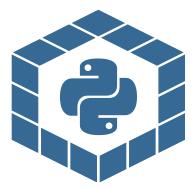
Status of Grid Python Toolkit (GPT)

Christoph Lehner (Uni Regensburg)

https://github.com/lehner/gpt

July 31st, 2023 - Lattice 2023

Grid Python Toolkit (GPT)



https://github.com/lehner/gpt

 A toolkit for lattice QCD and related theories as well as QIS (a parallel digital quantum computing simulator) and Machine Learning

- Python frontend, C++ backend
- Built on Grid data parallelism (MPI, OpenMP, SIMD, and SIMT)

Code co-authors:

- M. Bruno
- D. Richtmann
- T. Blum
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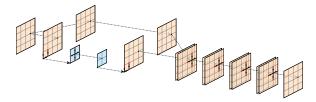
What's new since lattice 2022?

What is new since 2022 (1/3):

New Machine Learning features such as

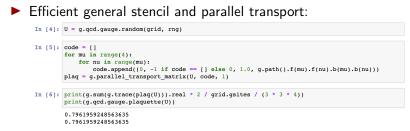
- Adam optimizer
- gauge-equivariant (local) parallel-transport layers
- gauge-equivariant (un)pooling layers
- classical multi-grid blocking layers

motivated by multi-grid gauge-equivariant models such as arXiv:2304.10438, arXiv:2302.05419 (to appear in PRD)



see also Tilo's talk today at 5pm in Algorithms session.

What is new since 2022 (2/3):



- Twisted Mass Fermions + DSDR term
- Quadruple precision global reduction support via Dekker tuples:

```
grid = g.grid([4,4,4,4], g.double)
```

 \Rightarrow

grid = g.grid([4,4,4,4], g.double_quadruple)

What is new since 2022 (3/3):

Performance on LUMI-G and Frontier (1 node):

Com	Initialized GPT /right (C) 2020 Christoph Lehner
GPT :	6.073338 s : : DWF Dslash Benchmark with : fdimensions : [64, 32, 32, 32] : precision : single : Ls : 12
GPT :	16.216618 s : 1000 applications of Dhop : Time to complete : 3.72 s : Total performance : 8926.87 GFlops/s : Effective memory bandwidth : 6167.65 GB/s
GPT :	16.217514 s : : DWF Dslash Benchmark with : fdimensions : [64, 32, 32, 32] : precision : double : Ls : 12
GPT :	27.783497 s : 1000 applications of Dhop : Time to complete : 8.45 s : Total performance : 3929.23 GFlops/s : Effective memory bandwidth : 5429.48 GB/s
	Finalized GPT

15 TF/s/node possible without inter-GCD communication. 5 TF/s/node in strong scaling up to 64 nodes for $64^3\times256$ problem size!

Overview 2020 - 2023

Guiding principles:

Performance Portability

common Grid-based framework for current and future (exascale) architectures

Modularity / Composability

build up from modular high-performance components, several layers of composability, "composition over parametrization"

Layout and dependencies

Python script / Jupyter notebook

gpt (Python)

- Defines data types and objects (group structures etc.)
- Expression engine (linear algebra)
- Algorithms (Solver, Eigensystem, ...)
- File formats
- · Stencils / global data transfers
- QCD, QIS, ML subsystems

cgpt (Python library written in C++)

- Global data transfer system (gpt creates pattern, cgpt optimizes data movement plan)
- Virtual lattices (tensors built from multiple Grid tensors)
- Optimized blocking, linear algebra, and Dirac operators
- Vectorized ranlux-like pRNG (parallel seed through 3xSHA256)



The QCD module

Example: Load QCD gauge configuration and test unitarity

Here: expression first parsed to a tree in Python (gpt), forwarded as abstract expression to C++ library (cgpt) for evaluation

