Numerical Quantum Physics – Foundations

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April 16, 2023



Organization

- No lectures on: 2023-05-01, 2023-05-18, 2023-05-29, 2023-06-08
- Final examination: One week coding project, most probably 2023-07-24 2023-07-30 (more information later)
- Exercises:
 - Group assignment this week
 - Every second week new sheet
 - First sheet: 2023-04-21
 - Total of 50% points on exercise sheets yields +0.3 bonus for final examination (only if passed)
 - Exercise git: git@gitlab.physik.uni-muenchen.de:nqp/nqp-exercises.git
 - HOME directory for lecture: /project/cip/2023-SS-NQP
- LMU Jupyterhub
 - https://jupyter.physik.uni-muenchen.de
 - Requires two-factor authentification (for instance Google Authenticator)
- Lecture homepage:



Article

Quantum supremacy using a programmable superconducting processor

https://doi.org/10.1038/s41586-019-1666-5

Received: 22 July 2019

Accepted: 20 September 2019

Published online: 23 October 2019

Frank Arute', Kunal Arya', Ryan Babbush', Dave Bacon', Joseph C. Bardin¹², Rami Barends', Rupak Biswas³, Sergio Boixo', Fernando G. S. L. Brandao¹⁴, David A. Buell', Brian Burkett', Yu Chen', Zjun Chen', Ben Chiaro', Roberto Collins', William Courtney', Andrew Dunsworth', Edward Farhi', Brooks Foxen¹⁴, Austin Fowler', Craig Gidney', Marisas Giustina', Rob Graff', Keith Guerin', Steve Habegger', Matthew P. Harrigan', Michael J. Hartmann⁴, Alan Ho', Markus Hoffmann', Trent Huang', Travis S. Humble', Sergei V. Isakov', Evan Jeffrey', Zhang Jiang', Dvir Kafri', Kostyantyn Kechedzhi', Julian Kelly', Paul V. Klimov', Sergey Knysh', Alexander Korotkov¹⁵, Fedor Kostritas', David Landhulis', Mike Lindmark', Erik Lucero', Dmitry Lyskh', Salvatore Mandrà¹⁰, Jarrod R. McClean', Matthew McEwen⁹, Anthory Megrant', Xiao Mi', Kristel Michielsen¹¹⁰, Masoud Mohseni', Josh Mutus', Ofer Naaman', Matthew Neeley', Charles Nell', Murphy Yuezhen Niu', Eric Ostby', Andre Petukhov', John C. Platt', Chris Quintana', Eleanor G. Rieffel³, Pedram Roushan', Nicholas C. Rubin', Daniel Sank', Kevin J. Satzinger', Vadim Smelyanskiv', Kovin J. Sung¹⁰, Matthew D. Trevithick', Amit Vainsencher', Benjamin Villalonga^{11,4}, Theodore White', J. Jamie Yao', John C. Platt', Janser Jacoma', Hartmut Neven's John M. Martinis^{16,4}

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- 69 authors
- 3 Supercomputing clusters
- Data analysis with external collaborators

Large Scale Numerics



Exploration of the ground-state phase diagram of electron-phonon system:

- 180TB raw data
- 5M files of raw data
- 2 Supercomputing clusters



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Analysis by Vincent Mourik (UNSW), Sergey Frolov (Pittsburgh)

Data manipulation and omission in 'Quantized Majorana conductance', Zhang et al, Nature 2018

On November 24th 2019 we received from one of the authors of the now retracted 'Quantized Majorana Conductance' paper in Nature a pdf file with experimental notebook-quality data. Within this pdf file, we found data that appear to contradict the central claim of the paper. We have found that the original source experimental data may have been manipulated, namely cut, as well as cut out and pasted together. Furthermore, entire datasets that contradict the central claim of the Nature paper were suppressed. Our analysis was carried out between December 2019 and March 2020. We are able to publish our analysis now, in March 2021, after the authors of the Nature paper have finalized their retraction and deposited data from their experiment in full on Zenodo.

Central claim from the bold paragraph of the Nature paper:

recent observation⁷ of a peak height close to 2e²/h. Here we report a quantized conductance plateau at 2e²/h in the zero-bias conductance measured in indium antimonide semiconductor nanowires covered with an aluminium superconducting shell. The height of our zerobias peak remains constant despite changing parameters such as the magnetic field and tunnet coupling, indicating that it is a quantized conductance plateau. We distinguish this quantized Majorana peak from possible non-Majorana origins by investigating its robustness

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Setback for Majorana fermion as Microsoft team retracts research paper

by Bob Yirka , Phys.org

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But things can go horribly wrong...

