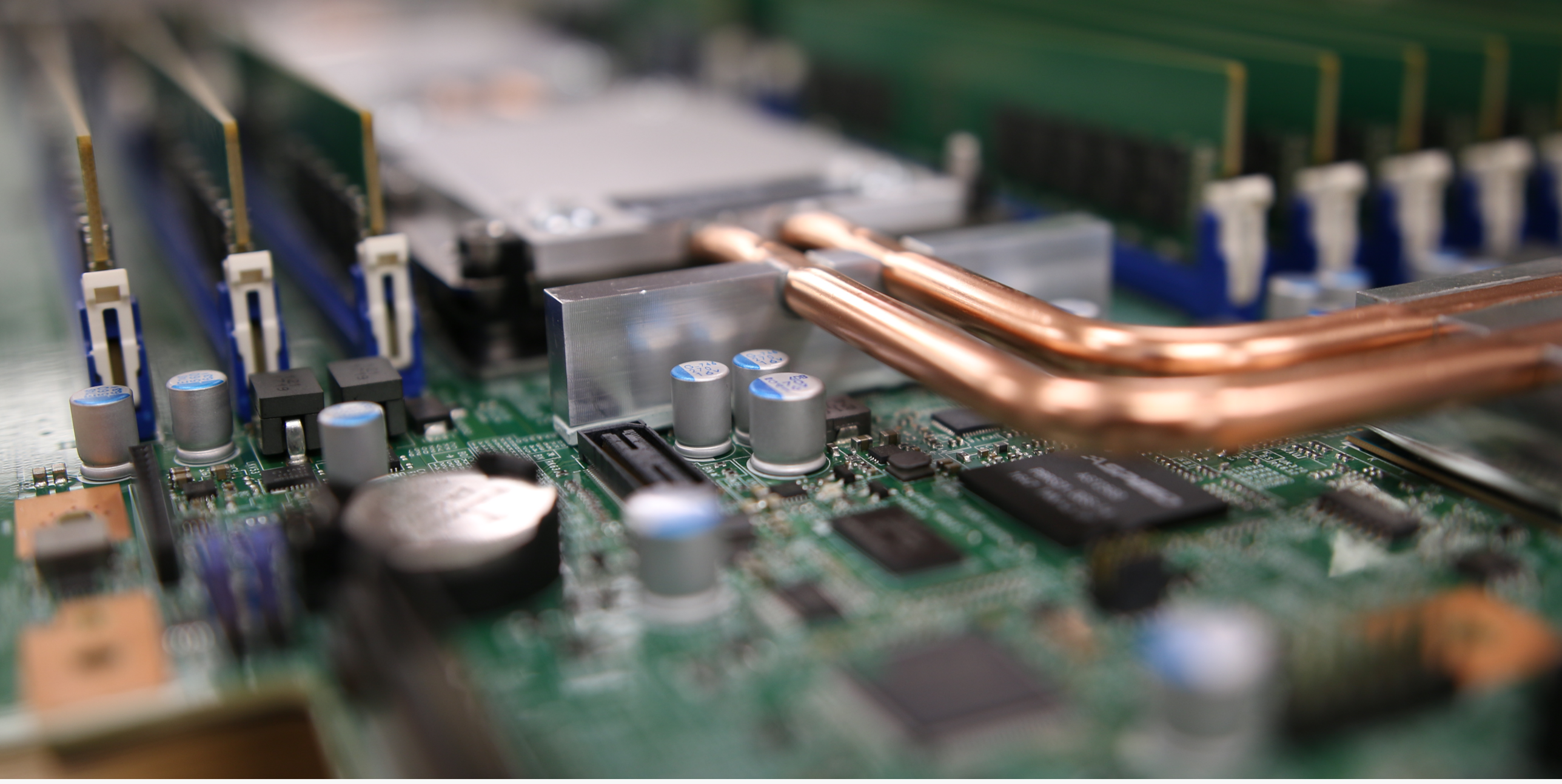


UKQCD perspective

Antonin Portelli

5th of March 2020

Lattice HPC meeting - Dublin, Ireland

THE UNIVERSITY *of* EDINBURGH

Image credit: The University of Edinburgh

- Lattice HPC in the UK
- UKQCD physics programme
- Grid & Hadrons
- Future plans

Lattice HPC in the UK

The DiRAC facility

DiRAC

"DiRAC is the integrated supercomputing facility for theoretical modelling and HPC-based research in particle physics, and astrophysics, cosmology, and nuclear physics […]"

https://dirac.ac.uk

DiRAC 2.5 systems

Data Intensive (Cambridge) - 2.3(CPU) + 1.2(GPU) PFlop/s

Data Intensive (Leicester) - 1(CPU) PFlop/s

Memory Intensive (Durham) - 0.9(CPU) PFlop/s

Extreme Scaling (Edinburgh) - 3.4(CPU) + 0.5(GPU) PFlop/s

DiRAC 3 soon?

The DiRAC facility

Science and Technology Facilities Council

- DiRAC is a UKRI/STFC facility, focused on **Astronomy, Nuclear, Particle and Particle Astrophysics**.

- Computer time is allocated through a yearly peer-reviewed call by the **Ressource Allocation Committee.**

- The RAC is composed by 2 sub-panels of experts (nuclear/particle & astro).

DiRAC lattice allocations

Cambridge (lattice only)

						CSD3 time			CSD3 storage			
Application ID	**SAFE ID**	**Project Title**	**P.I.**	**Start Date**	**End Date**	**CPU / Mhours**	**KNL / khours**	**GPU / khours**	**home / GB**	**work / TB**	**data / TB**	**RSE / month**
PPTM202	dp019	High Precision B physics from lattice QCD (HPQCD)	C. Davies	May '19	Mar '22	50.53			84.21	8.42	505.26	
PPTM203	dp007	Strong dynamics in the structure of matter	R. Horsley	May '19	Mar '22	31.88			500.00	1.05	1.05	
PPTM204	dp008	UKQCD–DWF: physics with dynamical chiral quarks	A. Juettner	May '19	Mar '22			151.70	3.61	1.81	1.81	18.00
PPTM205	dp099	Lattice Holographic Cosmology	A. Portelli	May '19	Mar '20	14.74			736.84	14.74	73.68	
PPTM207	dp051	Hadron Resonances from Lattice QCD	C. Thomas	May '19	Mar '21	15.37			28.21	28.21		
PPSP208	dp136	Simulation of Sp(2N) gauge theories for Composite Higgs models	L. Biagio, E. Bennett	May '19	Mar '20	13.13			7.05	4.94	28.21	5.00
PPSP209	dp098	High-order NSPT for IR conformal theories	L. Del Debbio	May '19	Mar '20	5.89			73.68	36.84		
PPSP210	dp137	Spontaneous Symmetry Breaking in the 3d Thirring Model	S. Hands	May '19	Mar '20	1.00			500.00	0.50		3.00

https://dirac.ac.uk

DiRAC lattice allocations

Edinburgh (all projects)

						time	storage			
Application ID	**SAFE ID**	**Project Title**	**P.I.**	**Start Date**	**End Date**	**ES / Mhours**	**home / GB**	**work / TB**	**data / TB**	**RSE / month**
PPTM201	dp006	Extreme QCD: Quantifying the QCD Phase Diagram IIb	C. Allton	May '19	Mar '22	309.91	57.93	5.79	28.96	3.00
PPTM203	dp007	Strong dynamics in the structure of matter	R. Horsley	May '19	Mar '22	109.22	1456.31	2.91	2.91	
PPTM204	dp008	UKQCD–DWF: physics with dynamical chiral quarks	A. Juettner	May '19	Mar '22	688.83	41747.57	333.98	1603.11	18.00

https://dirac.ac.uk

UKQCD-DWF: ~60 % of Edinburgh service

UKQCD physics programme

General structure

- Mainly focused on **light and heavy flavour physics**, using domain-wall fermions.

- In collaboration with RBC in the US, access to USQCD.

