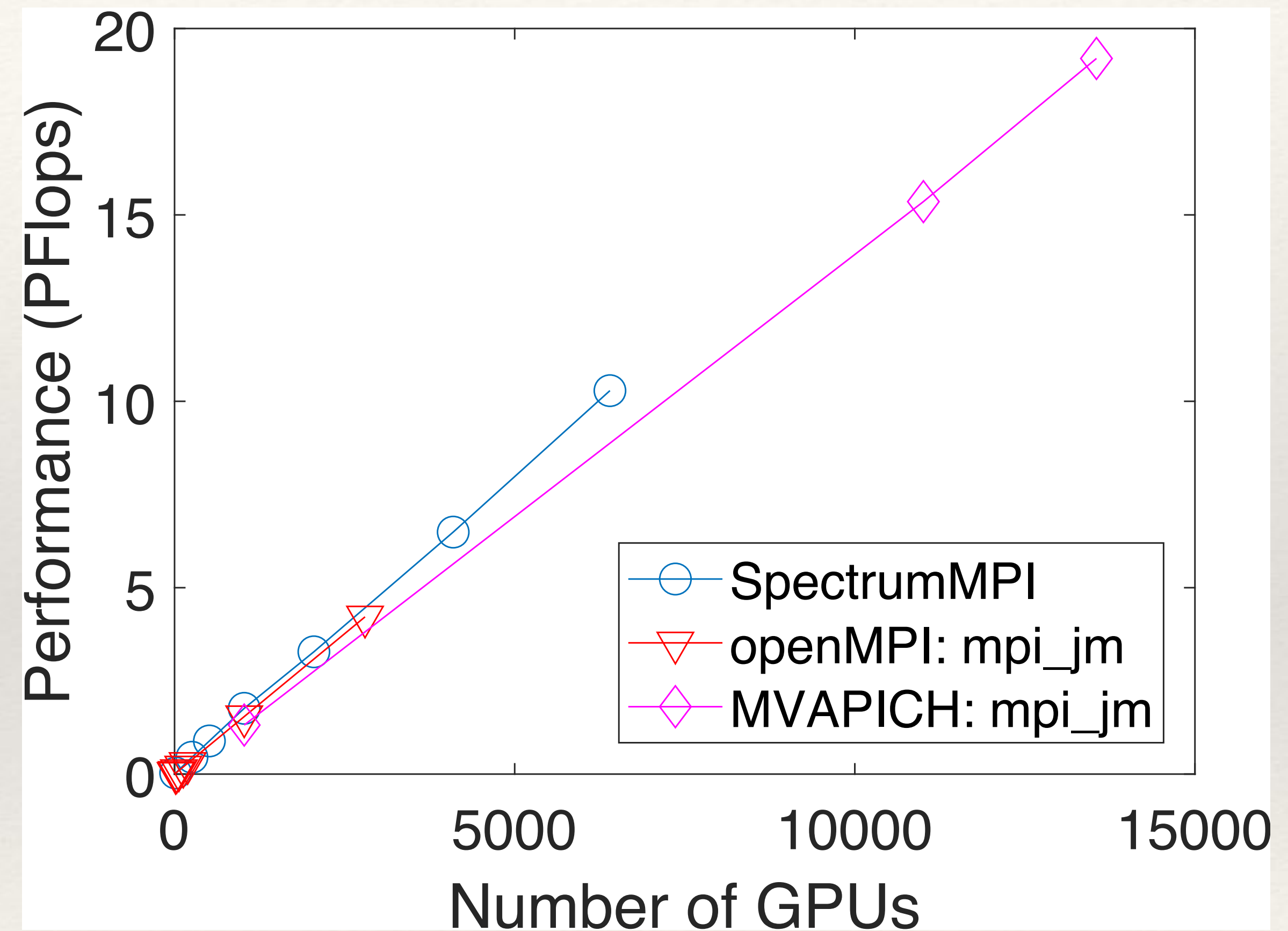
For our research

Sierra (~4300) is **~10 times** faster than Titan

Summit (~4600) is **~15 times** faster than Titan

These machines are **disruptively** faster than previous computers

MVAPICH runs done with single job



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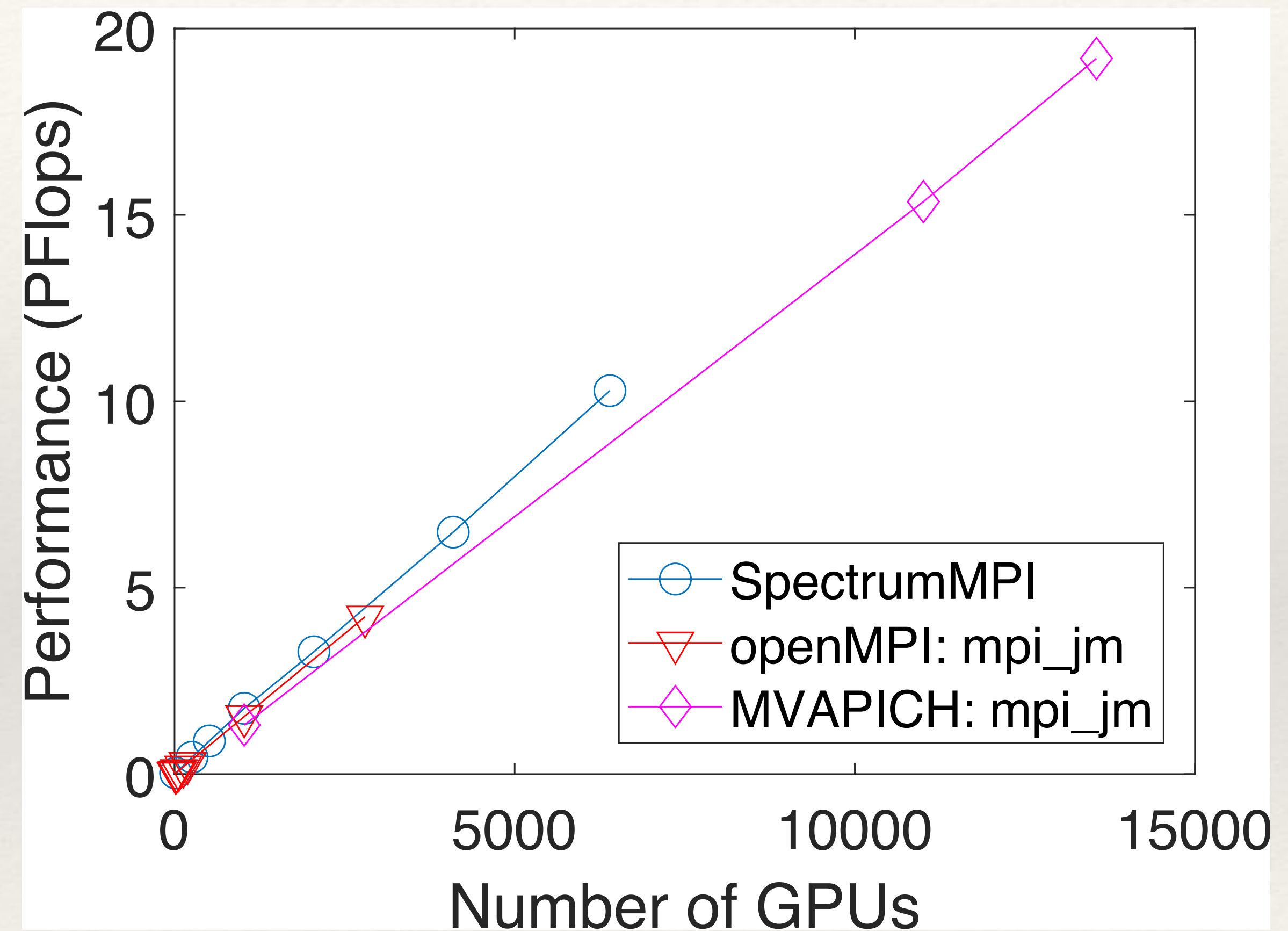
Sierra (~4300) is **~10 times** faster than Titan

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These machines are **disruptively** faster than previous computers

- ❑ In 2.5 weekends on Sierra - we accomplished 5x more than in 1 year on Titan

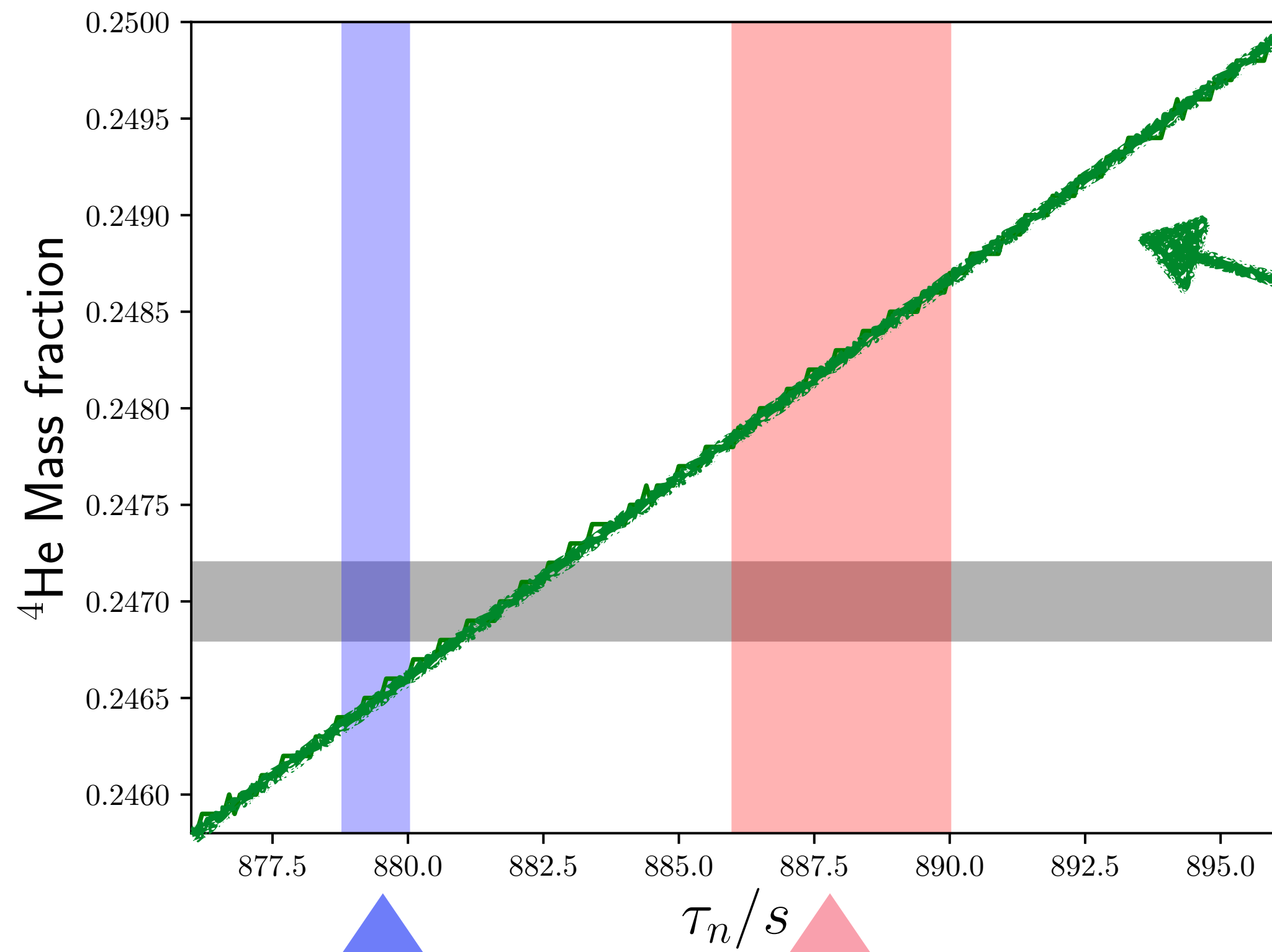
MVAPICH runs done with single job



What did this get us?