For peer review we need:

- Documentation
- Reproducibility
- Data consistency

And only after that comes the good story!

Large Scale Numerics



Distributed version control systems

- Control system
 - Content tracking
 - Backup functionality



Distributed version control systems

- Control system
 - Content tracking
 - Backup functionality
- Version control system
 - Structured project evolution
 - Roll-back/Push-forward functionality



Distributed version control systems

- Control system
 - Content tracking
 - Backup functionality
- Version control system
 - Structured project evolution
 - Roll-back/Push-forward functionality
- Distributed version control system
 - Parallel development branches
 - Branching/Merging from common project base
 - Issue fixing and task assignments



Distributed version control systems at the example of Git

- Control system
 - git add, git stash
 - git clone, git push, git pull



Distributed version control systems at the example of Git

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 - git add, git stash
 - git clone, git push, git pull
- Version control system
 - git commit
 - git checkout



Distributed version control systems at the example of Git

- Control system
 - git add, git stash
 - git clone, git push, git pull
- Version control system
 - git commit
 - git checkout
- Distributed version control system
 - git branch, git merge, git cherry-pick, git reset
 - git log



Large Scale Numerics

High Performance Computing (HPC): When do you really need a cluster?

Parallelization! But it's not all the same ...



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- OpenMP parallelization (single node computation)
 - Shared memory, dependent processes
 - Large RAM per CPU ratio



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- MPI parallelization (multi node computation)
 - Independent processes with independent memory
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- OpenMP parallelization (single node computation)
 - Shared memory, dependent processes
 - Large RAM per CPU ratio
- MPI parallelization (multi node computation)
 - Independent processes with independent memory
 - Fast interconnect between nodes
- Architecture specific solutions
 - Graphics Processing Unit cluster
 - <u>Tensor</u> <u>Processing</u> <u>Unit</u> cluster

PRX QUANTUM 3, 020331 (2022)

Editors' Suggestion

Simulation of Quantum Many-Body Dynamics with Tensor Processing Units: Floquet Prethermalization

Alan Morningstar^(*),^{1,2,*} Markus Hauru^(*), ² Jackson Beall^(*), ² Martin Ganahl,² Adam G.M. Lewis,² Vedika Khemani,³ and Guifre Vidal²

Department of Physics, Princeton University, Princeton, New Jersey 08544, USA
 ²Sandbox@Alphabet, Mountain View, California 94043, USA
 ³Department of Physics, Stanford University, Stanford, California 94305, USA



You have a code but how to use it?

- Write jobscript which performs desired computation
 - Wrap computation into a few commands
 - Specify hardware/software requirements, runtime, used resources, ...
 - Setup/Change job directories



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 - Specify hardware/software requirements, runtime, used resources, ...
 - Setup/Change job directories
- Submit jobscript to queueing system
 - <u>Simple Linux Utility for Resource</u> <u>Management (SLURM)</u>
 - Specify job dependencies
 - Wait 🛡 ...



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 - <u>Simple Linux Utility for Resource</u> <u>Management (SLURM)</u>
 - Specify job dependencies
 - Wait 🛡 ...
 - ...until 🛡 ...finished 🛡
 - sinfo, squeue, scontrol, ...



SLURM example for ASC cluster

• Open SSH-tunnel to login-node

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mkdir: cannot create directory '/scratch-local': Permission denied schestion_postelle/gis=v=logind0:=4

SLURM example for ASC cluster

- Open SSH-tunnel to login-node
- Setup SLURM jobscript
 - Specify SLURM parameter with preceeding #SBATCH
 - Repeated violation of job constraints reduces job priorities
 - Checkout available node types to avoid impossible constraints

#!/bin/bash

```
#SBATCH --export=ALL
#SBATCH --mail-type=ALL
#SBATCH --mail-user=sebastian.paeckel@physik.uni-muenchen.de
#SBATCH --partition=th-ws,th-cl,cluster,large
#SBATCH --constraint=avx2
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
```

```
#SBATCH --time=3-00:00:00
#SBATCH --mem=126
##SBATCH --chdir=/project/th-scratch/s/Sebastian.Paeckel/
##SBATCH --output=/project/th-scratch/s/Sebastian.Paeckel/
##SBATCH --error=/project/th-scratch/s/Sebastian.Paeckel/
```

```
echo Hello world from $(hostname)
```