<u>Edinburgh University:</u>
Peter Boyle (BNL)
Luigi Del Debbio
Felix Erben
Vera Gülpers
Nelson Lachini
Michael Marshall
Fionn Ó hÓgáin
Raoul Hodgson
Antonin Portelli
Andrew Yong
Azusa Yamaguchi

<u>University of Southampton:</u>
Nils Asmussen
Jonathan Flynn
Ryan Hill
Andreas Jüttner
James Richings
Chris Sachrajda

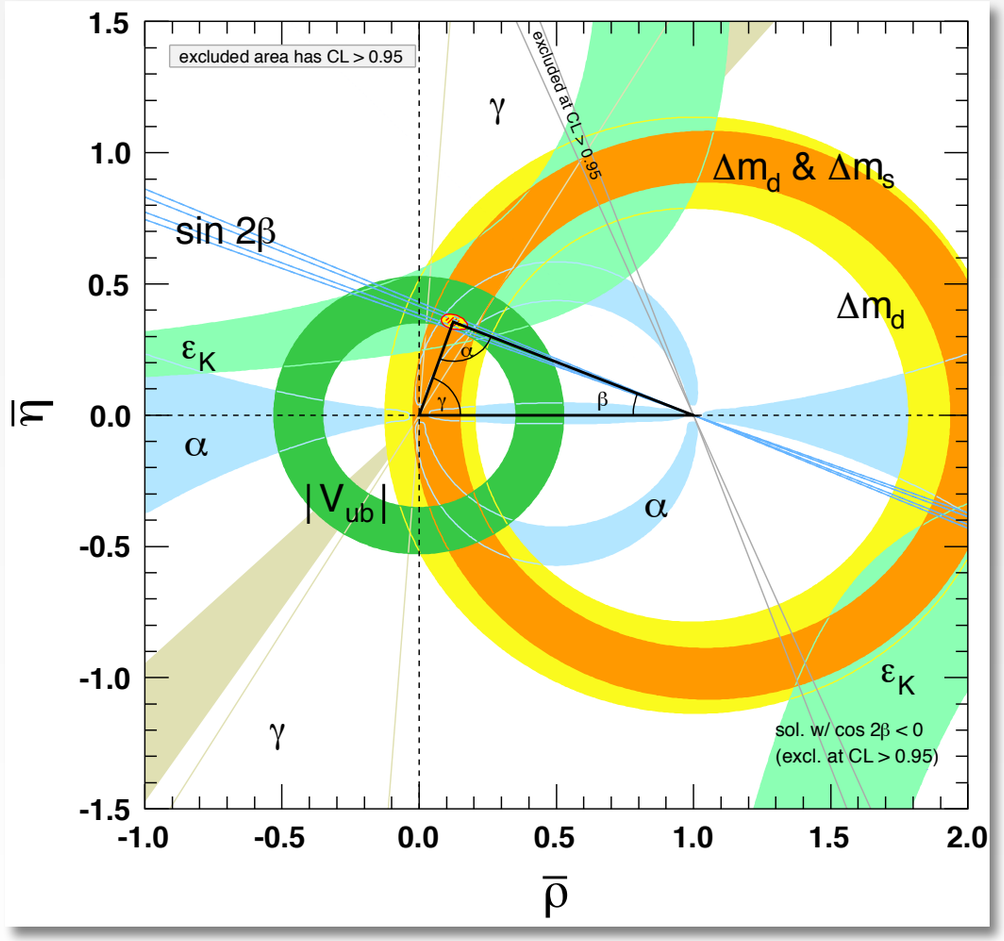
<u>University of Liverpool:</u>
Nicolas Garron

<u>CP3:</u>
Toby Tsang

2 tenured faculty, 4 postdocs coming to Edinburgh 2020-2021

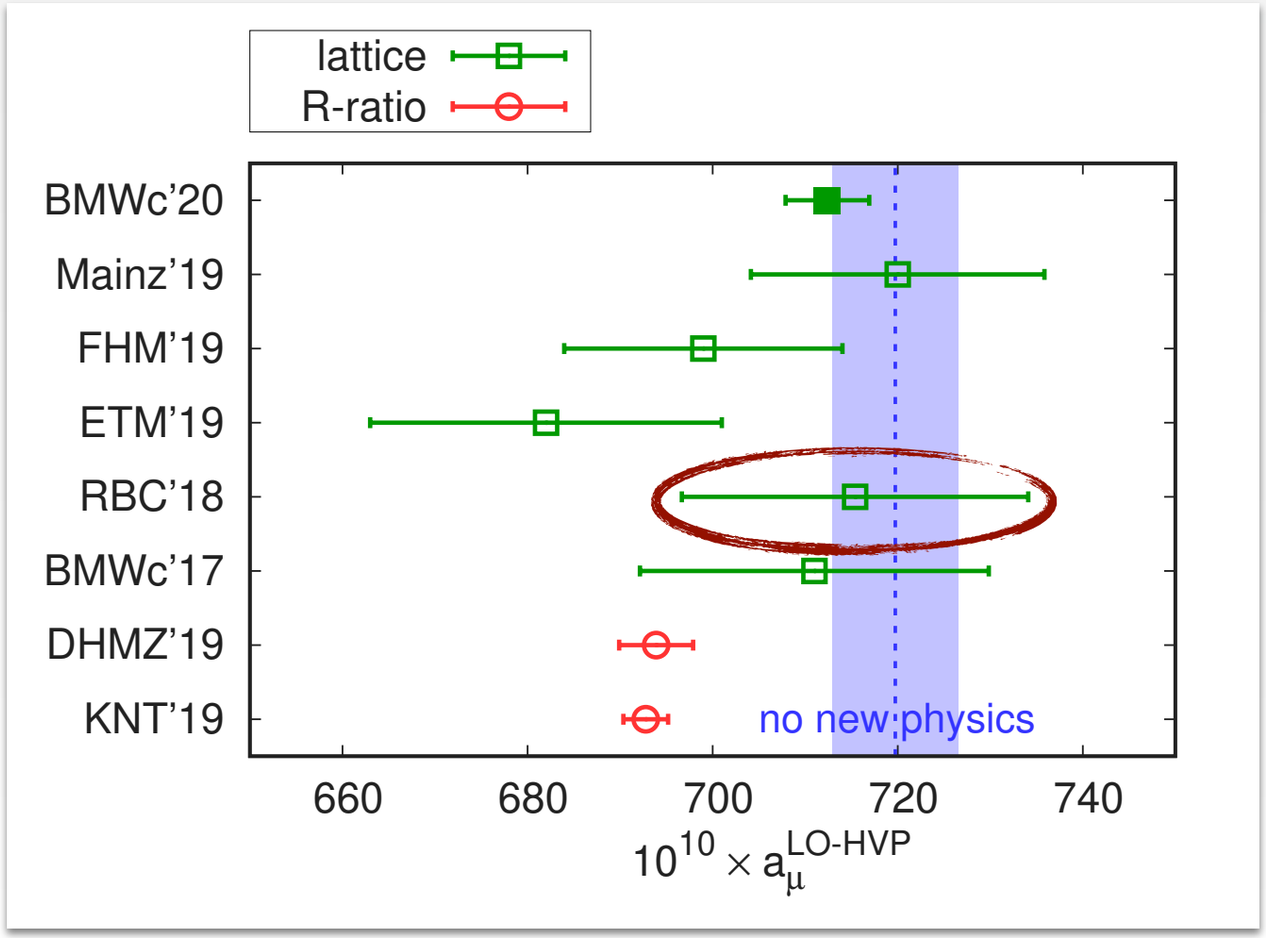
Flavour physics

- Radiative corrections to kaon leptonic and semi-leptonic decays.
- B & D leptonic and semi-leptonic decays.
- B & D bag parameters.
- Light quark masses.
- Rare $K \to \pi \ell^+ \ell^-$ decays.
- Rare $\Sigma \to p \ell^+ \ell^-$ decays.
- $K - \bar{K}$ mixing.