- ~3 months Early Science Time on Sierra @ LLNL
Sep. - Dec. 2018
- Early Science Time on Summit @ ORNL
Jan. +
- 2019 DOE INCITE Allocation on Summit
Jan. +

Why is understanding the neutron lifetime interesting?



$$\tau_n = \frac{(5172.0 \pm 1.1) \text{ seconds}}{1 + 3g_A^2}$$

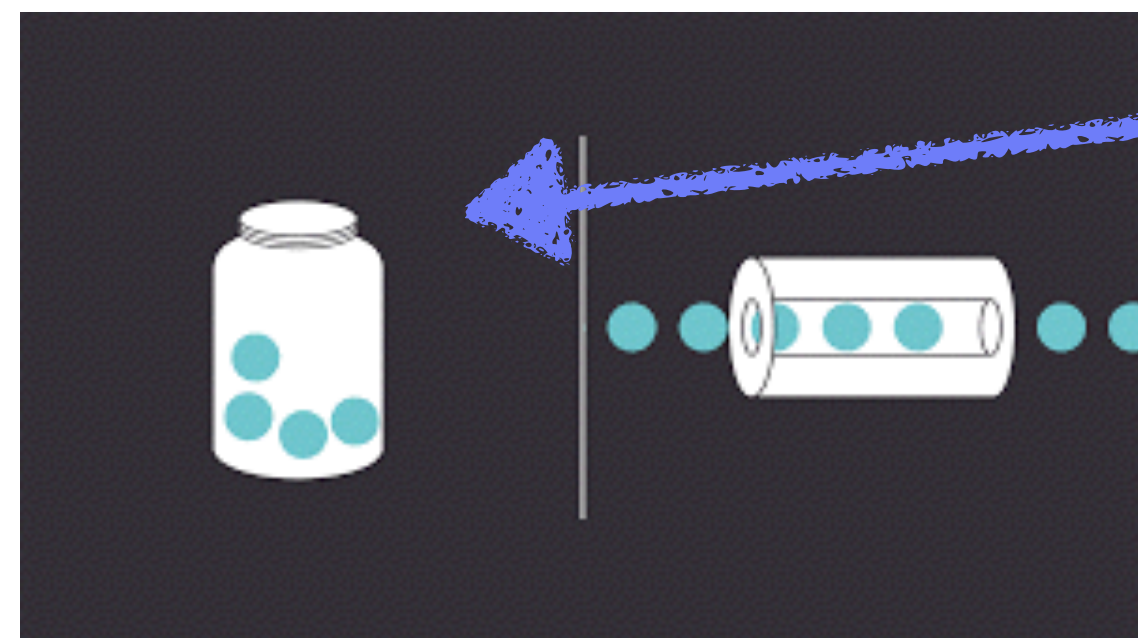
Czarnecki, Marciano, Sirlin

Predicted primordial ${}^4\text{He}$ mass fraction of the universe as a function of the neutron lifetime

Observed primordial ${}^4\text{He}$ mass fraction of the universe

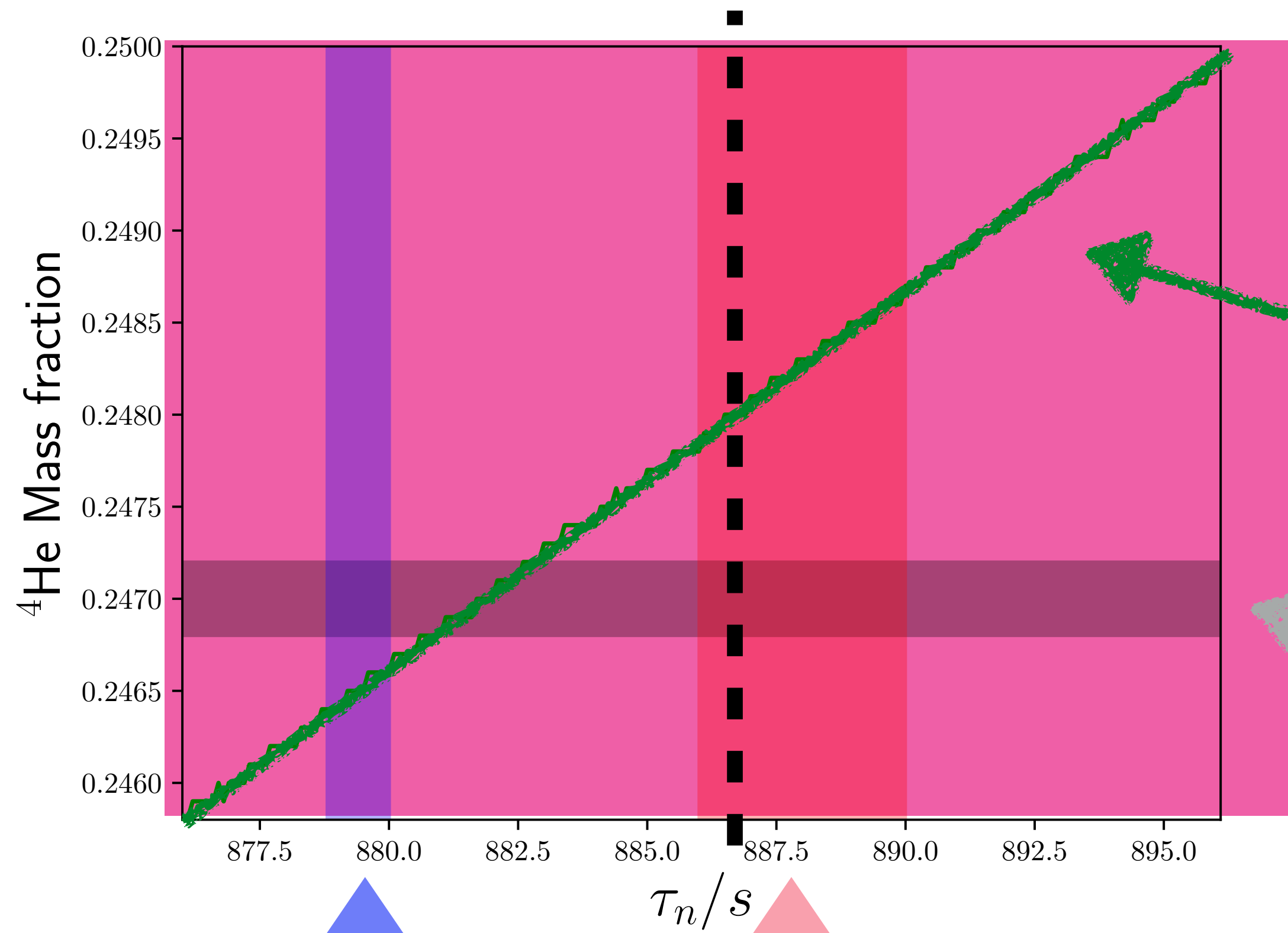
Two different methods of measuring the neutron lifetime disagree at the 99% level

bottle and beam



Is one of the experiments wrong? Or is there new physics hiding here?