Example: create a pion propagator on a random gauge field

```
# double-precision 8^4 arid
qrid = q.qrid([8,8,8,8], q.double)
# pRNG
rng = g.random("seed text")
# random gauge field
U = q.qcd.qauge.random(grid, rnq)
# Mobius domain-wall fermion
fermion = g.gcd.fermion.mobius(U, mass=0.1, M5=1.8, b=1.0, c=0.0, Ls=24,
                               boundary phases=[1,1,1,-1])
# Short-cuts
inv = g.algorithms.inverter
pc = q.qcd.fermion.preconditioner
# even-odd-preconditioned CG solver
slv 5d = inv.preconditioned(pc.eo2 ne(), inv.cq(eps = 1e-4, maxiter = 1000))
# Abstract fermion propagator using this solver
fermion propagator = fermion.propagator(slv 5d)
# Create point source
src = q.mspincolor(U[0].grid)
g.create.point(src. [0, 0, 0, 0])
# Solve propagator on 12 spin-color components
prop = q(fermion propagator * src)
# Pion correlator
q.message(q.slice(q.trace(prop * q.adj(prop)), 3))
```

Example: solvers are modular and can be mixed

General design principle: use modularity of python code instead of large number of parameters to configure solvers/algorithms; Python can also be used in configuration files

```
# Create an coarse-grid deflated, even-odd preconditioned CG inverter
# (eig is a previously loaded multi-grid eigensystem)
sloppy_light_inverter = g.algorithms.inverter.preconditioned(
    q.gcd.fermion.preconditioner.eo1 ne(parity=q.odd),
   q.algorithms.inverter.sequence(
        g.algorithms.inverter.coarse_deflate(
            eig[1],
            eiq[0].
            eig[2],
            block=200,
        ),
        q.algorithms.inverter.split(
            g.algorithms.inverter.cg({"eps": 1e-8, "maxiter": 200}),
            mpi_split=[1,1,1,1],
        ).
   ),
```

Further example: Multi-Grid solver

```
def find near null vectors(w, cgrid):
    slv = i.fgmres(eps=1e-3, maxiter=50, restartlen=25, checkres=False)(w)
    basis = g.orthonormalize(
        rng.cnormal([g.lattice(w.grid[0], w.otype[0]) for i in range(30)])
    null = g.lattice(basis[0])
    null[:] = 0
    for h in basis:
        slv(b, null)
    g.gcd.fermion.coarse.split chiral(basis)
    bm = q.block.map(cgrid, basis)
    bm.orthonormalize()
    bm.check orthogonality()
    return hasis
mg_setup_3lvl = i.multi_grid_setup(
    block_size=[[2, 2, 2, 2], [2, 1, 1, 1]], projector=find_near_null_vectors
)
wrapper solver = i.fgmres(
    {"eps": 1e-1, "maxiter": 10, "restartlen": 5, "checkres": False}
smooth_solver = i.fgmres(
    {"eps": 1e-14, "maxiter": 8, "restartlen": 4, "checkres": False}
coarsest solver = i.fgmres(
    {"eps": 5e-2, "maxiter": 50, "restartlen": 25, "checkres": False}
mg 3lvl kcycle = i.sequence(
     i.coarse grid(
        wrapper_solver.modified(
             prec=i.sequence(
                 i, coarse grid(coarsest solver, *mg setup 3lvl[1]), smooth solver
         ),
         *mg setup 3lvl[0].
     ),
     smooth solver.
```

All algorithms implemented in Python – Example: Euler-Langevin stochastig DGL integrator

```
21
22
     class langevin_euler:
         @g.params_convention(epsilon=0.01)
        def __init__(self, rng, params):
24
             self.rng = rng
26
             self.eps = params["epsilon"]
28
        def call (self, fields, action):
29
             qr = action.gradient(fields, fields)
30
             for d, f in zip(qr, fields):
31
                 f @= q.qroup.compose(
32
                     -d * self.eps
33
                     + self.rng.normal element(g,lattice(d)) * (self.eps * 2.0) ** 0.5.
                     f.
34
35
                 )
36
```

Implemented algorithms:

- ▶ BiCGSTAB, CG, CAGCR, FGCR, FGMRES, MR solvers
- Multi-grid, split-grid, mixed-precision, and defect-correcting solver combinations
- Coarse and fine-grid deflation
- Implicitly restarted Arnoldi and Lanczos, power iteration
- Chebyshev polynomials
- All-to-all vector generation
- SAP and even-odd preconditioners
- MSPCG (additive Schwarz)
- Gradient descent, non-linear CG, Adam optimizers
- Runge-Kutta integrators, Wilson flow
- Fourier acceleration
- Coulomb and Landau gauge fixing
- Domain-wall–overlap transformation and MADWF
- Symplectic integrators (leapfrog, OMF2, and OMF4)
- Markov: Metropolis, heatbath, Langevin, (DD-)HMC

Implemented fermion actions:

- Domain-wall fermions: Mobius and zMobius
- Twisted-mass fermions

})

 Wilson-clover fermions both isotropic and anisotropic (RHQ/Fermilab actions); Open boundary conditions available

Example: stout-smeared heavy-quark Mobius DWF

```
# load configuration
U = g.load(config)
qrid = U[0].qrid
# smeared aauae link
U \text{ stout} = U
for n in range(3):
    U_stout = q.qcd.gauge.smear.stout(U_stout, rho=0.1)
fermion_exact = q.qcd.fermion.mobius(U_stout,{
    "mass": 0.6.
    "M5": 1.0.
    "b": 1.5,
    "c": 0.5.
    "Ls": 12.
    "boundary_phases": [1.0, 1.0, 1.0, -1.0],
```

Performance

Benchmark results committed to github

https://github.com/lehner/gpt/tree/master/benchmarks/ reference

^{9.9} master → gpt / benchmarks / reference /		Rank	System	Cores	Rmax (PFlog/s)	Rpeak (PFlop/s)	Power (kW)
😫 lehner supermuc-ng timing 📖	on Apr 1 🕚 History	1	Prontier - HPE Cray EX235a, AND Optimized 3rd Generation EPYC 64C 20Hz, AND Instinct MI250X, Stingshet-11, HPE	8,699,904	1,194.00	1,679.82	22,703
			DOE/SC/Oak Ridge National Laboratory United States				
bnl_knl 8 months ago		2	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.28Hz, Tofu interconnect D, Fujitsu	7,630,848	442.01	537.21	29,899
juron juron	8 months ago		RIKEN Center for Computational Science Japan				
juwels_booster 2 months ago		3	LUNI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 44C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE	2,220,288	309.10	428.70	6,016
Irz_supermuc_ng	last month		EuroHPC/CSC Finland				
dpace3	8 months ago	4	Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA	1,824,768	238.70	304.47	7,404
gpace4	4 months ago		HDR100 Infiniband, Atos EuroHPC/CINECA Italy				
stampede2_knl	6 months ago	5	Summit - IBM Power System AC\$22, IBM POWER9 22C	2,414,592	148.60	200.79	10,096
summit summit	8 months ago		3.076Hz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiliband, IBM DOE/SC/Oak Ridge National Laboratory United States				

Results available for GPU and CPU architectures. In the following, focus on Frontier/LUMI-G (AMD MI250X), Juwels/Leonardo booster (NVIDIA A100) and Fugaku/QPace4 (A64FX).

Juwels Booster (node has $4 \times A100-40$ GB): Single-node domain-wall fermion D operator

```
Initialized GPT
   Copyright (C) 2020 Christoph Lehner
GPT ·
        1.543473 s :
                 : DWF Dslash Benchmark with
                     fdimensions : [64, 32, 32, 32]
                     precision : single
                     Ls
                               : 12
        7.958636 s : 1000 applications of Dhop
GPT :
                     Time to complete
                                         : 2.93 s
                     Total performance
                                         : 11325.46 GFlops/s
                 :
                     Effective memory bandwidth : 7824.86 GB/s
GPT :
        7.959499 s :
                 : DWE Dslash Benchmark with
                     fdimensions : [64, 32, 32, 32]
                 .
                     precision : double
                 :
                     Ls
                            : 12
        17.420620 s : 1000 applications of Dhop
GPT :
                     Time to complete
                                          : 5.78 s
                     Total performance
                                         : 5749.77 GElops/s
                     Effective memory bandwidth : 7945.14 GB/s
Finalized GPT
```