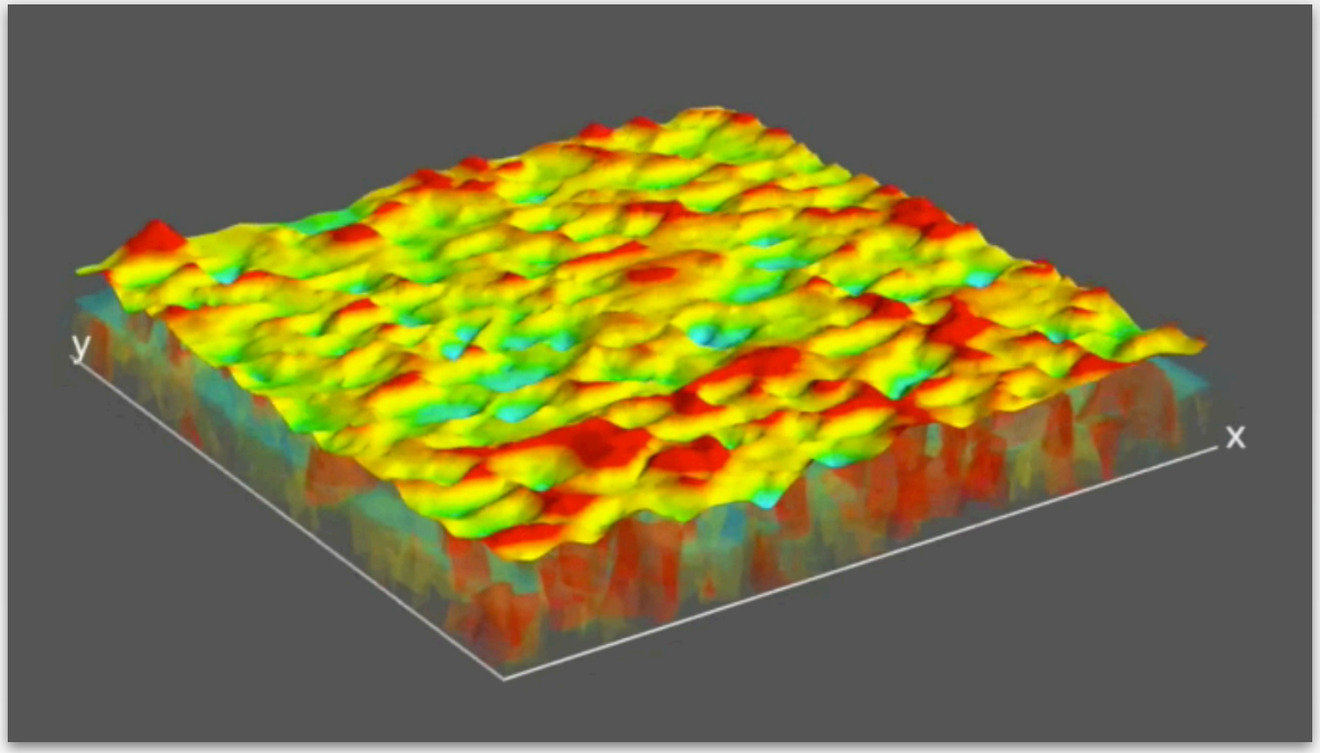
Hadronic physics

- $K\pi$ & $\pi\pi$ scattering at physical quark masses.
- Muon anomalous magnetic moment.



[BMW, arXiv:2002.12347]

BSM physics



[A. Jüttner, private comm.]

- Composite Higgs models, strong Yang-Mills in non-fundamental representations.
- Holographic cosmological models, critical phase of scalar gauge theories in 3D.

Grid & Hadrons

The Grid library

- Free (GPLv2) data parallel C++11 library.
  https://github.com/paboyle/Grid

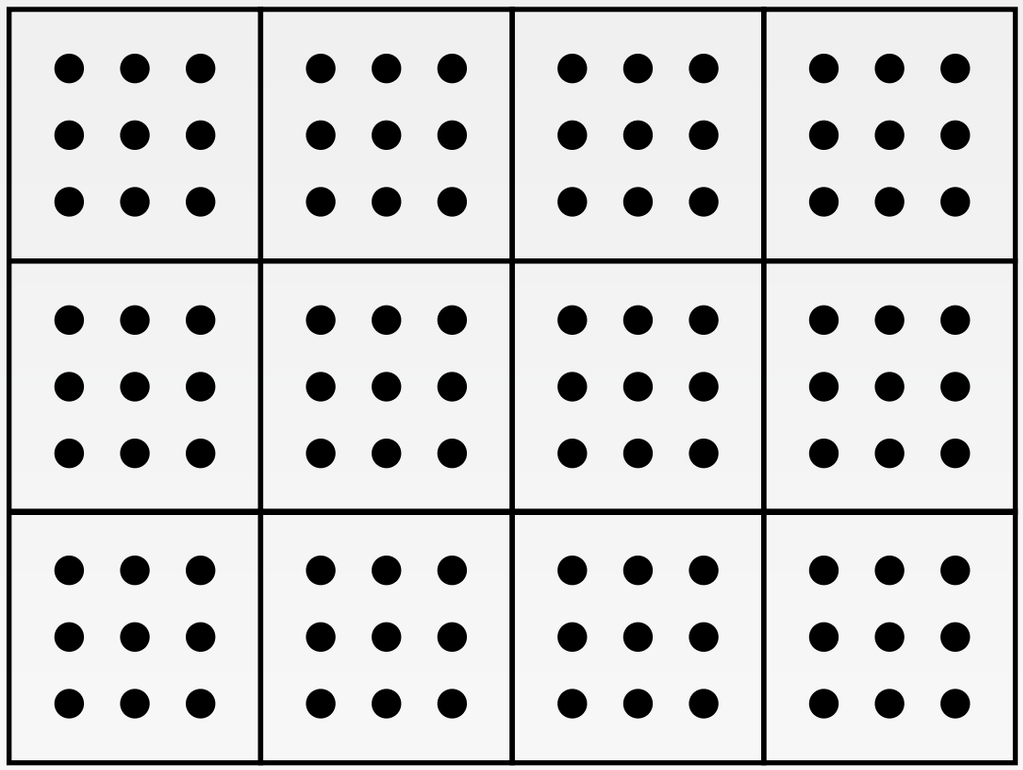
- Multi-platform, most code platform-agnostic.
  SSE, AVX, AVX2, AVX512, QPX, NEONv8, NVIDIA (post-Pascal)

- Implements popular lattice fermion actions
  (Wilson, DWF, Staggered, …)

- Implements many solvers
  (CG (many flavours), multi-grid CG, Lanczos, …)

- Implements full HMC/RHMC interface

Grid lattice layout



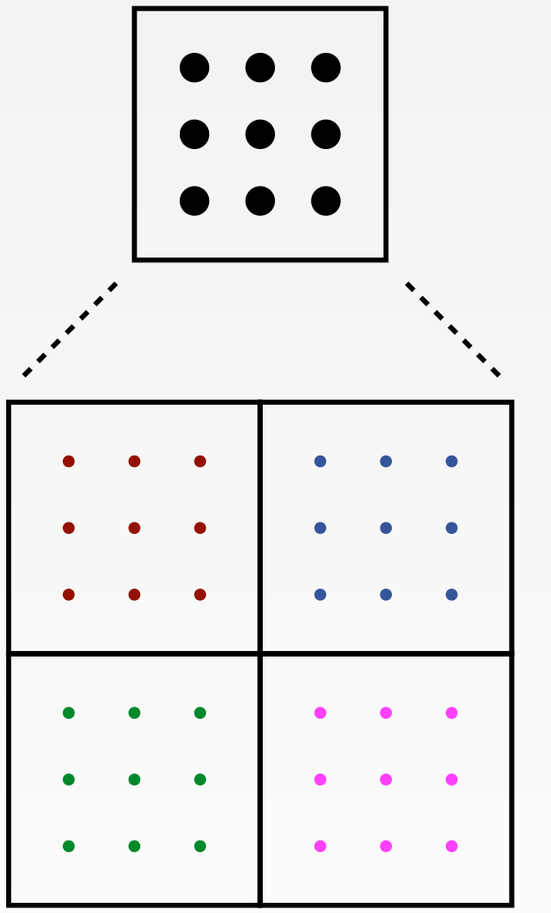
MPI Cartesian layout

High-efficiency halo exchange

Shared buffer and multi-endpoint comms

● = [· · · ·]