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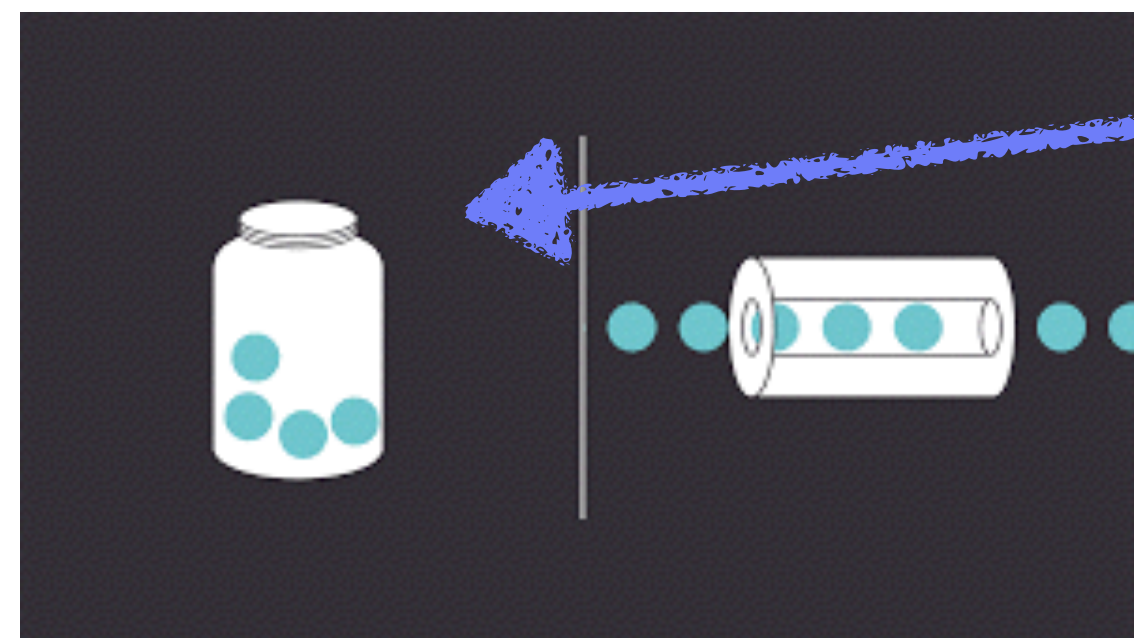
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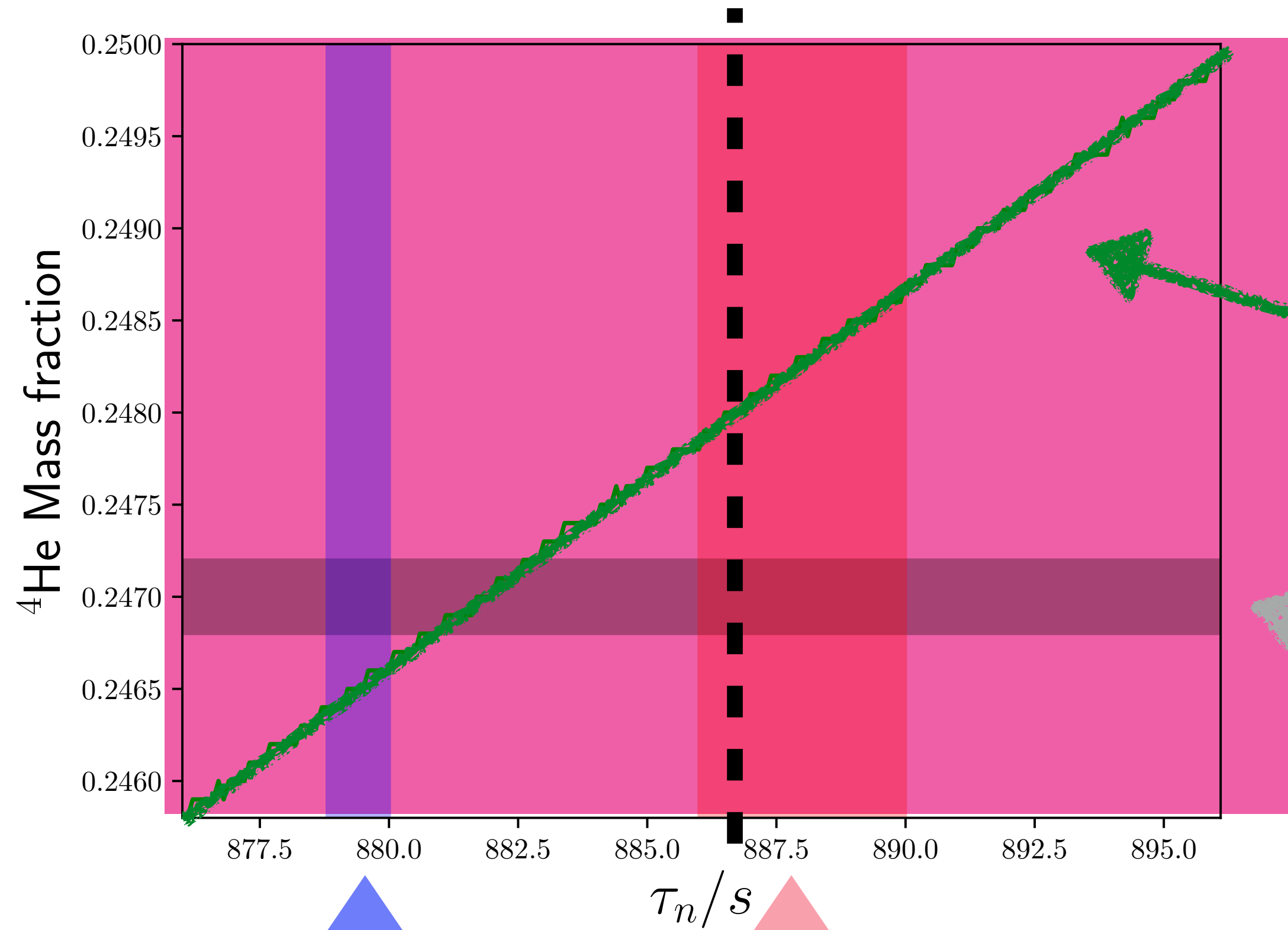
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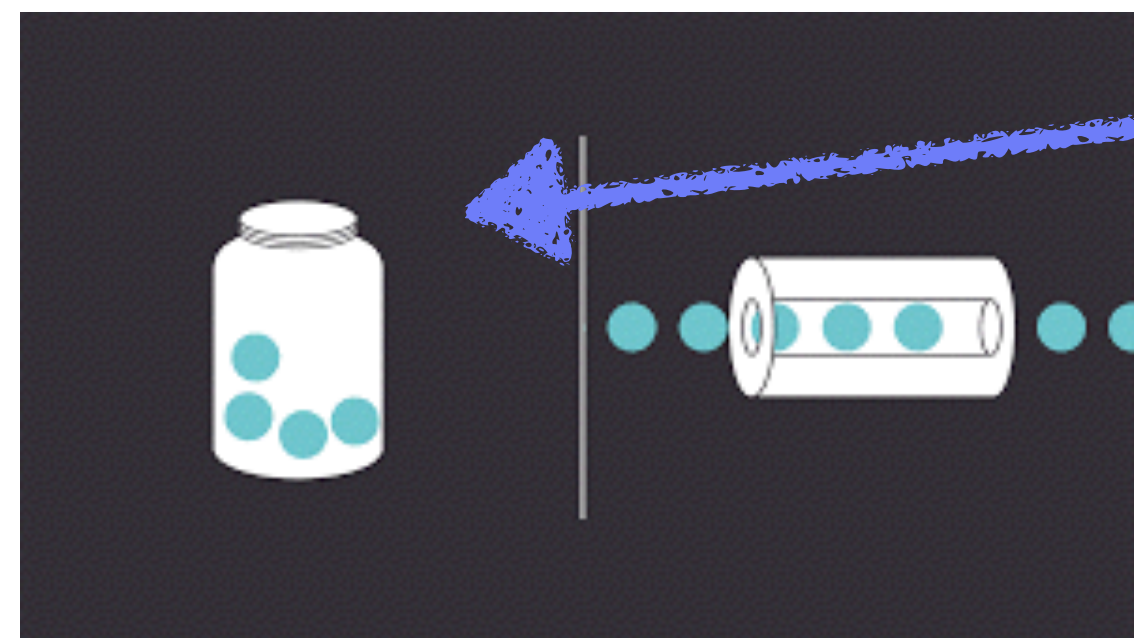
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Can we reduce the uncertainty to a discriminating level?

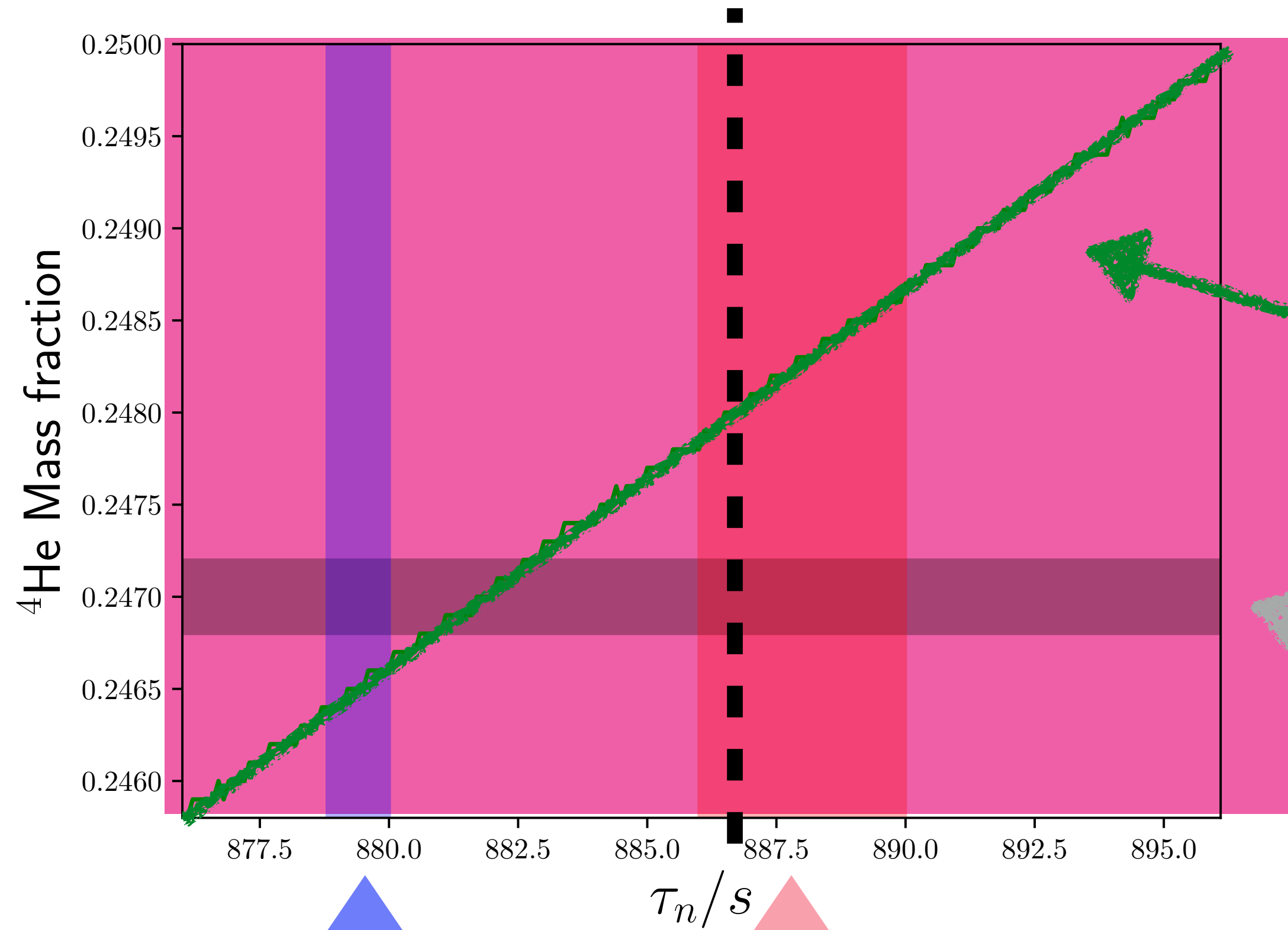
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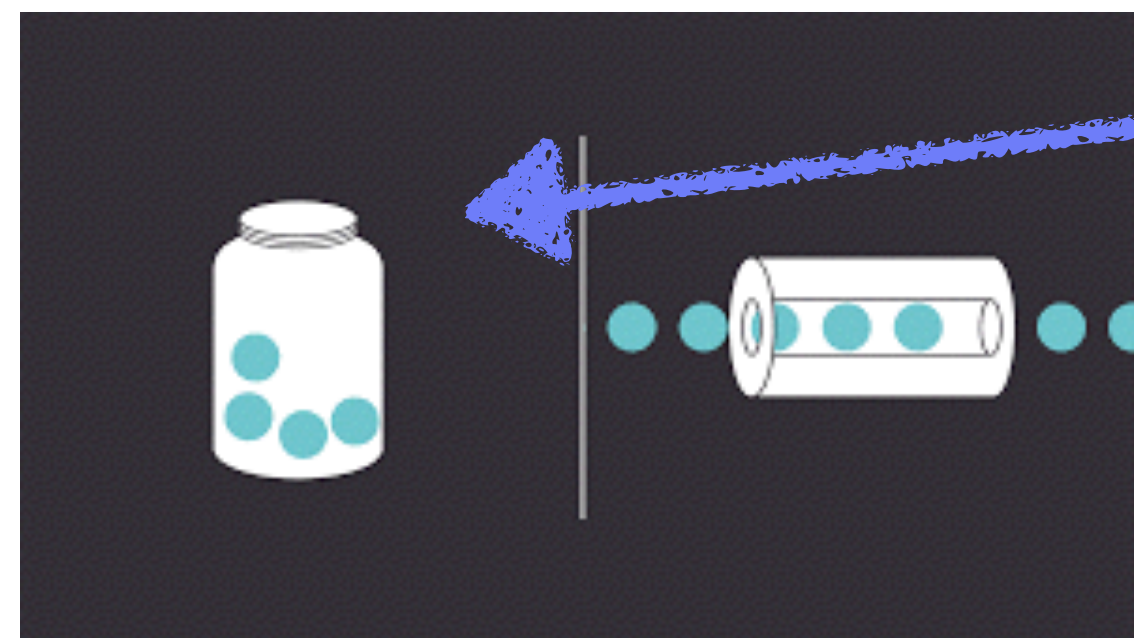
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Can we reduce the uncertainty to a discriminating level?

