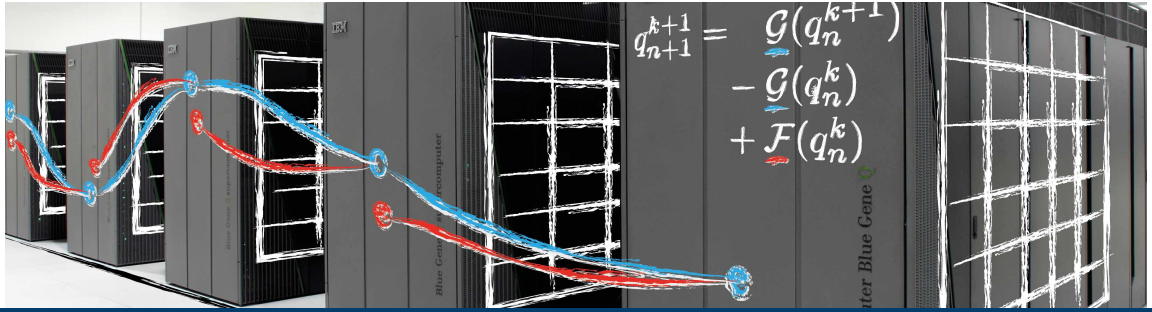


Massively parallel adaptive spectral deferred correction in Python

December 9, 2024 | Thomas Baumann | Jülich Supercomputing Centre

Agenda

Introduction to SDC

Adaptivity in SDC
- Boosting computational efficiency
- Boosting resilience

Python on HPC
- Python on GPUs
- Parallel scaling
- Large space-time parallel simulation

Spectral deferred correction (SDC)[1]

Goal

Solve initial value problem (IVP): $u_t = f(u), \quad u(0) = u_0$

SDC idea

- Integrate IVP w.r.t. time: $u(t) = u_0 + \int_0^t f(u(s))ds$
- Compute integral over interval $(0,\Delta t]$ numerically with quadrature rule Q
  $\rightarrow$ defines a fully implicit Runge-Kutta method (RKM)
- Solve fully implicit RKM iteratively using preconditioned Picard iteration

[1] [Dutt et al., 2000]

SDC: Numerical integration with quadrature rule

Compute quadrature rule

- Divide the interval into M quadrature nodes $0 \leq \tau_m \leq \Delta t$, with $u_m \approx u(\tau_m)$
- Compute interpolating Lagrange polynomials: $l_j^\tau(t)$ with $l_j^\tau(\tau_i) = \delta_{ij}$
  $\rightarrow$ Use for polynomial approximation of $f(t) = \sum_{m=1}^{M} l_m^\tau(t) f(u_m)$
- Integrate polynomial approximation:
  $u_m = u_0 + \int_0^{\tau_m} \sum_{j=1}^{M} l_j^\tau(t) f(u_j) dt = u_0 + \sum_{j=1}^{M} f(u_j) \int_0^{\tau_m} l_j^\tau(t) dt = u_0 + \sum_{j=1}^{M} q_{mj} f(u_j)$

Collocation problem: Exact integral of order M polynomial approximation

$$\boxed{u_m = u_0 + \sum_{j=1}^{M} q_{mj} f(u_j), \quad m = 1,...,M} \iff \vec{u} = \vec{u}_0 + Qf(\vec{u})$$

Collocation problem

Pros

- Polynomial approximation is order M accurate anywhere within $(0, \Delta t]$
- For spectral quadrature rules: Get up to order $2M$ at Δt

Cons

- $Q \in \mathbb{R}^{M \times M}$ is dense
- For PDE with N degrees of freedom, need to solve $MN \times MN$ systems in collocation problem

SDC to the rescue

Solve collocation problem iteratively with forward substitution $\rightsquigarrow$ solve kM-many $N \times N$ systems