SIMD/SIMT vector



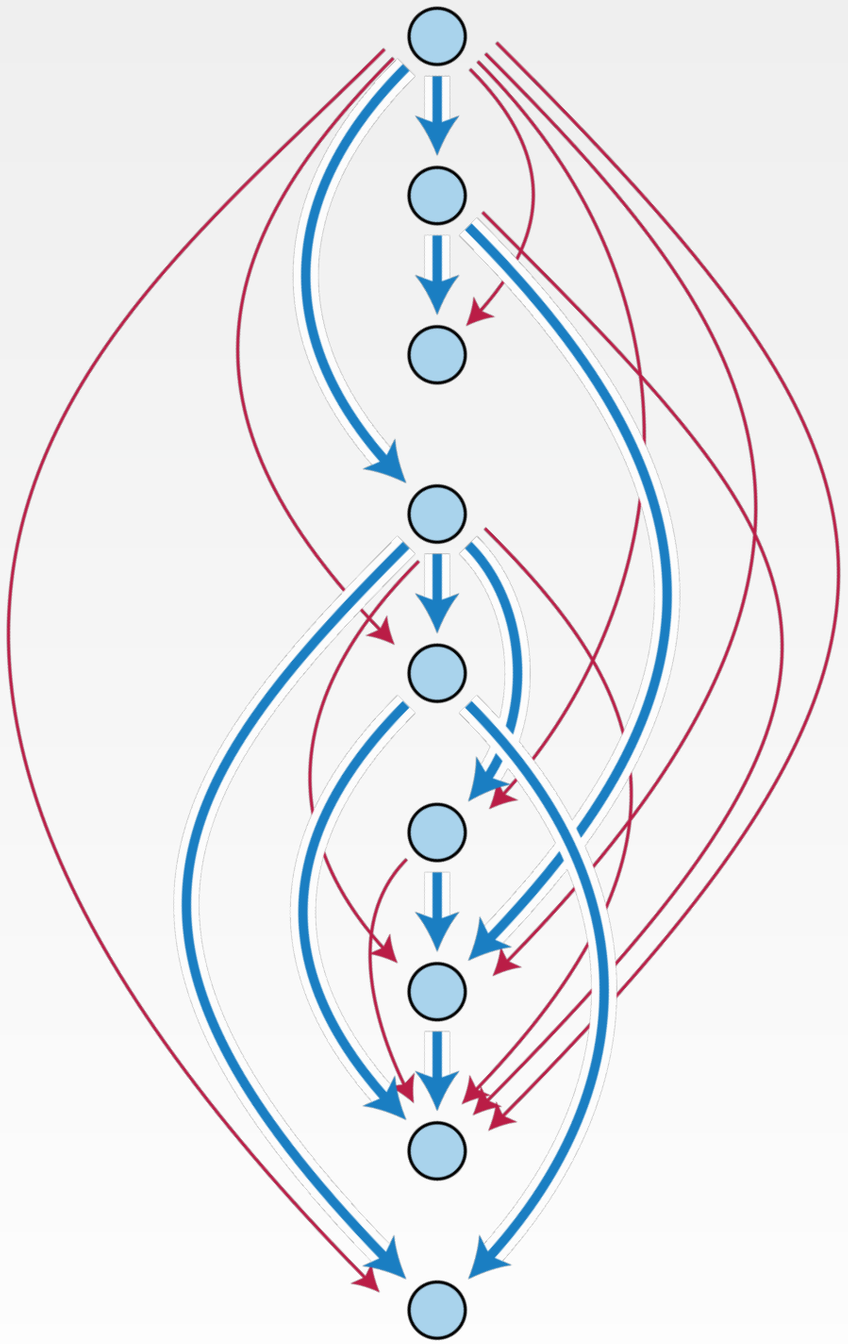
Vectorised layout

Grid lattice expressions

```
C = tr(g5*gSnk*q1*adj(gSrc)*g5*adj(q2));
```

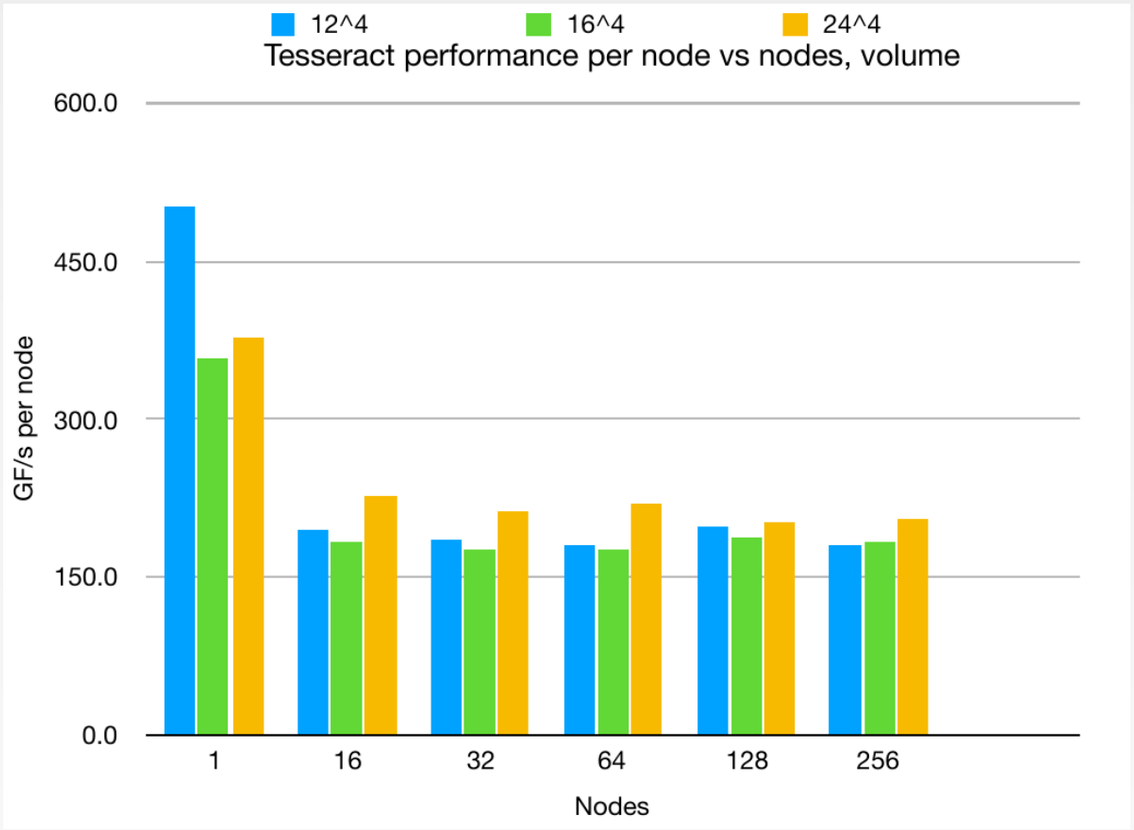
- C++ expression template engine
- Site-wise operation automatically parallelised
- 100% vectorised thanks to vector layout
- Loops over sites multi-threaded
- Symbolic gamma matrix algebra
- High-level circular shift operator & stencil interfaces

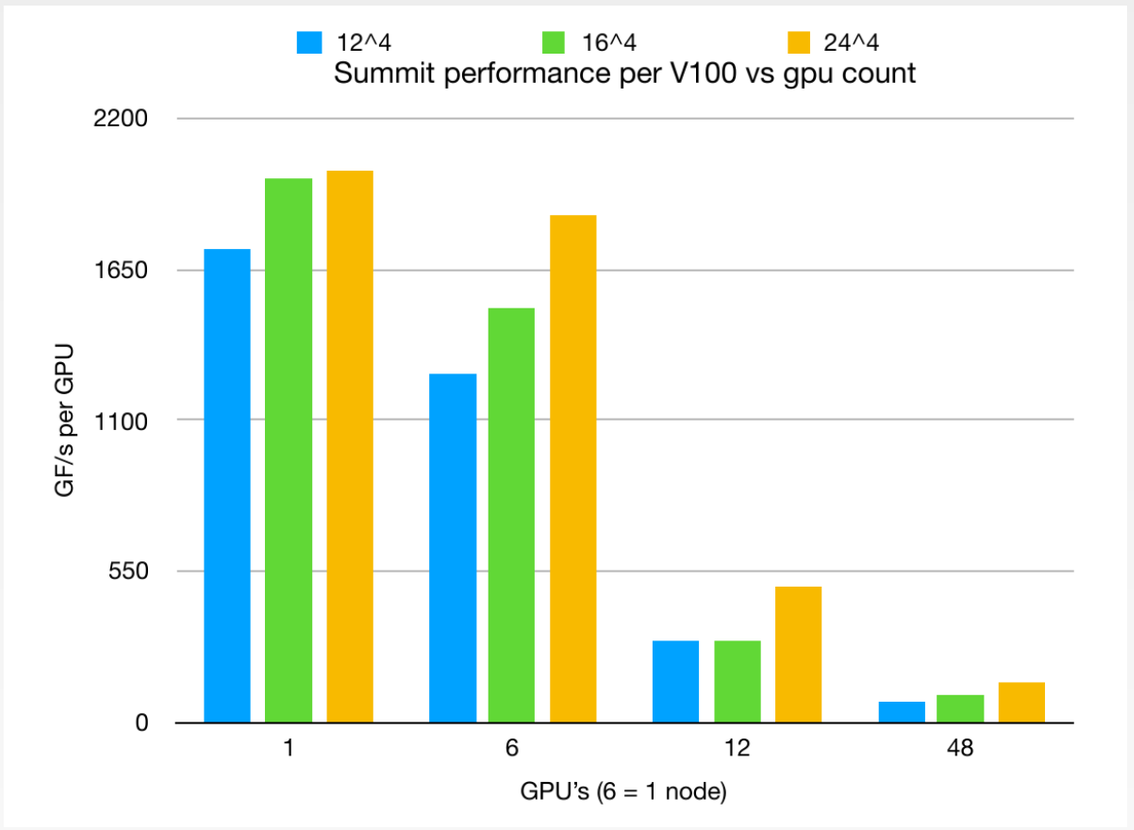
Hadrons



- Measurement steps: modules with inputs/outputs
- Measurement: DAG of modules
- Schedule through topological ordering minimising memory consumption
- Global, generic object store shared by modules
- Part of Grid (Lattice 2019 talk)