Yes!
With **summit!**

Two different methods of measuring the neutron lifetime disagree at the 99% level

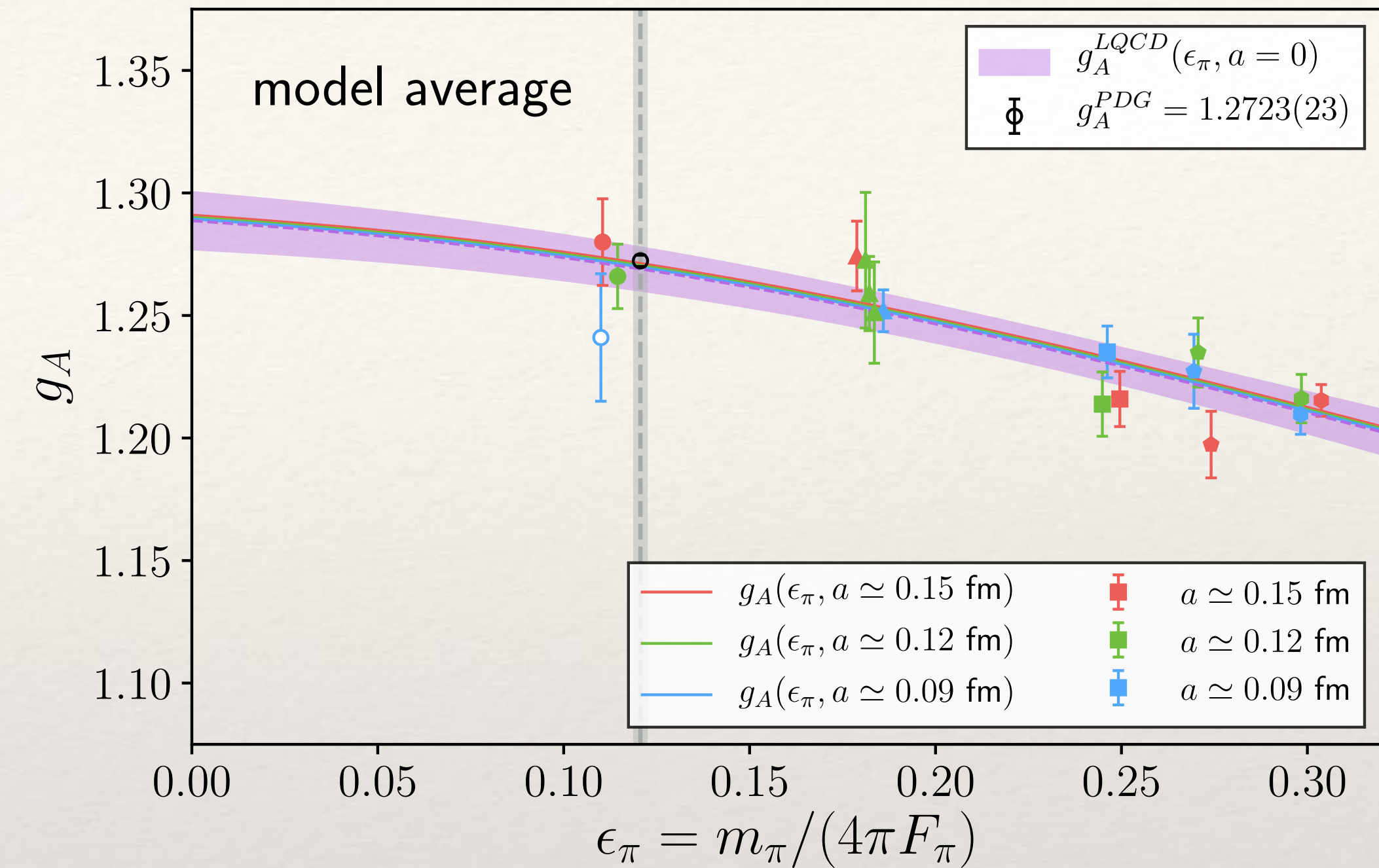
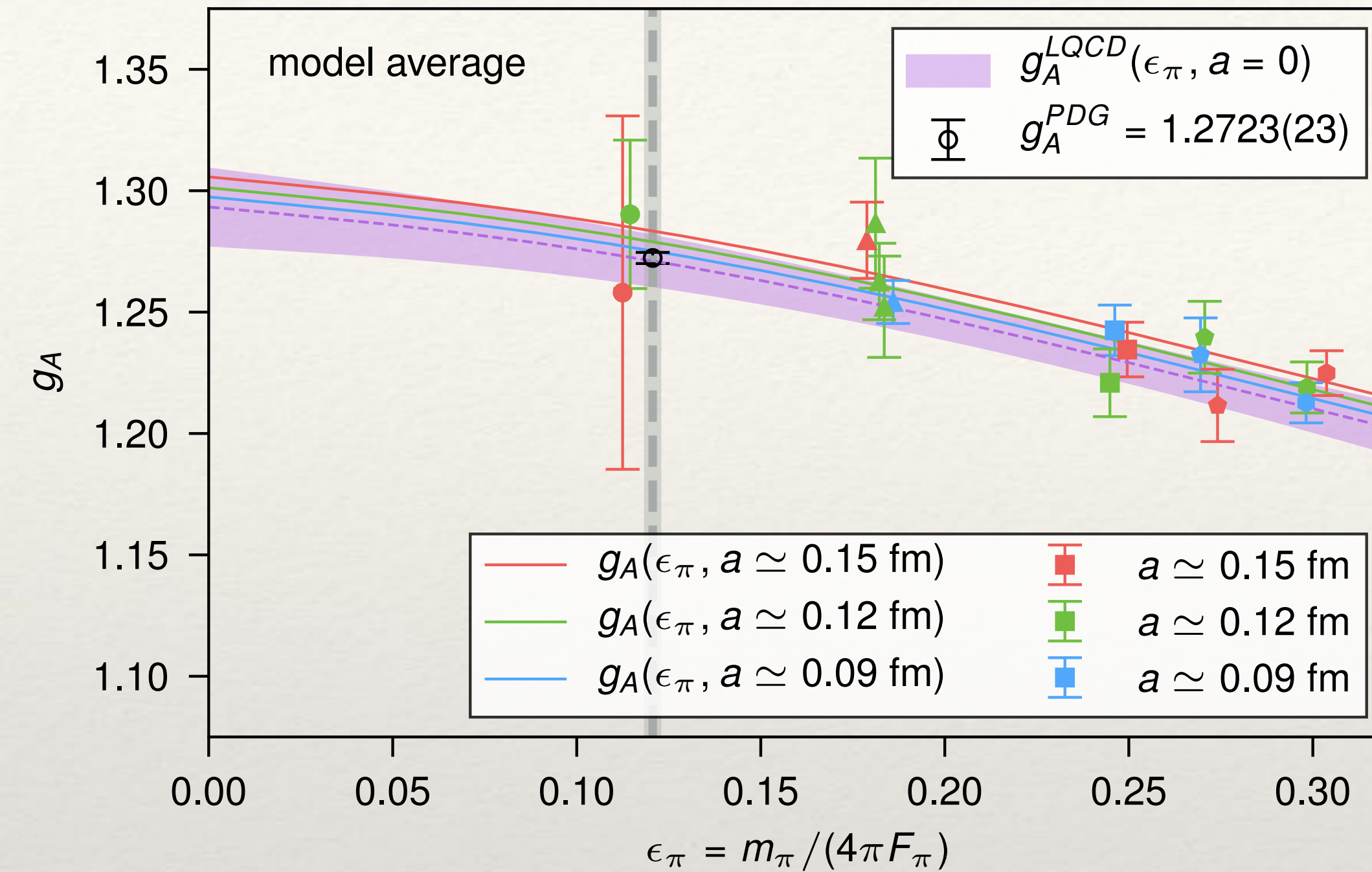
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The Neutron Lifetime on Sierra Early Science