Compare to HBM bandwidth of 1,555 GB/s per GPU

QPace4 (node has one A64FX): Single-node domain-wall fermion $D \hspace{-1.5mm}/$ operator

```
Initialized GPT
   Copyright (C) 2020 Christoph Lehner
GPT :
        0.265714 s :
                 : DWF Dslash Benchmark with
                     fdimensions : [24, 24, 24, 24]
                     precision : single
                            : 8
                     LS
        20.218240 s : 1000 applications of Dhop
GPT :
                     Time to complete
                 ÷.,
                                       : 3.67 s
                     Total performance
                                      : 954.90 GFlops/s
                     Effective memory bandwidth : 677.11 GB/s
GPT :
        20.218842 s :
                 : DWF Dslash Benchmark with
                     fdimensions : [24, 24, 24, 24]
                     precision : double
                     Ls
                               : 8
        45.245379 s : 1000 applications of Dhop
GPT :
                     Time to complete
                                      : 7.36 s
                     Total performance
                                         : 475.80 GFlops/s
                     Effective memory bandwidth : 674.77 GB/s
Finalized GPT
```

Compare to HBM bandwidth of 1,000 GB/s per A64FX

Juwels Booster (node has $4 \times$ A100-40GB): Single-node site-local matrix products

	Initialized GP	т		GPT :	62.262581 s :		
Cop	right (C) 2020 Chr:	istoph Lehner			: Ma	atrix Multiply Benchmark with	
						fdimensions : [48, 48, 48,	128]
GPT :	1.589357 s :				:	precision : double	
	: Mat	rix Multiply Benchmark with			:		
	:	fdimensions : [48, 48, 48,	128]	GPT :	72.003471 s : 10	<pre>matrix_multiply</pre>	
	:	precision : single				Object type	: ot_matrix_color(3)
	:					Time to complete	: 0.012 s
GPT :	10.985099 s : 10	matrix_multiply				Effective memory bandwidth	: 5264.01 GB/s
	:	Object type	: ot_matrix_color(3)				
	:	Time to complete	: 0.0058 s	GPT :	78.174681 s : 10	∂ matrix_multiply	
	:	Effective memory bandwidth	: 5271.36 GB/s		:	Object type	: ot_matrix_spin(4)
						Time to complete	: 0.02 s
GPT :	16.689329 s : 10	matrix_multiply				Effective memory bandwidth	: 5439.91 GB/s
	:	Object type	: ot_matrix_spin(4)				
	:	Time to complete	: 0.01 s	GPT :	128.232979 s : 10	0 matrix_multiply	
	:	Effective memory bandwidth	: 5333.21 GB/s		:	Object type	: ot_matrix_spin_color(4,3)
						Time to complete	: 0.22 s
GPT :	62.092583 s : 10	matrix_multiply			:	Effective memory bandwidth	: 4416.45 GB/s
	:	Object type	: ot_matrix_spin_color(4,3)		:		
	:	Time to complete	: 0.097 s				
		Effective memory bandwidth	: 5057.37 GB/s		Finalized GF	т	
	:						

Compare to HBM bandwidth of 1,555 GB/s per GPU

Juwels Booster (node has $4 \times$ A100-40GB): Inner product (reduction)

:	28.406798 s :	100 rank_inner_product	
	:	Object type	: ot_vector_singlet(12)
	:	Block	: 4 × 4
	:	Data resides in	: accelerator
	:	Performed on	: accelerator
	:	Time to complete	: 0.13 s
	:	Effective memory bandwidth	: 4827.16 GB/s
	:		
	:	rip: timing: unprofiled	= 0.000000e+00 s (= 0.00 %)
	:	rip: timing: rip: view	= 9.706020e-04 s (= 0.70 %)
	:	rip: timing: rip: loop	= 1.369879e-01 s (= 99.30 %)
	:	rip: timing: total	= 1.379585e-01 s (= 100.00 %)
	:		