Scaling





Grid single precision Dslash, [P. Boyle, USQCD All-Hands Collaboration Meeting 2019]

- DiRAC Extreme Scaling (Tesseract):
  hypercubic network topology (HPE SGI-8600 blades)

Future plans

Radiative corrections

- Radiative corrections to semi-leptonic decays.
- Radiative corrections to 2-body scattering.

Computational challenges

- Volume scaling, **large volumes**.
- Non-trivial phase space, deflation with **non-trivial BCs**.

Hadronic long-distance effects

- Rare decays at high precision.
- Heavy meson rare decays.
- $D \to \pi\pi$ decays.

Computational challenges

- Reliable spectral reconstruction, **very-large volumes**.
- Non-trivial phase space, deflation with **non-trivial BCs**.

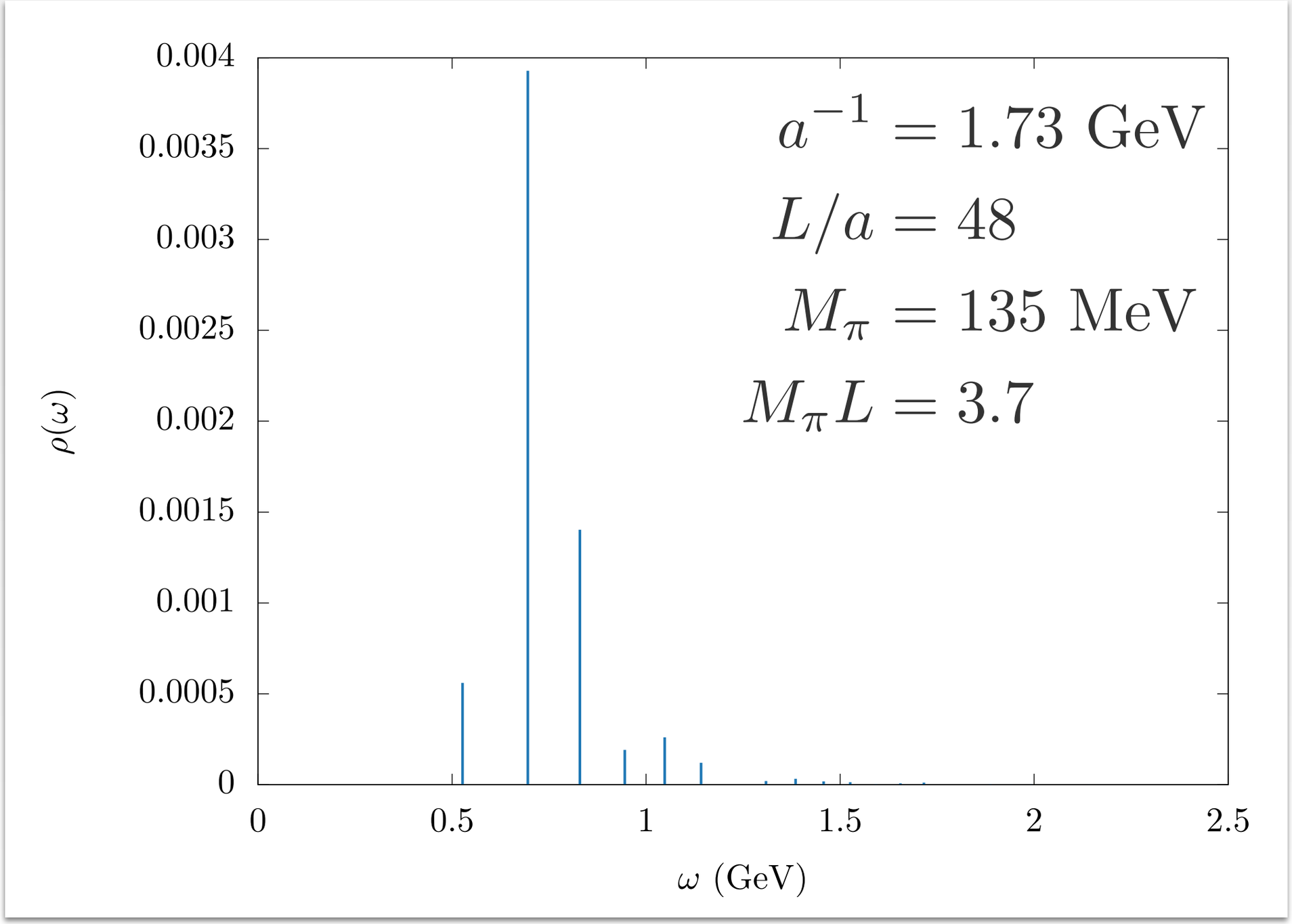
Spectral reconstruction

- Lattice simulation at high density of states.
- Scattering amplitudes beyond GEVP.

Computational challenges

- Reliable **spectral reconstruction methodology**.
- Large to **extremely large volumes**.

Ok, but how large is “very” large?



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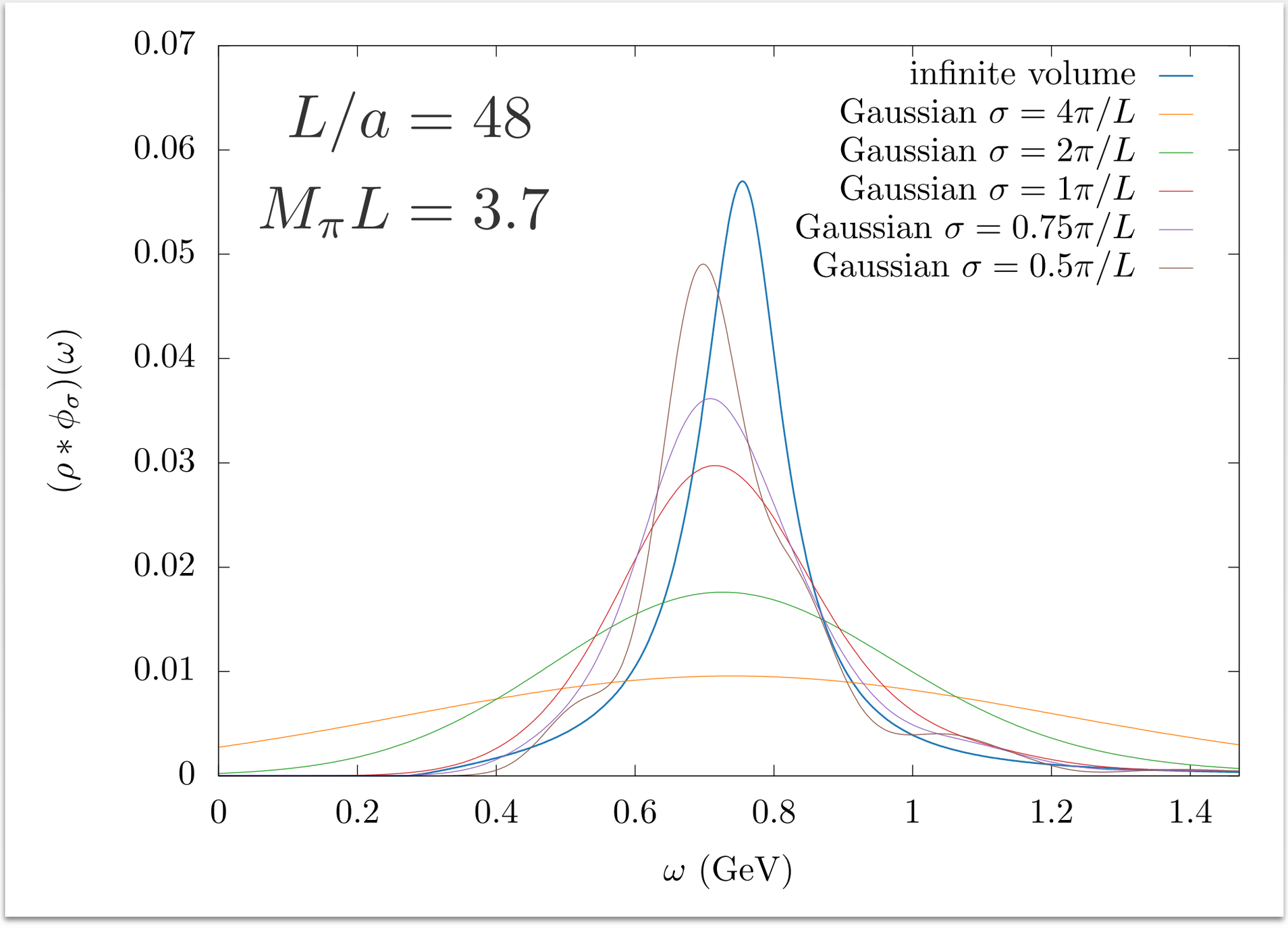