1 year on Titan (ORNL) + 2 years on GPU machines at LLNL



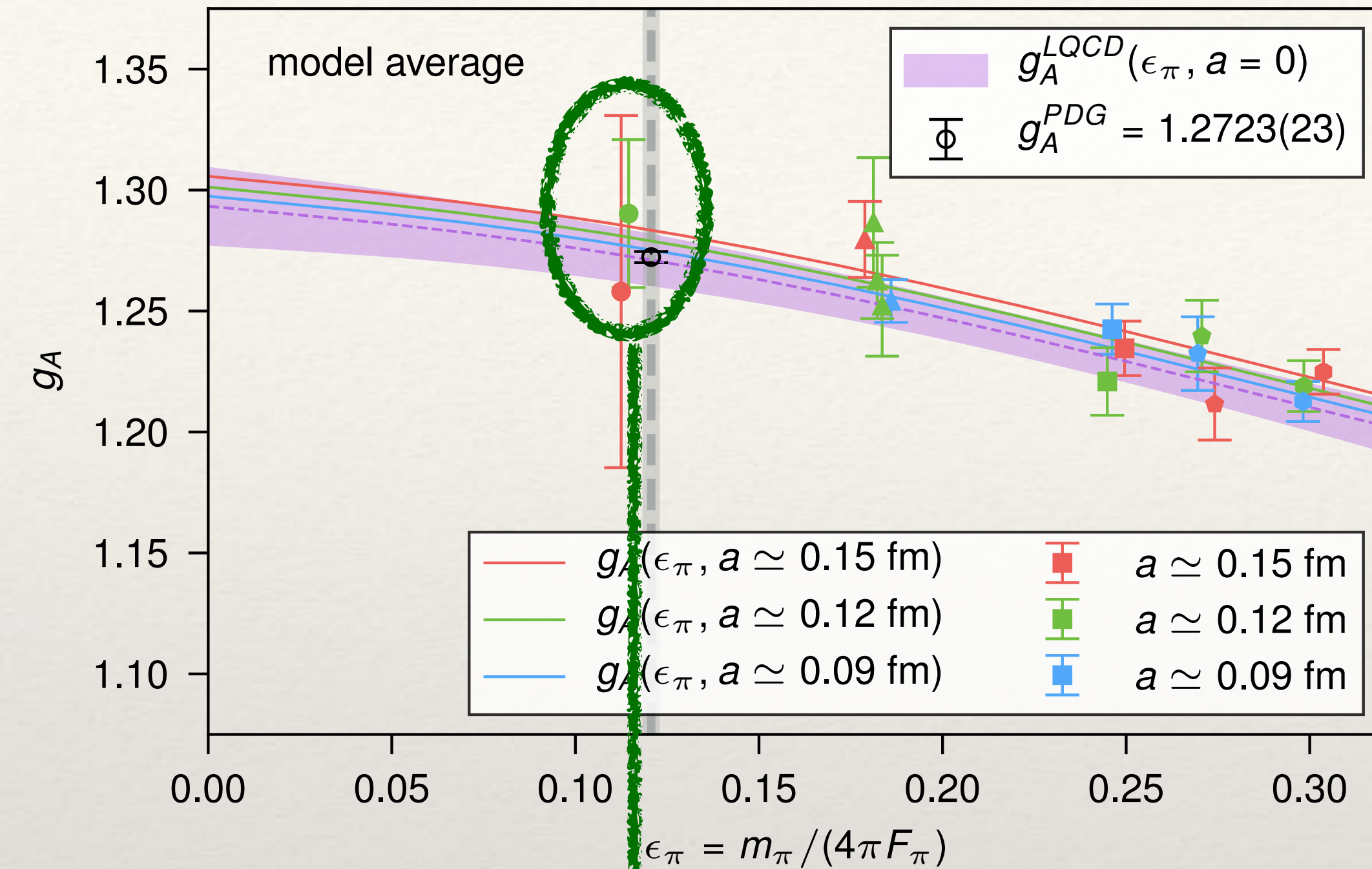
Nature 558 (2018) no. 7708, 91-94

Sierra Early Science

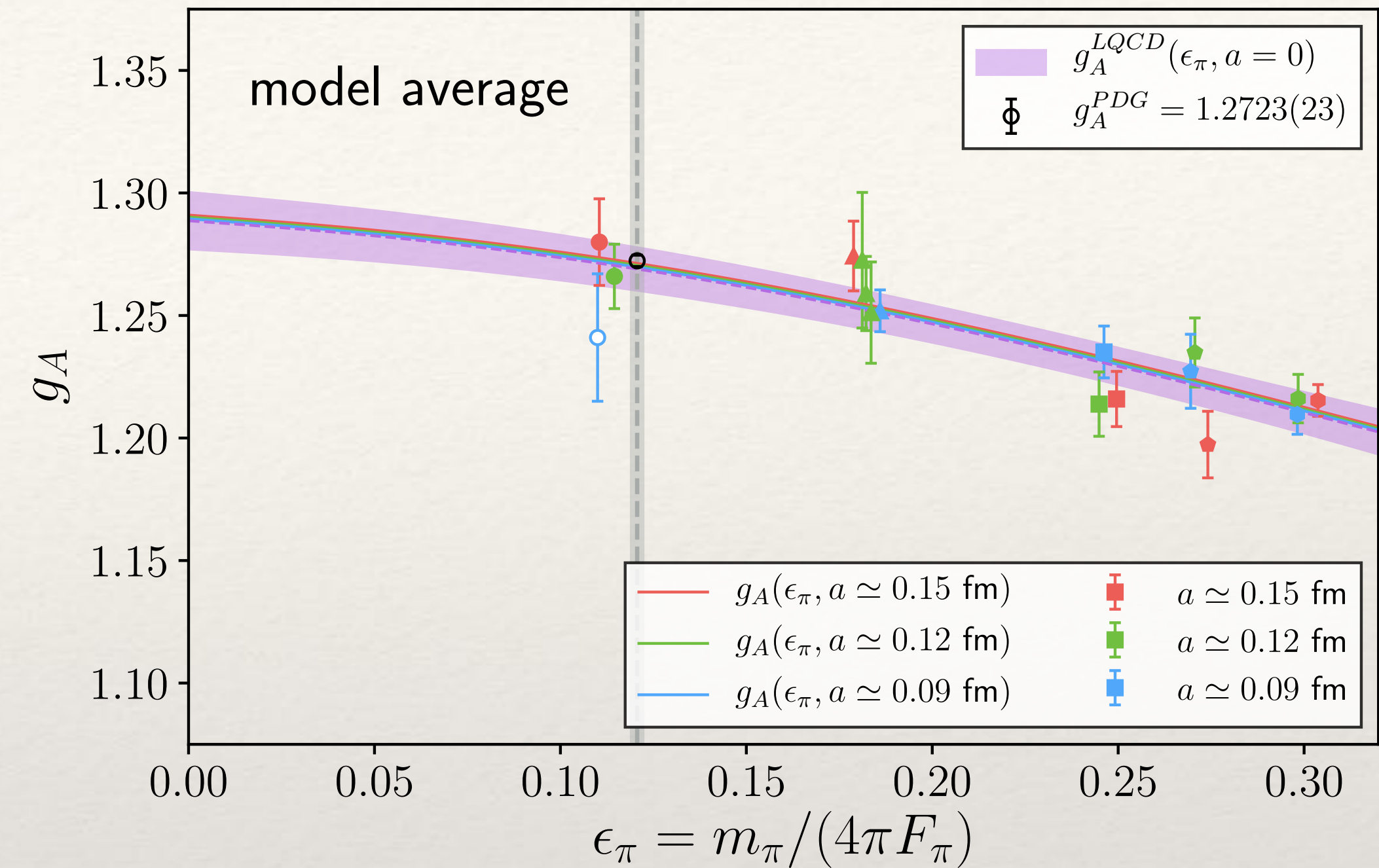
- ❑ The vertical gray band denotes the physical value of pion mass - these points are significantly more expensive than the rest to compute - but the most valuable for the final predictions
- ❑ The green point in our publication cost as much computing time as all the other points combined
- ❑ The green point from Sierra has 10x more statistics than our publication
- ❑ The red point from our publication was not useful
- ❑ The red point from Sierra came from an entirely new calculation and is now very useful
- ❑ The blue point from Sierra was entirely unattainable from previous computers (it still needs more statistics to be useful)

The Neutron Lifetime on Sierra Early Science

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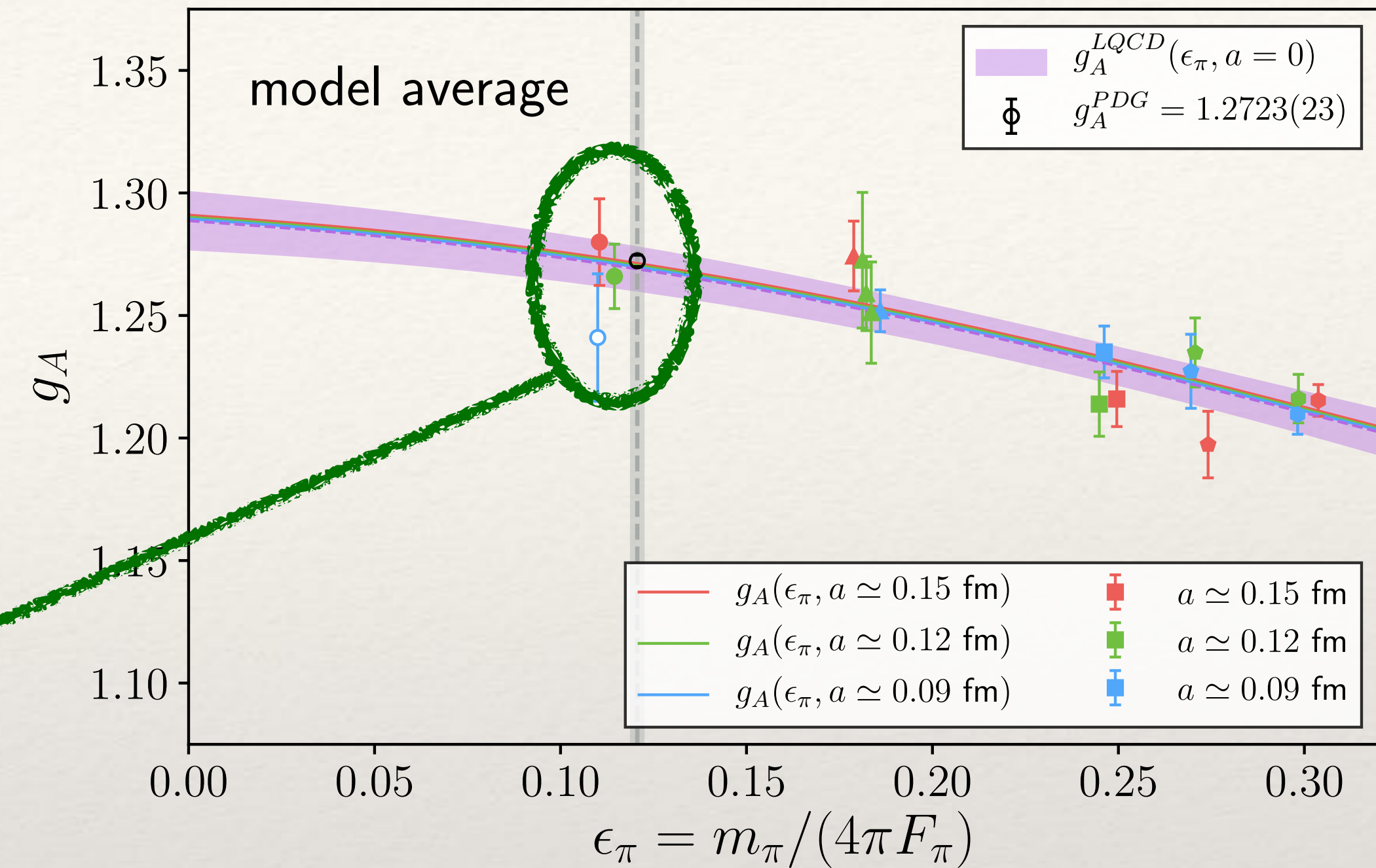
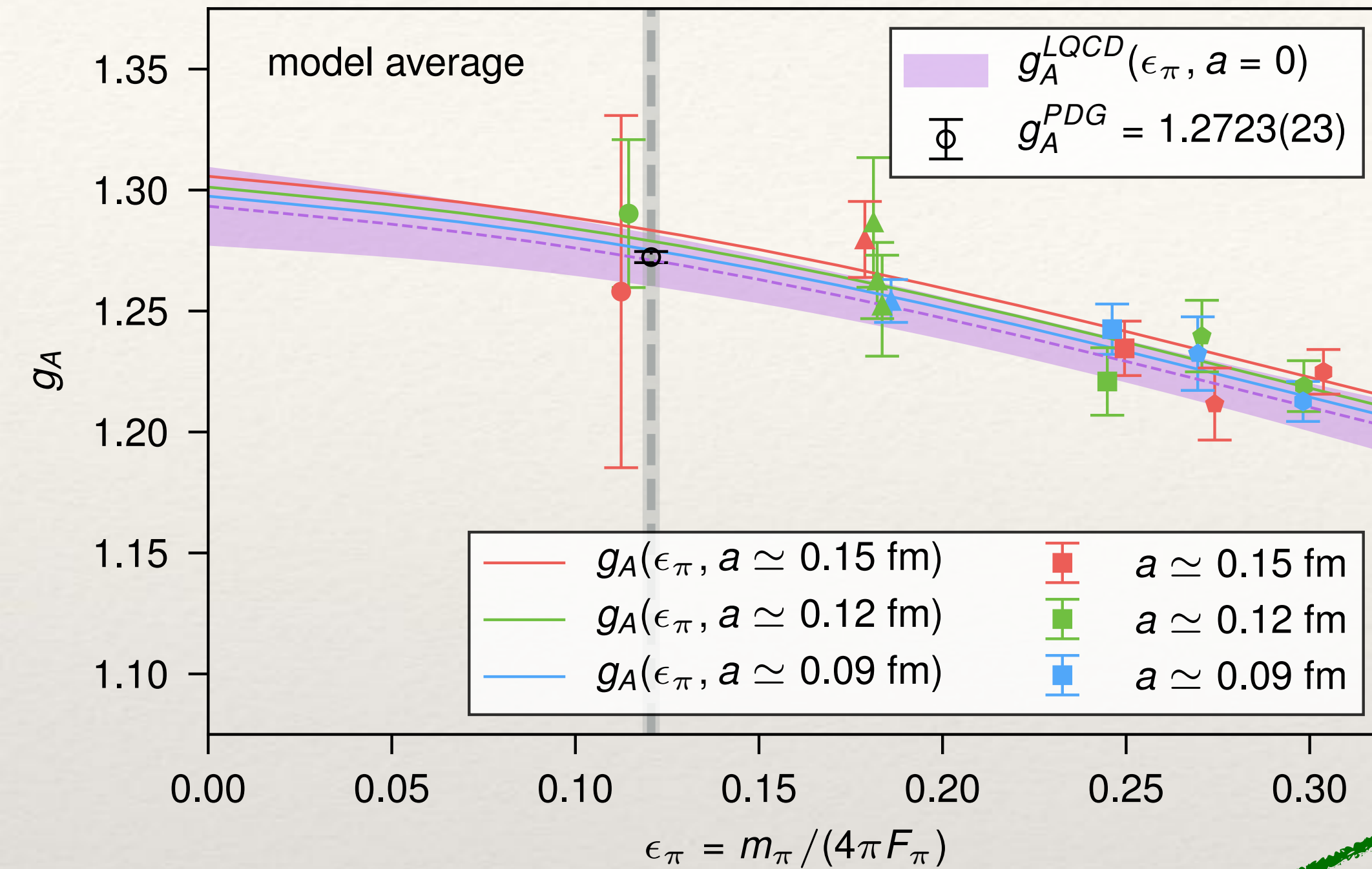


Sierra Early Science

- The vertical gray band denotes the physical value of pion mass - these points are significantly more expensive than the rest to compute but the most valuable for the final predictions
- The green point in our publication cost as much computing time as all the other points combined
- The green point from Sierra has 10x more statistics than our publication
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The Neutron Lifetime on Sierra Early Science