SLURM example for ASC cluster

- Open SSH-tunnel to login-node
- Setup SLURM jobscript
 - Specify SLURM parameter with preceeding #SBATCH
 - Repeated violation of job constraints reduces job priorities
 - Checkout available node types to avoid impossible constraints
- Submit job to queue using
 - sbatch for non-interactive jobs
 - srun/salloc for interactive jobs
- Watch job status using squeue

Sabastian.Packal@th-ab-lawabp31:/Documents/Teaching/nap-lecture/lectures/chapter_15 sub Sabastian.Packal@cip-sv-login.cip.physik.uni-mumchan.de Warning: Persenently adad the RBA host kay for IP address '10.55.21.53' to the list of known hosts. Sebastian.Packal@cip-sv-Dgin.cip.physik.ut-mumchen.de's parseroid

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File systems at ASC cluster

- Always check your quota!
- If home directory is full → account de-facto dead (with all your data)!

(sepastian.paeckei@cip-sv-ioginez:~\$ quota									
ţ	ath type	I	SPACE: used	soft	hard	I	FILES: used	soft	hard
/project/ /r	cip lustre	-	2.4 Gi 5.1 Gi	300.0 Gi	400.0 Gi 40.0 Gi		37043	75000	100000

Large Scale Numerics

High Performance Computing (HPC): How to use cluster?

File systems at ASC cluster

- Always check your quota!
- If home directory is full → account de-facto dead (with all your data)!
- Virtual drives
 - always available
 - smaller bandwidth $\sim 10-100 {\rm MBit/s}$
- Local drives
 - only available on current machine
 - large bandwidth > 1GBit/s
- Backups are important but expensive if number of files is large (file limit)

Mount	Speed	Availability	Total Size	def. Quota	Backup	Period of storage
/home	**	network wide (see <u>details</u>)	8 TB	40GB	snapshot & tape	unlimited
/project/theorie	**	network wide	30 TB	100 GB	snapshot & tape	unlimited
/scratch	***	network wide	67 TB	500 GB	snapshot	unlimited
/scratch-local	****	local	depending	no	no	Deletion after 30 days
/tmp	*****	local	depending	no	no	Deletion after 7 days or the next reboot

Working on problem sheets using the LMU Jupyterhub

LMU Jupyterhub provides a simple user interface for interactive SLURM jobs at the ASC cluster

• Before login set up two-factor authentification

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Working on problem sheets using the LMU Jupyterhub

LMU Jupyterhub provides a simple user interface for interactive SLURM jobs at the ASC cluster

- Before login set up two-factor authentification
- Setup job specifics
 - Choose cluster
 - Specify hardware: CPUs, RAM
 - Choose max. runtime

Job Parameters

PARAMETER	VALUE
Requested number of logical CPUs (max. avail.: 40): We use Hyper-threading on most computers, e.g., one core has two logical CPUs. Cores are always allocated completely:	2
GPU Type: Select the type of GPU you want to use. Some partitions may contain different types. This setting is ignored, if the number of GPUs is zero.	A40 ~
Requested number of GPUs (max. avail.: 2): If you request more than one, please make sure that you know how to use them in parallel. We use the environment variable science.com science.com science.com science.com science.com <a href="https://wwwwwwwwwwwwwwwwwwwwwwwwwwwwwwwwwww</th> <th>0</th>	0
Requested memory (max. avail.: 613 GB): Memory is an expensive and limited resource. Request only as much as you really need.	4 0 GB
Requested runtime in hours (max. avail.: 48 h):	12 🖸 h
Environment Costum modifications can be made by providing a file <i>a</i> /jupy(crhuk, environment, sh.) If existed, this file will be sourced within the SLUMB poblekov the Jupyreland is started. It can contain additional reduite load <i>a</i> , command or <i>any</i> other modifications of the environment.	python/3.10-2022.08 v
Reservation:	none v

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Working on problem sheets using the LMU Jupyterhub

LMU Jupyterhub provides a simple user interface for interactive SLURM jobs at the ASC cluster

- Before login set up two-factor authentification
- Setup job specifics
 - Choose cluster
 - Specify hardware: CPUs, RAM
 - Choose max. runtime
- In terminal: initialize environment
 - First login: Create symbolic link to lecture's home directory:
 - ln -s /project/cip/2023-SS-NQP/ ~/2023-SS-NQP
 - Load default modules: source ~/2023-SS-NQP/init_modules.sh