SDC iteration

Recall: Want to solve $\vec{u} = \vec{u}_0 + Qf(\vec{u})$

Simplest iterative scheme: Picard iteration

$$\vec{u}^{k+1} = \vec{u}^k + \vec{r}^k, \quad \vec{r}^k := \vec{u}_0 + \Delta t Q F(\vec{u}^k) - \vec{u}^k$$

- Gain one order of accuracy per iteration up to the order of Q
- Method is explicit $\rightarrow$ poor stability

Use preconditioner Q_Δ

$$(I_M - \Delta t Q_\Delta F)\left(\vec{u}^{k+1}\right) = \vec{u}_0 + \Delta t \left(Q - Q_\Delta\right) F\left(\vec{u}^k\right)$$

- Still gain one order of accuracy per iteration up to the order of Q (most of the time... [Causley and Seal, 2019, Christlieb et al., 2009])
- Q_Δ is lower triangular $\rightsquigarrow$ forward substitution

SDC preconditioners

Easy splitting

$$\left(I_M - \Delta t \sum_i Q_\Delta^i F\right)\left(\vec{u}^{k+1}\right) = \vec{u}_0 + \Delta t \left(Q - \sum_i Q_\Delta^i\right) F\left(\vec{u}^k\right)$$

$\rightarrow$ We will later use IMEX splitting by using one preconditioner that is strictly lower triangular and one with non-zero diagonal entries [Ruprecht and Speck, 2016]

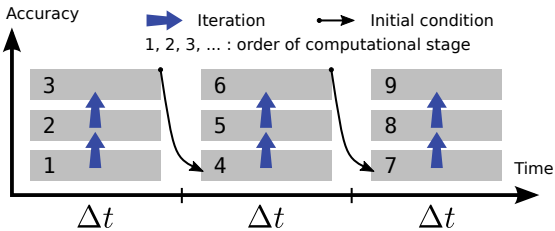
Small scale time-parallelism via diagonal Q_Δ [van der Houwen and Sommeijer, 1991]

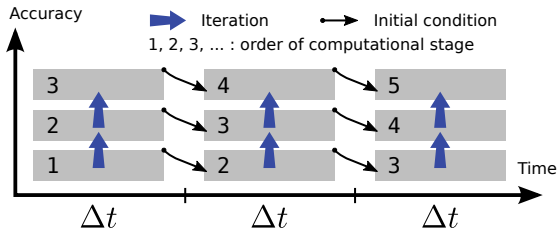
- Update the nodes in parallel on M tasks
- Very good preconditioners where recently published by Gaya and Thibaut [Čaklović et al., 2024]

Optimal preconditioner is problem dependent, not known a priori and an active area of research

Parallel-in-time extension: Block Gauß-Seidel SDC

[Guibert and Tromeur-Dervout, 2007]





Start iteration on step as soon as one iteration has been performed on previous step

Figures by Thibaut Lunet

Adaptive step size selection in SDC

- SDC has a lot in common with RKM
- Step size adaptivity is mature in RKM with embedded methods

$\rightarrow$ transfer concepts from embedded RKM to SDC

Embedded Runge-Kutta methods

- Idea: Control step size to match local error to target tolerance ϵ_{TOL}
- Error estimate: subtract solutions of different orders p and q, $q > p$:

$$\epsilon = \|u^{(p)} - u^{(q)}\| = e^{(p)} + \mathcal{O}(\Delta t^{q+1})$$

  $\rightarrow$ This estimates local error of lower order method
- Step size update: Infer "optimal" step size via the order ($\beta = 0.9$: safety factor)

$$\Delta t_{\mathrm{opt}} = \beta \left(\frac{\epsilon_{\mathrm{TOL}}}{\epsilon} \right)^{1/(p+1)}$$

- Restart current step if $\epsilon > \epsilon_{\mathrm{TOL}}$
- Obtain lower order methods from same stages but different weights as higher order method

Step size adaptivity in SDC

Transfer ideas from embedded RKM

- Use same step size update equation
- Use bespoke error estimates

Resulting algorithms

- Δt-adaptivity: Constant number of iterations, adaptive step size
- Δt-k-adaptivity: Choose both adaptively