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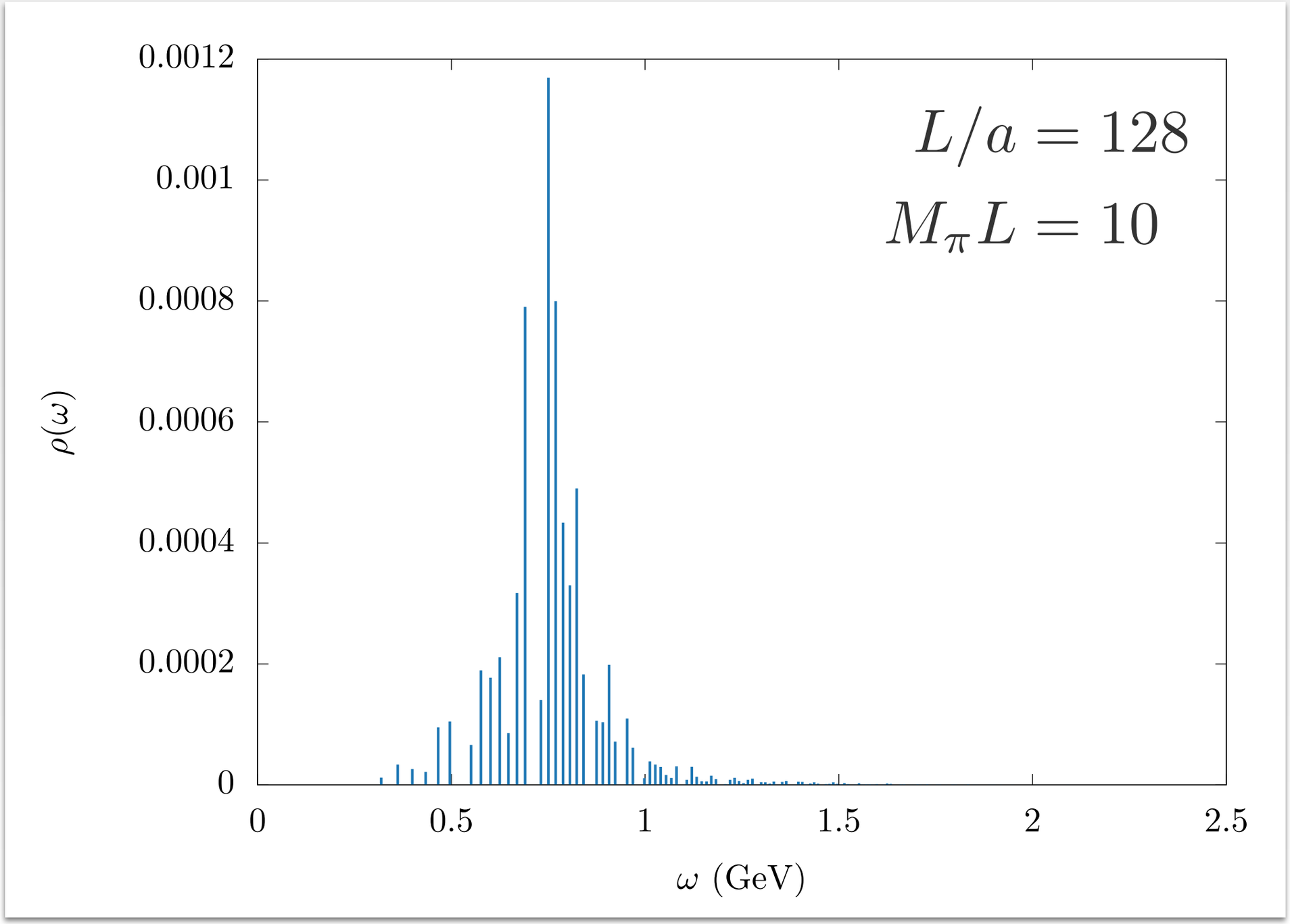

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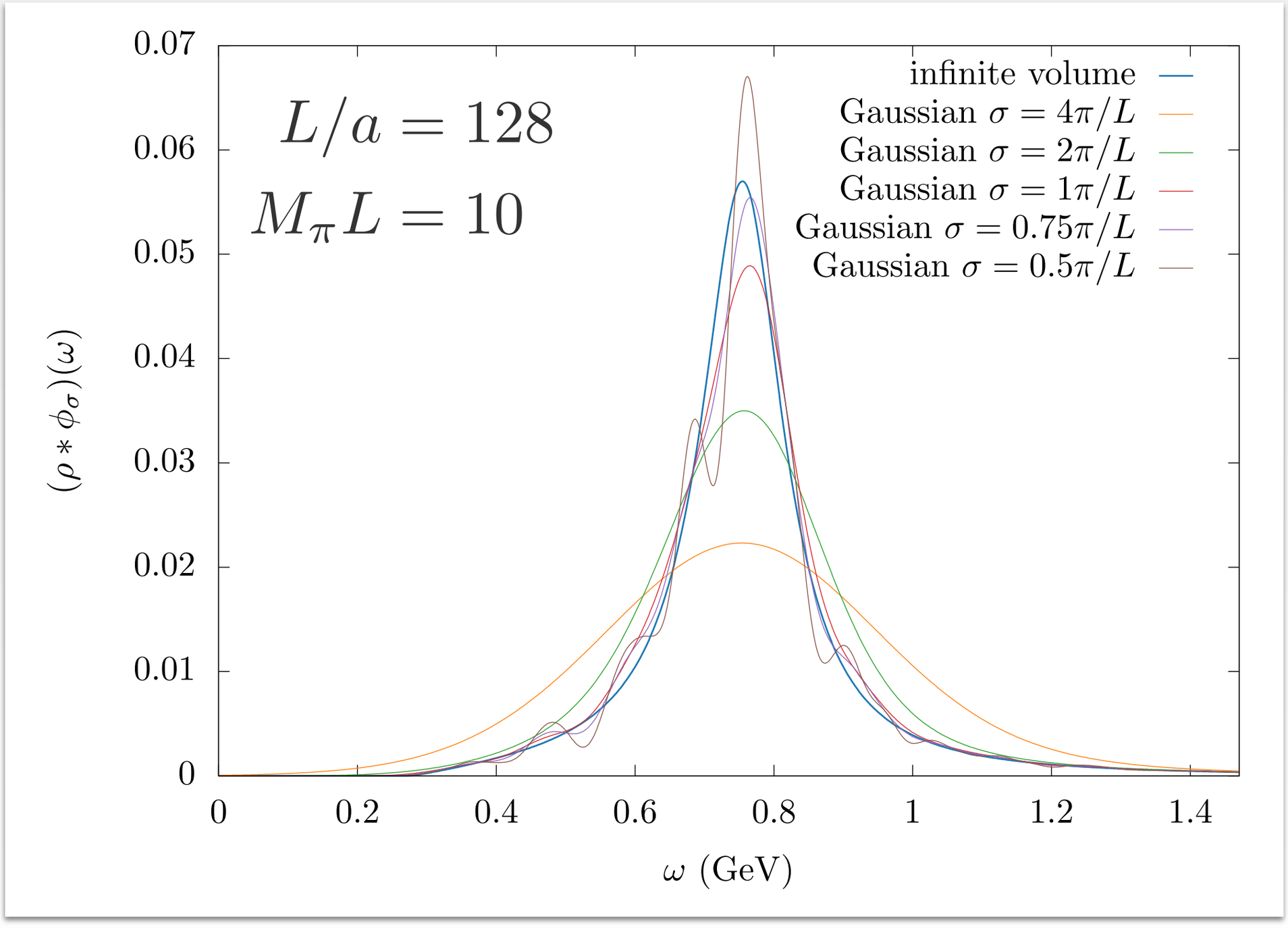