1 year on Titan (ORNL) + 2 years on GPU machines at LLNL



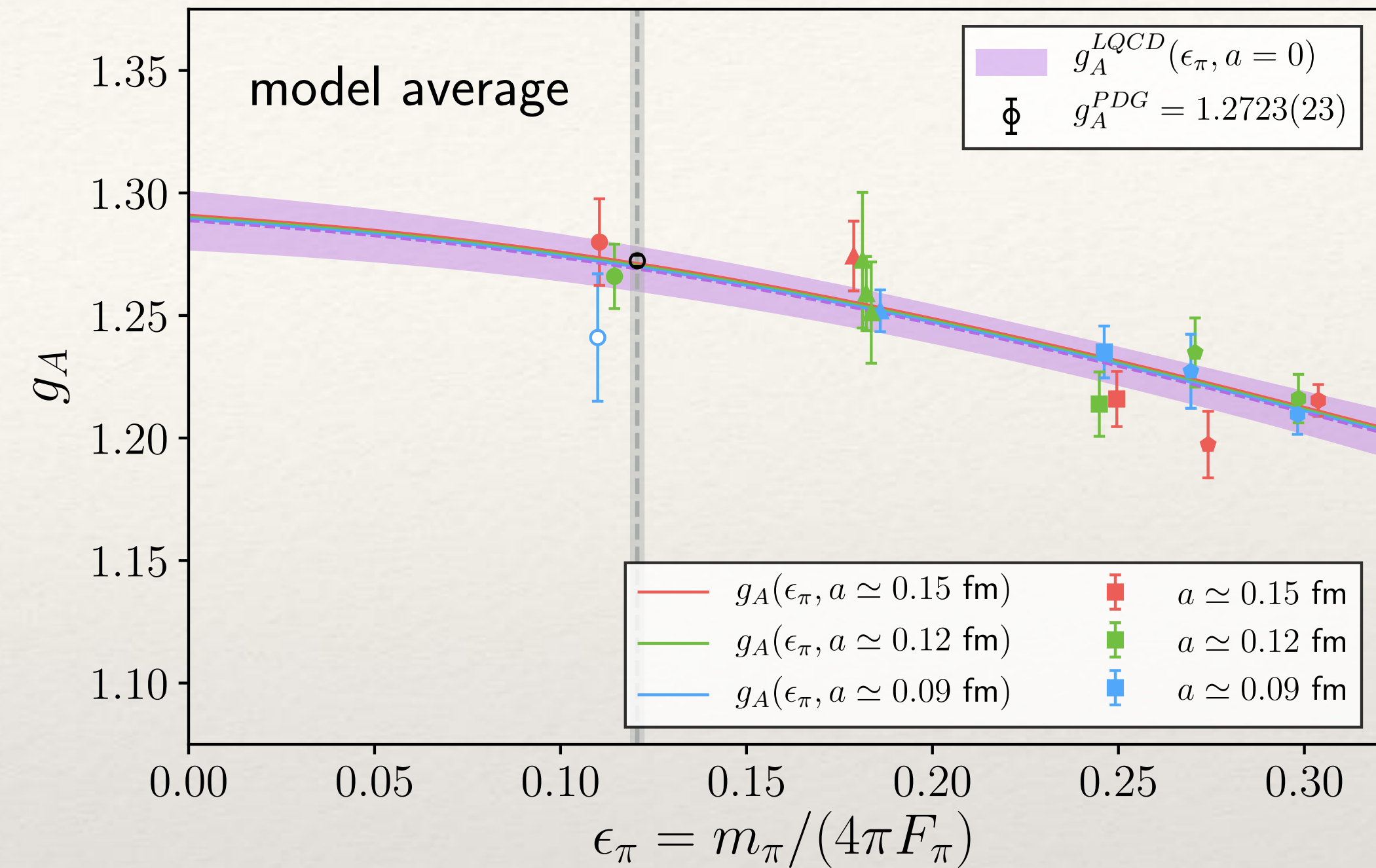
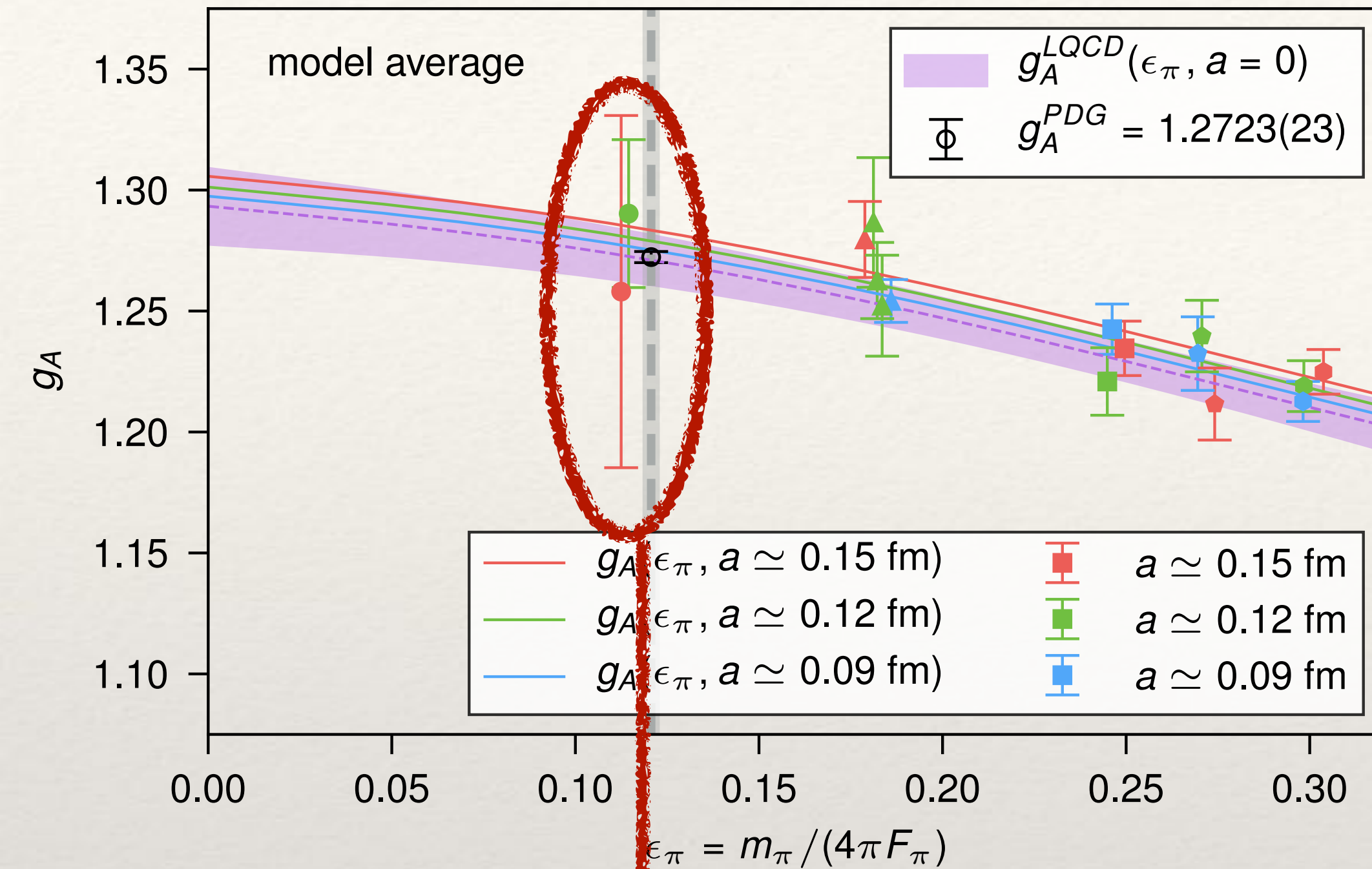
Nature 558 (2018) no. 7708, 91-94