Δt-adaptivity

Error estimate

Order of SDC after k iterations: k
(conditions apply)

$$\epsilon = \|u^{k-1} - u^k\|$$

Step size update

$$\Delta t_{\text{opt}} = \beta \left(\frac{\epsilon_{\text{TOL}}}{\epsilon}\right)^{1/k}$$

Δt-k-adaptivity

- Recall: Solution to collocation problem is order M polynomial approximation in $(0,\Delta t]$ by u_m, $m = 0,...,M$
- Idea: Construct secondary order $M-1$ solution via polynomial interpolation at τ_{M-1}
  - Select nodes $\tau^* = \{\tau_i, i = 0,1,...,M-2,M\}$
  - Compute interpolation weights via Lagrange polynomials $w_j = l_j^{\tau^*}(t = \tau_{M-1})$

Error estimate

$$\epsilon = \| \sum_{m=0}^{M-2} w_j u_j + w_{M-1} u_M - u_{M-1} \|_\infty$$

Step size update

$$\Delta t_{\text{opt}} = \beta \left(\frac{\epsilon_{\text{TOL}}}{\epsilon} \right)^{1/M}$$

Step size adaptivity for diagonal SDC

Diagonal SDC

Use diagonal Q_Δ, everything else is the same

Δt-adaptivity

Numerically verify you get the expected order after every iteration

Δt-k-adaptivity

Business as usual

Step size adaptivity for Block Gauß-Seidel SDC

Block Gauß-Seidel SDC

Solve entire block with first order method, then solve entire block with second order method, ...

Δt-adaptivity

- Increment on last step in block behaves like global error within the block
  $\rightarrow$ Make sure error due to parallelization does not get out of hand
- Overestimates local error a bit, but can be used as usual

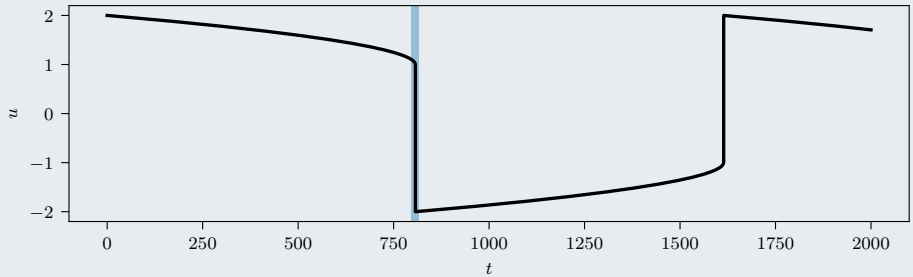
Δt-k-adaptivity

Business as usual

Benchmark problems

Van der Pol Oscillator

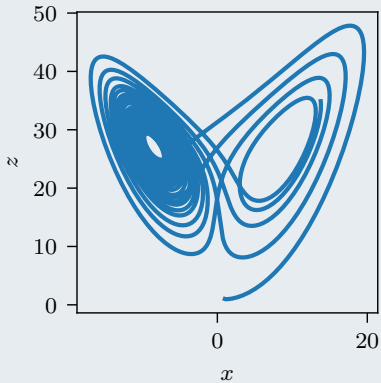
$$u_{tt} - \mu \left(1 - u^2\right) u_t + u = 0$$