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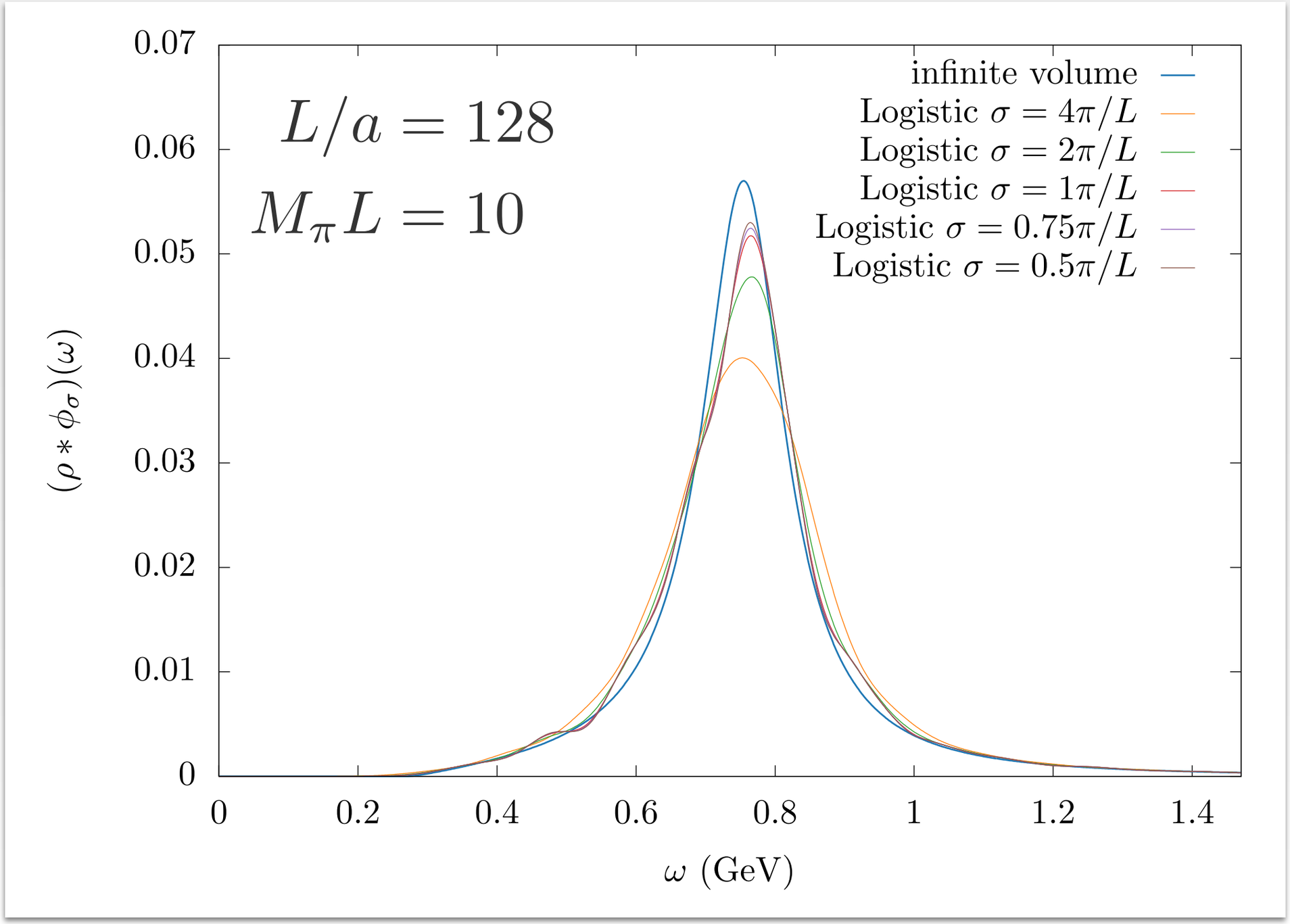

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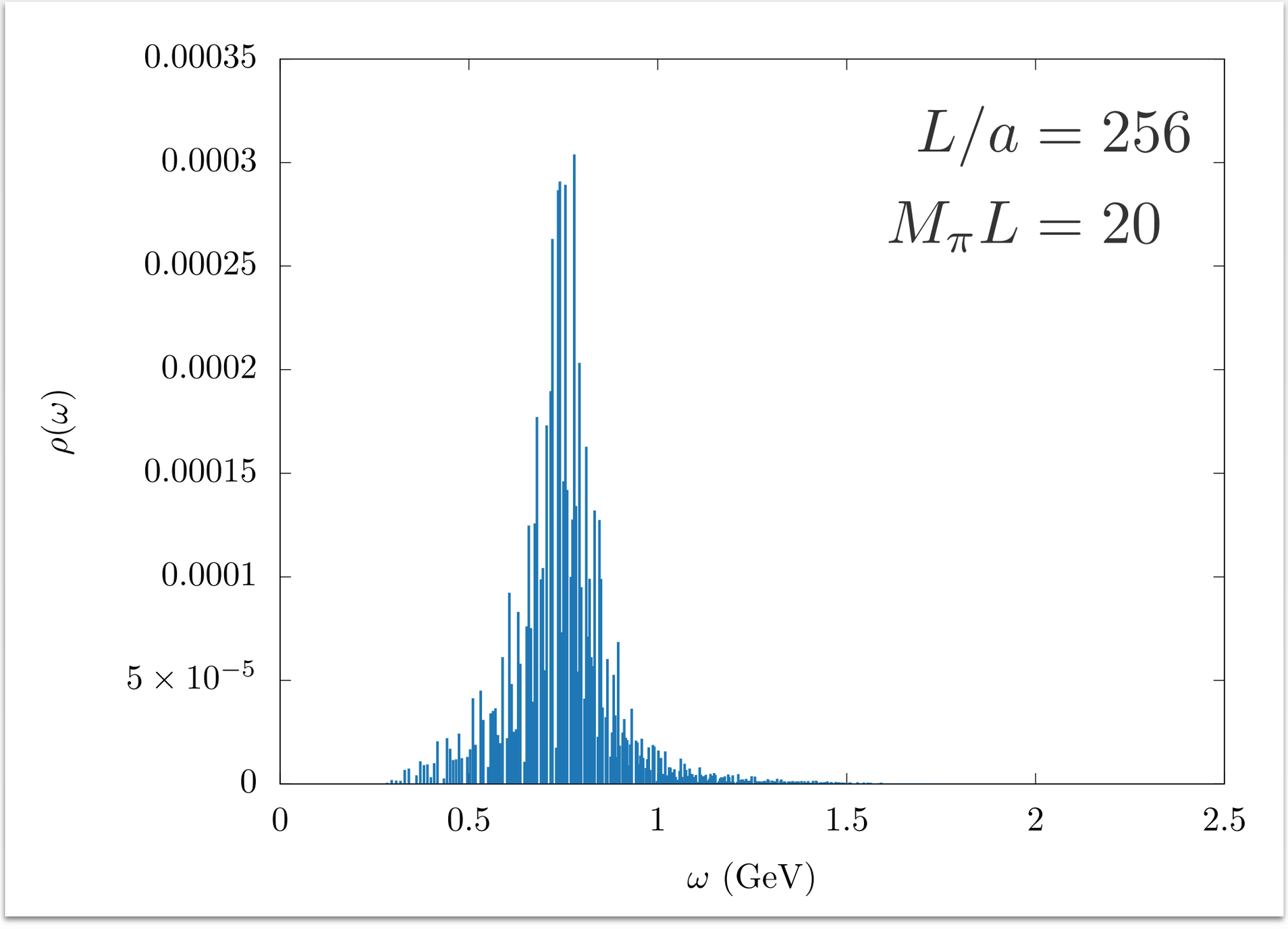