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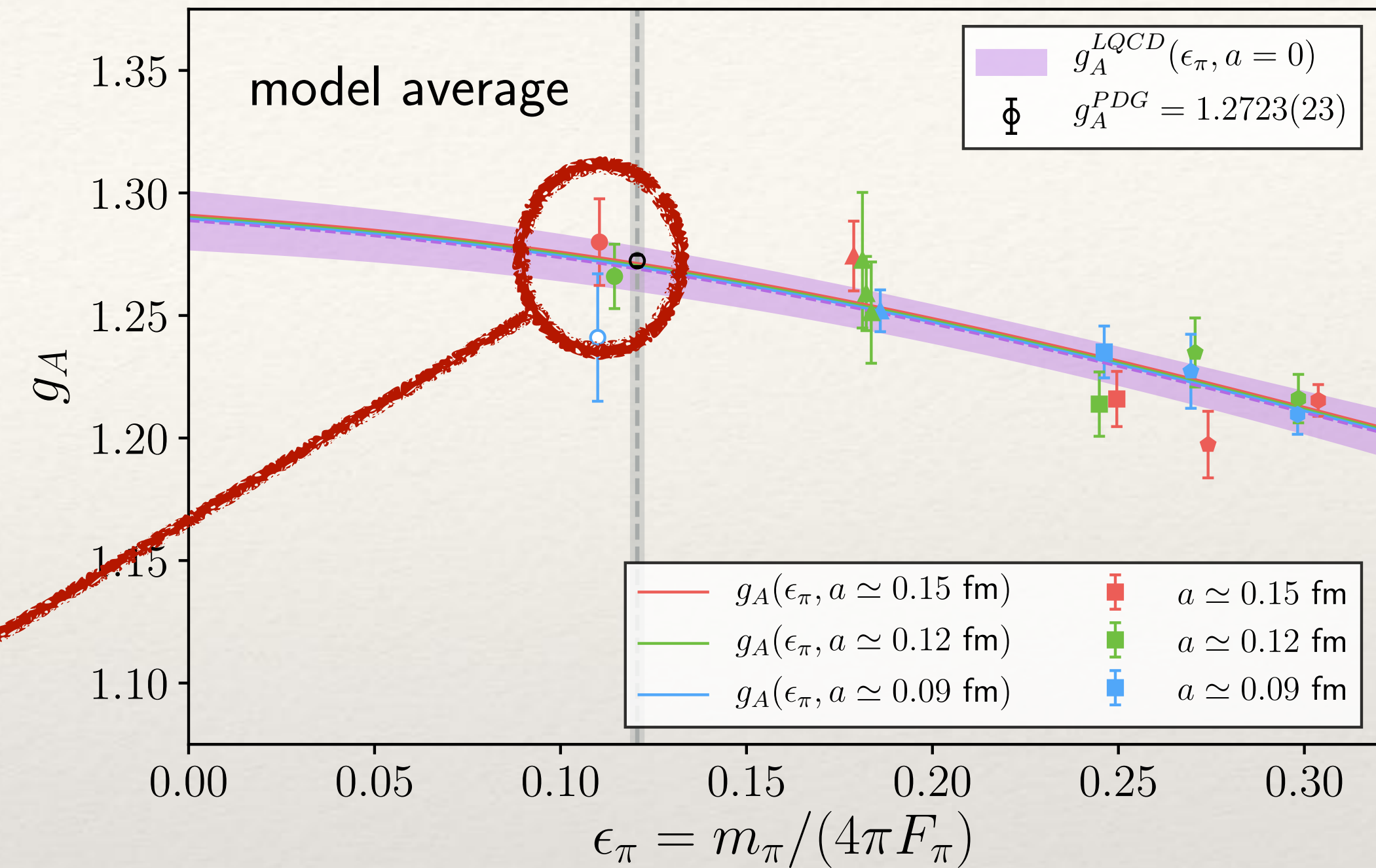
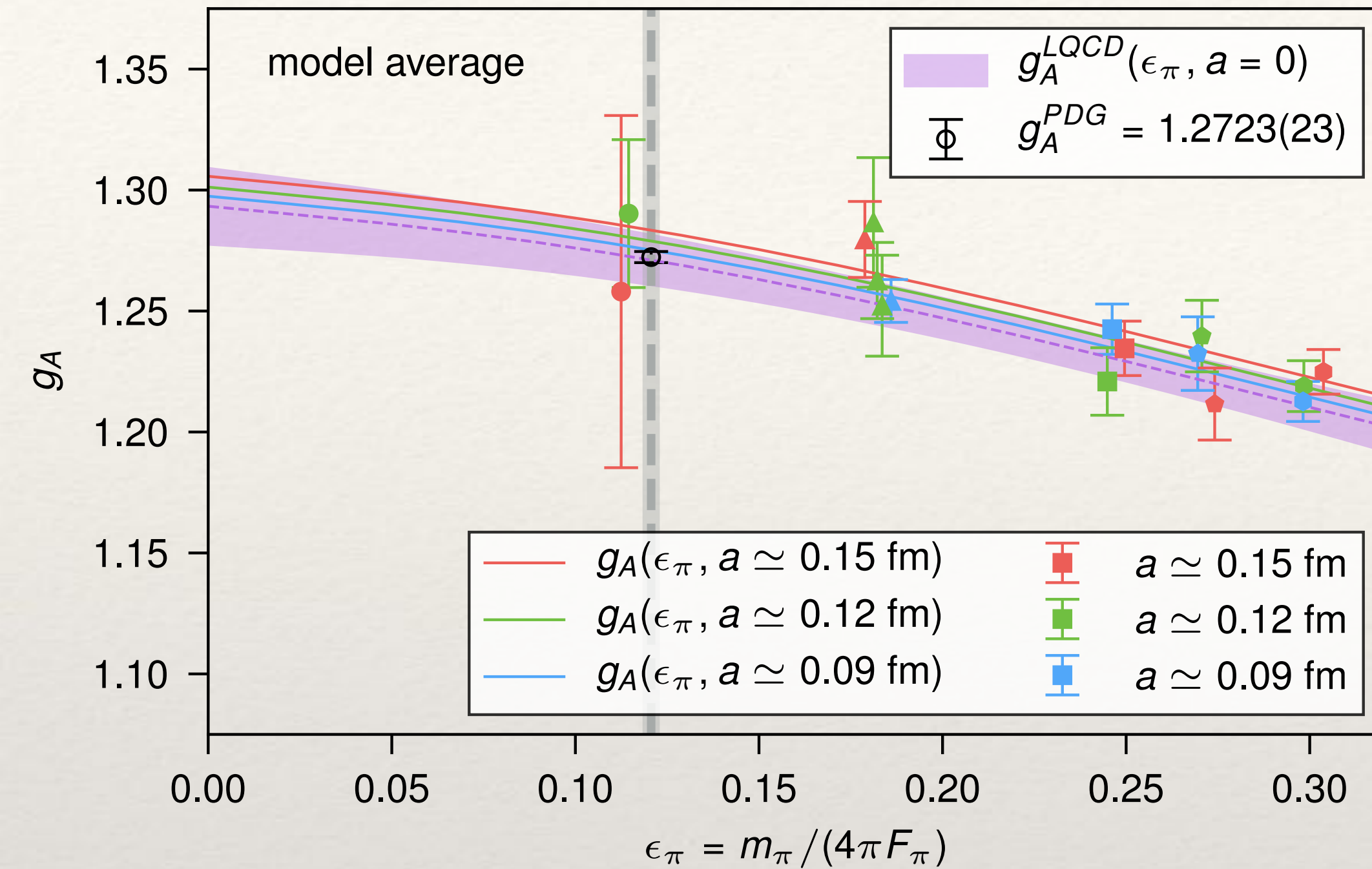
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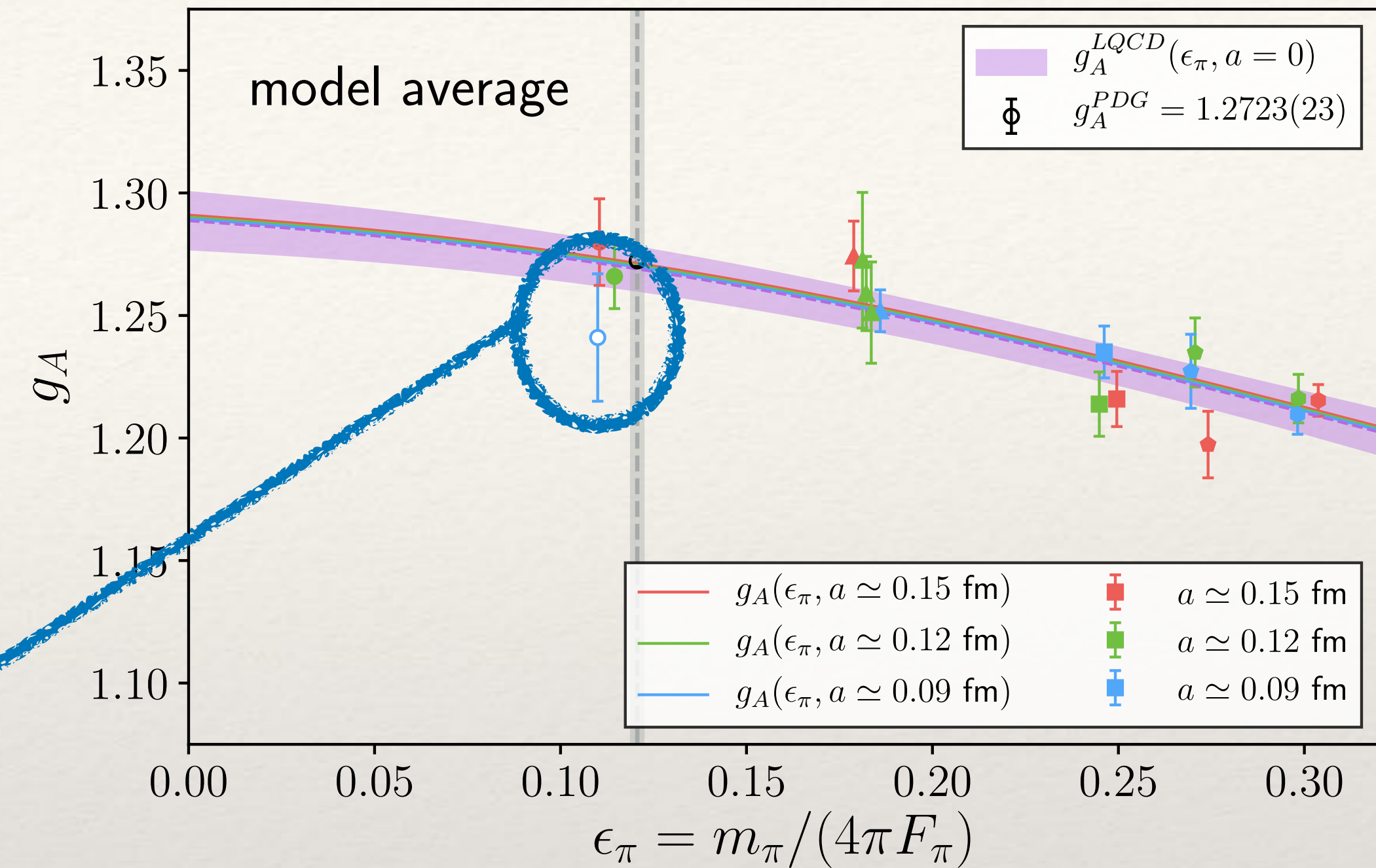
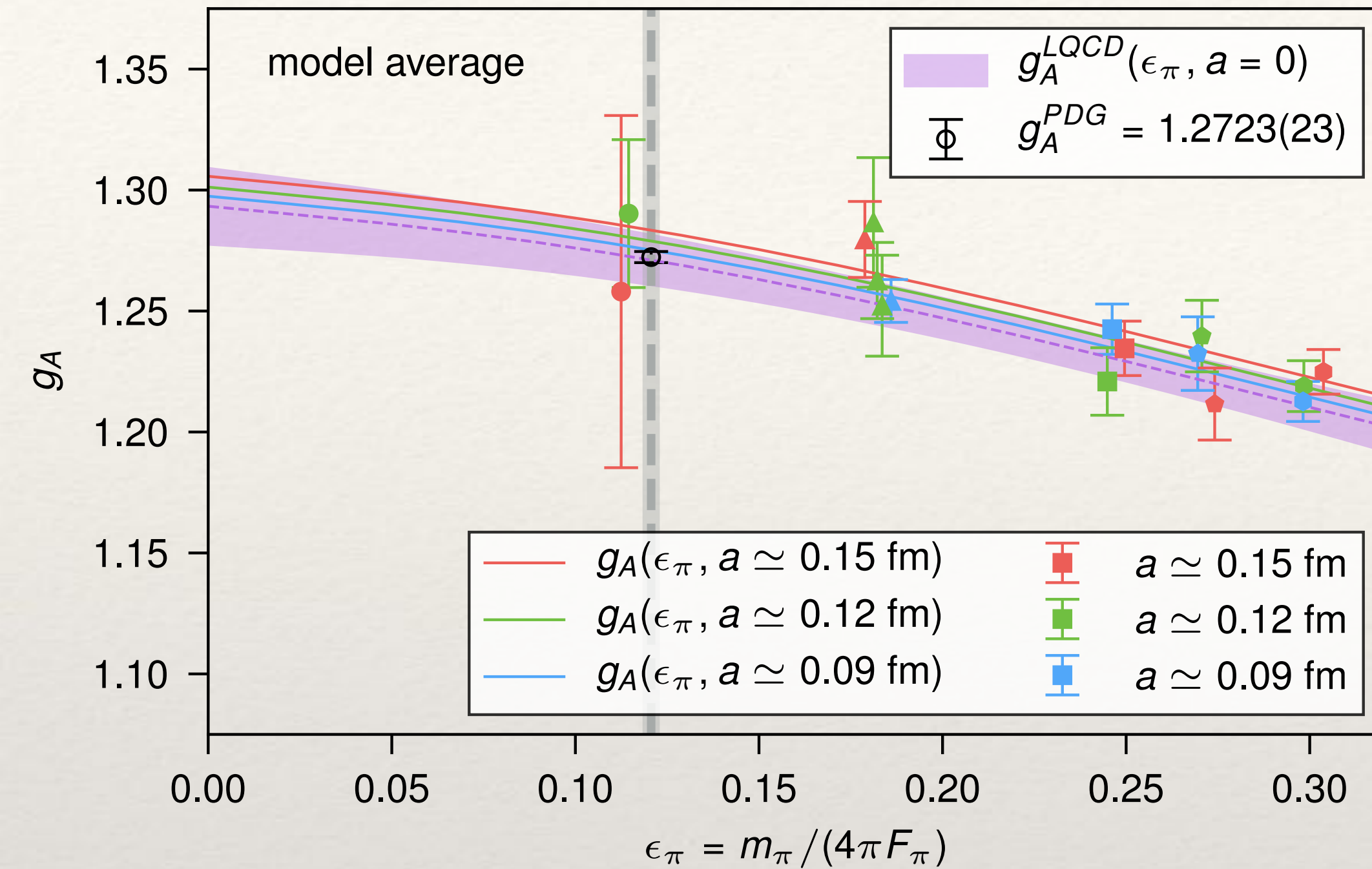
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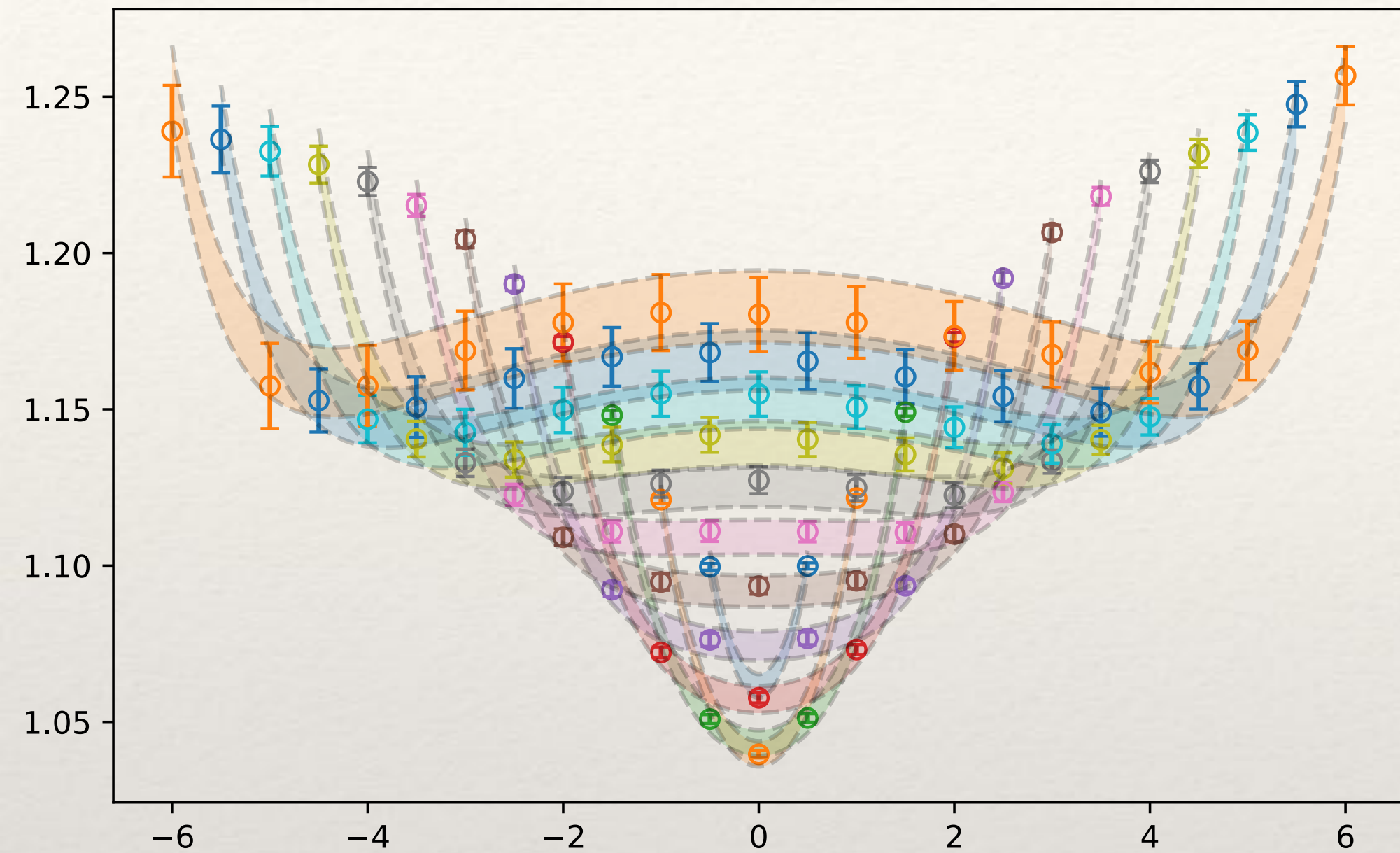