GPT

Compare to HBM bandwidth of 1,555 GB/s per GPU

Performance summary

Machine	Operation	Performance	Bandwidth
Frontier	Ø	9 TF/s	6.2 TB/s
Booster	$ ot\!$	12 TF/s	7.8 TB/s
Booster	ColorMatrix $ imes$		5.2 TB/s
Booster	${\sf SpinColorMatrix}\ \times$		5.1 TB/s
Booster	SpinColorVector $\langle \cdot, \cdot angle$		4.8 TB/s
QPace4	$ ot\!$	0.95 TF/s	0.68 TB/s
SuperMUC-NG	$ ot\!$	0.72 TF/s	0.51 TB/s

Single-node SP performance of Wilson \not{D} and linear algebra on Juwels Booster (4xA100, HBM BW 1.6 TB/s per A100), Qpace4 (A64FX, HBM BW of 1 TB/s per node), and the SuperMUC-NG (Skylake 8174). The \not{D} performance is inherited from Grid, the linear algebra performance is based on cgpt.

Example applications

RBC ensemble generation

(the generating GPT scripts are linked below; around 200 lines of Python script each)

ID	a^{-1}/GeV	N _f	$L^3 \times T \times L_s$	b + c	$m_{\rm res} \times 10^4$	$m_\pi/{ m MeV}$	$m_K/{ m MeV}$	$m_{D_s}/{ m GeV}$	$m_{\pi}L$	Code
481	1.73	2+1	$48^3 \times 96 \times 24$	2	6.1	139	499	-	3.87	CPS
64I	2.35	$^{2+1}$	$64^3 \times 128 \times 12$	2	3.1	139	507	-	3.77	CPS
96I	2.69	$^{2+1}$	$96^3 \times 192 \times 12$	2	2.3	132	486	-	4.70	CPS
1	1.73	2+1	$32^3 \times 64 \times 24$	2	6.3	208	513	-	3.85	GPT script
2	1.73	$^{2+1}$	$24^3 \times 48 \times 32$	2	4.6	284	534	-	3.96	GPT script
3	1.73	$^{2+1}$	$32^3 \times 64 \times 24$	2	6.5	210	597	-	3.88	GPT script
4	1.74	$^{2+1}$	$24^3 \times 48 \times 24$	2	6.2	279	534	-	3.84	GPT script
5	1.75	2+1+1	$24^3 \times 48 \times 24$	2	6.7	280	536	1.99	3.84	GPT script
6	1.75	2+1+1	$24^3 imes 48 imes 24$	2	6.7	280	536	1.5	3.84	GPT script
7	1.76	2+1+1	$24^3 \times 48 \times 24$	2	7.9	284	540	1.39	3.88	GPT script
8	2.37	2+1+1	$32^3 \times 64 \times 12$	2	3.0	280	536	1.99	3.88	GPT script
9	2.37	$^{2+1}$	$32^3 \times 64 \times 12$	2	3.0	281	535	-	3.80	GPT script
А	1.76	$^{2+1}$	$24^3 \times 48 \times 8$	2	41.5	303	548	-	4.15	GPT script
В	1.73	$^{2+1}$	$32^3 \times 64 \times 24$	2	6.1	139	499	-	2.58	GPT script
С	1.73	$^{2+1}$	$64^3 \times 128 \times 24$	2	6.1	139	499	-	5.16	GPT script
D	1.74	$^{2+1}$	$32^3 \times 64 \times 24$	2	6.2	279	534	-	5.12	GPT script
Е	3.50	$^{2+1}$	$48^3 \times 192 \times 12$, openBC	2	1.4	280	535	-	3.87	GPT script

Further examples

- QED corrections to g-2 HVP and tau decays of RBC/UKQCD
- Ensemble parameters and g-2 HVP (Tuesday talk C.L.)
- g-2 HLbL project of RBC/UKQCD (combined with QLattice)
- Scattering studies in scalar field theory (Bruno et al.)
- Testing stochastic locality with CP(n) models (Bruno, Morandi)

Also applied by BNL and Bielefeld groups for ongoing projects.