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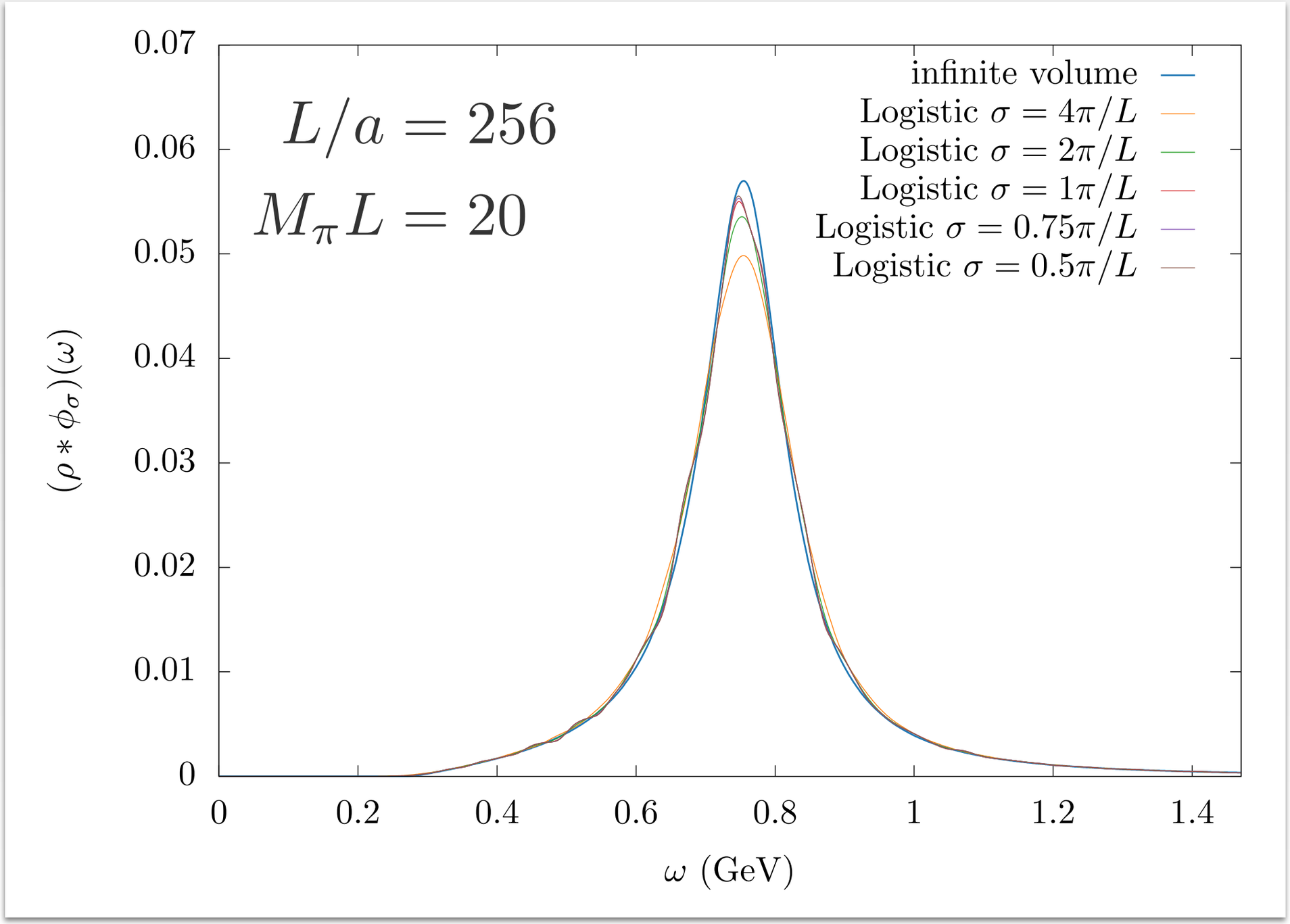
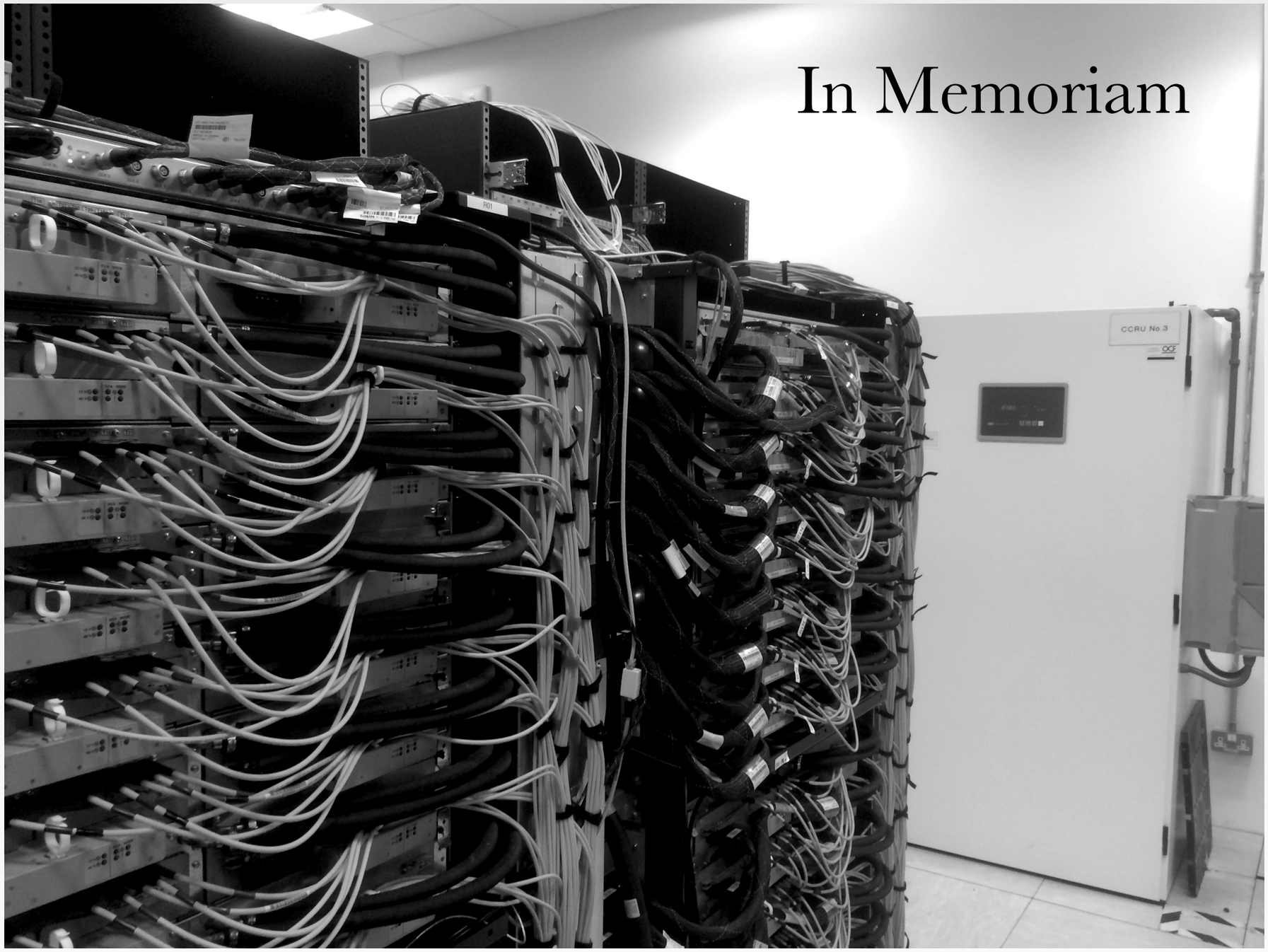


Future HPC requirements

- This is quite rough, but very likely need partitions with **very large memory footprint**.
- Lattice is becoming much more **memory-intensive** that it used to be (deflation, distillation, A2A, etc…)
- **We will still need "real" parallel machines**
  i.e. machines where computation vs. network is balanced, and network is topology-aware.
- NVME is promising for **high-speed FS caching**.
- Balanced parallel machines with GPU?
  (Nvidia bought Mellanox, HPE-Cray Slingshot)



Thank you!

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