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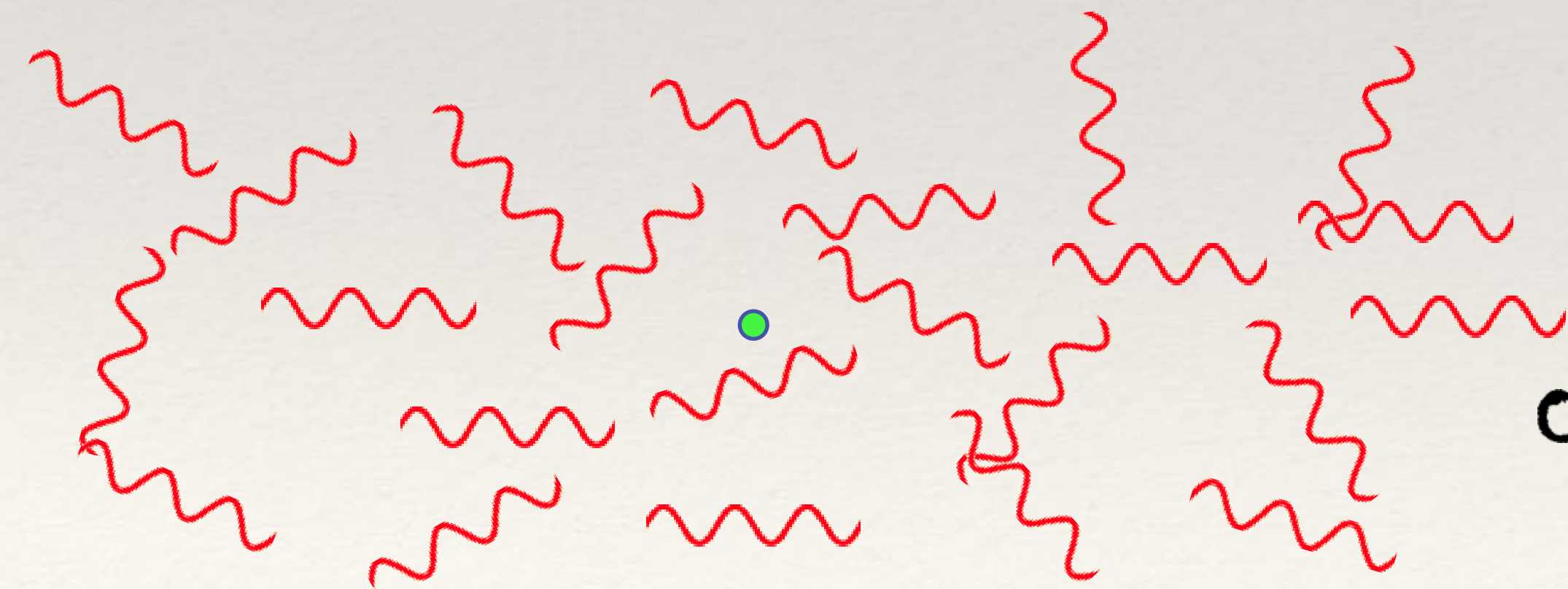
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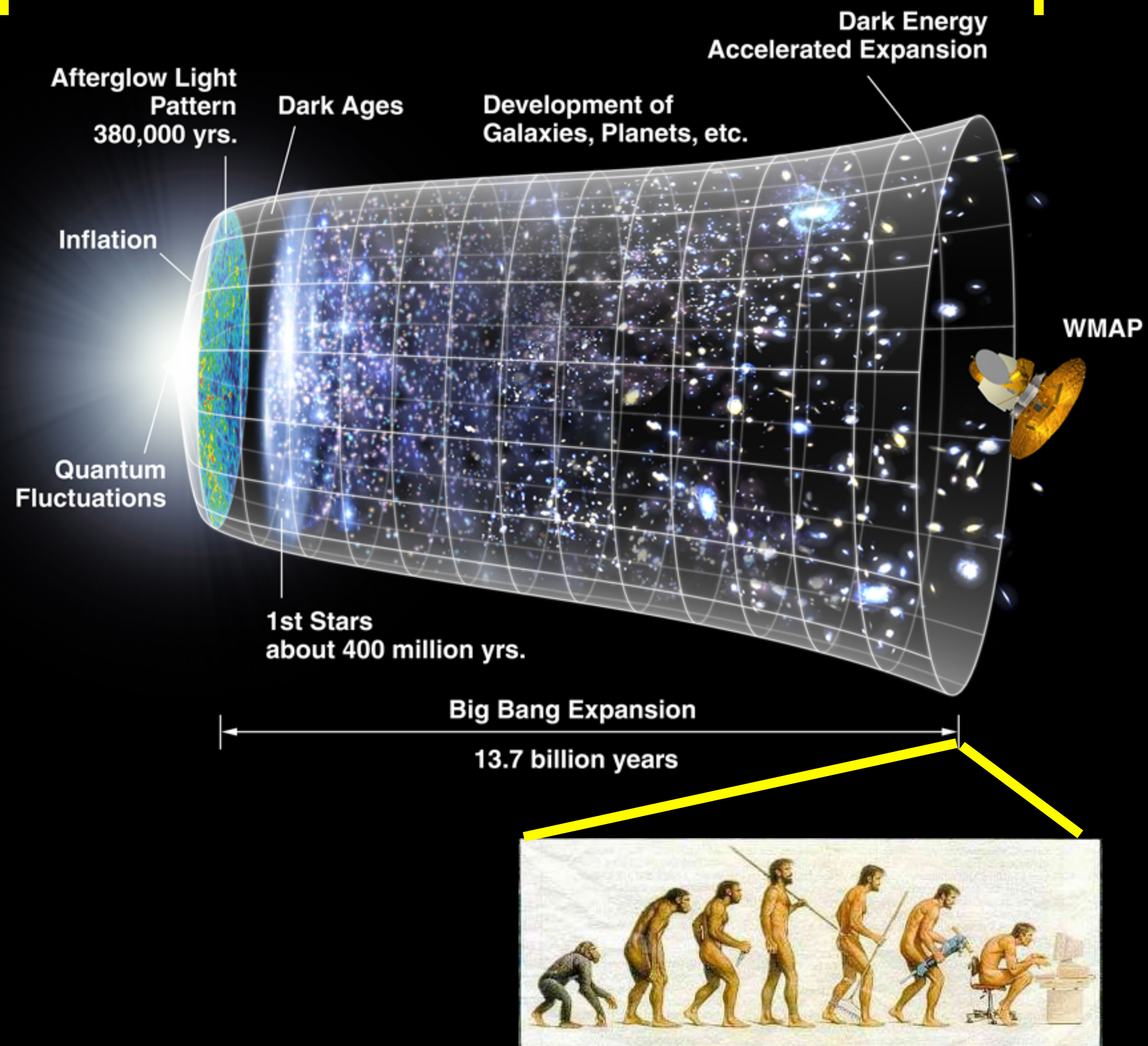
Sneak peak of Results



- We recently finished a “tuning” run on Summit
- not yet processed into a nice result
- This data set is about **5x** larger than ever created for such a calculation (it also temporarily occupies about 1 PetaByte of scratch space)
- Our theoretical understanding (fit bands) is in remarkable agreement with the numerical results
- This will provide us with an unprecedented ability extract the physics of interest
- The results we obtain this year will help in the quest to understand the origin of matter over anti-matter in the universe



Standard Model of Particle Physics



- ★ This is a very exciting time for basic science research with high-performance-computing
- ★ Titan (K20) brought us to the edge of making predictive contact with basic nuclear physics quantities relevant to our understanding of the universe
- ★ Summit is **disruptively** faster than Titan
 - ★ we are still learning to expand our vision of what can be accomplished
- ★ Making full use of the new heterogeneous architecture requires
 - ★ Optimized GPU libraries, QUDA
 - ★ the development of sophisticated, and light-weight job managers
MetaQ, MPI_JM