Teaching

LGT lecture based on interactive GPT notebooks

(link to lecture)

Chapters:

- Chapter 1: path integral formulation of quantum mechanics (Jupyter Notebook, PDF)
- Chapter 2: Markov Chain Monte Carlo (MCMC) methods (Jupyter Notebook, PDF, last update 09.11.10:14)
- Chapter 3: statistics of continous variables (Jupyter Notebook, PDF, last update 07.11. 21:00)
- Chapter 4: scalar field theory on a lattice (Jupyter Notebook, PDF, last update 02.12. 10:45)
- Chapter 5: symmetries of fundamental field theories (Jupyter Notebook, PDF, last update 21.11. 18:30)
- Chapter 6: gauge theories on a lattice (Jupyter Notebook, PDF, last update 28.11. 16:30)
- Chapter 7: static quark potential and spectrum of pure QCD (Jupyter Notebook, PDF, last update 03.12. 10:11)
- Chapter 8: strong coupling expansion (Jupyter Notebook, PDF, last update 05.12. 21:11)
- Chapter 9: continuum limit and phase transitions (Jupyter Notebook, PDF, last update 13.12. 10:14)
- Chapter 10: fermions on a lattice (Jupyter Notebook, PDF, last update 19.12. 18:04)
- Chapter 11: symmetries of the Wilson action (Jupyter Notebook, PDF, last update 10.01.09:35)
- Chapter 12: chiral symmetry on a lattice (Jupyter Notebook, PDF, last update 24.01. 10:00)
- Chapter 13: Hybrid Monte Carlo (HMC) (Jupyter Notebook, PDF, last update 28.01.09:46)
- Chapter 14: Hadron spectroscopy (Jupyter Notebook, PDF, last update 04.02. 09:56)

The machine learning module

Example: train simple feed-forward network

```
In []: import gpt as g
grid = g.grid([4, 4, 4], g.double)
rng = g.random("test")
# network and training data
n = g.ml.network.feed_forward([g.ml.layer.nearest_neighbor(grid)] * 2)
training_input = [rng.uniform_real(g.complex(grid)) for i in range(2)]
training_output = [rng.uniform_real(g.complex(grid)) for i in range(2)]
# cost functional
c = n.cost(training_input, training_output)
# train network
W = n.random_weights(rng)
gd = g.algorithms.optimize.gradient_descent
gd(maxiter=4000, eps=1e-4, step=0.2)(c)(W, W)
```

The quantum computing module

Example: create and measure a 5-qubit bell state

```
import gpt as g
from apt.gis.gate import *
rng = g.random("qis_test")
# initial state with 5 qubits. stored in double-precision
st = g.gis.backends.dvnamic.state(rng. 5. precision=g.double)
g.message("Initial state:\n".st)
# prepare Bell-type state
st = (H(0) | CNOT(0,1) | CNOT(0,2) | CNOT(0,3) | CNOT(0,4)) * st
g.message("Bell-type state:\n",st)
# measure
st = M() * st
q.message("After single measurement:\n",st)
q.message("Classically measured bits:\n",st.classical bit)
GPT :
          197.943668 s : Initial state:
                           + (1+0j) |00000>
GPT :
          197.949198 s : Bell-type state:
                       : + (0.7071067811865475+0j) |00000>
                       : + (0.7071067811865475+0j) |11111>
GPT :
          197.951478 s : After single measurement:
                       : + (1+0j) |11111>
GPT :
          197.952545 s : Classically measured bits:
                       : [1, 1, 1, 1, 1]
```

How to use GPT?

https://github.com/lehner/gpt

Quick Start

The fastest way to try GPT is to install Docker, start a Jupyter notebook server with the latest GPT version by running

docker run --rm -p 8888:8888 gptdev/notebook

and then open the shown link http://127.0.0.1:8888/?token=<token> in a browser. You should see the tutorials folder pre-installed.

The docker images are automatically generated for each version that passes the CI interface.

CI currently has test coverage of 96%, running on each pushed commit.

Thank you