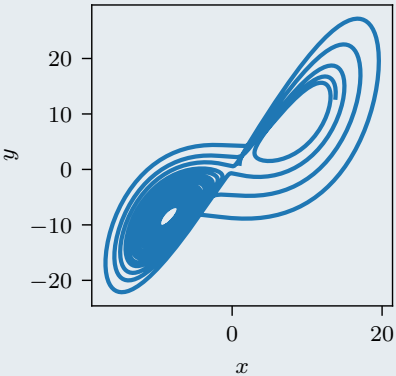


Benchmark problems

Lorenz attractor

$$x_t = \sigma(y - x)$$
$$y_t = \rho x - y - xz$$
$$z_t = xy - \beta z$$



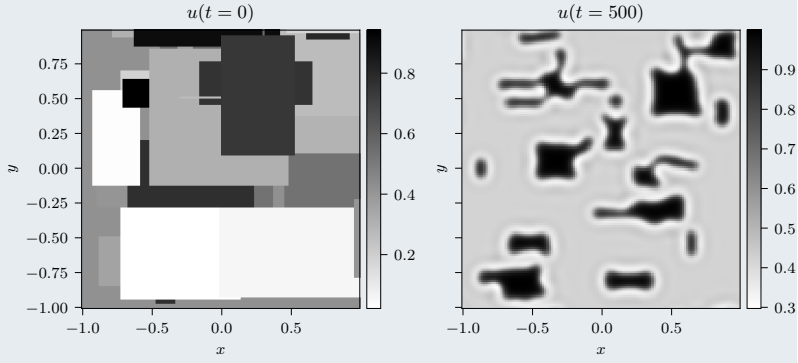


Benchmark problems

Gray-Scott

$$u_t = \nu_u \Delta u - uv^2 + F(1-u)$$
$$v_t = \nu_v \Delta v + uv^2 - (F+k)v$$

Solve IMEX with Fourier pseudo-spectral discretization



Benchmark problems

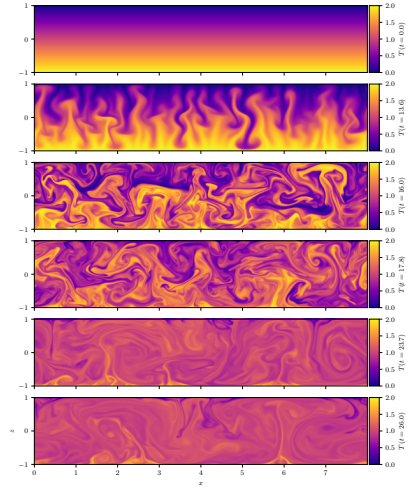
Rayleigh-Benard convection

Incompressible fluid dynamics:

$$
\begin{aligned}
u_t - \nu(u_{xx} + u_{zz}) + p_x &= -uu_x - vu_z \\
v_t - \nu(v_{xx} + v_{zz}) + p_z - T &= -uv_x - vv_z \\
T_t - \kappa(T_{xx} + T_{zz}) &= -uT_x - vT_z \\
u_x + v_z &= 0
\end{aligned}
$$

Space discretization

- Solve IMEX with Fourier + ultraspherical pseudo-spectral discretization
- Differential algebraic equation $\rightarrow$ need stiffly accurate integrator



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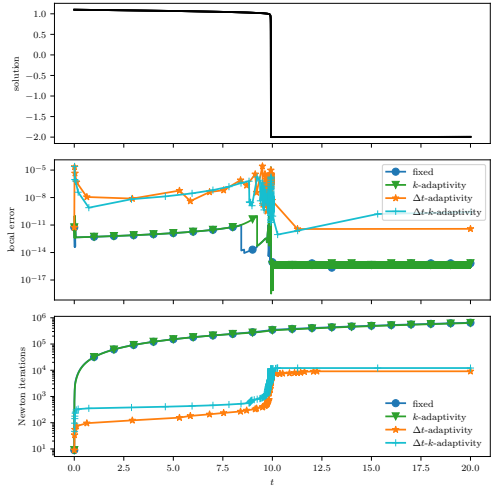
Boosting computational efficiency with adaptivity



SDC strategies

- fixed: fixed iteration number k and step size Δt
- k-adaptivity: adaptive k, fixed Δt
- Δt-adaptivity: adaptive Δt, fixed k
- Δt-k-adaptivity both adaptive

Results

- k-adaptivity: Can't tune k finely enough
- Need adaptive Δt to accommodate changes in timescale

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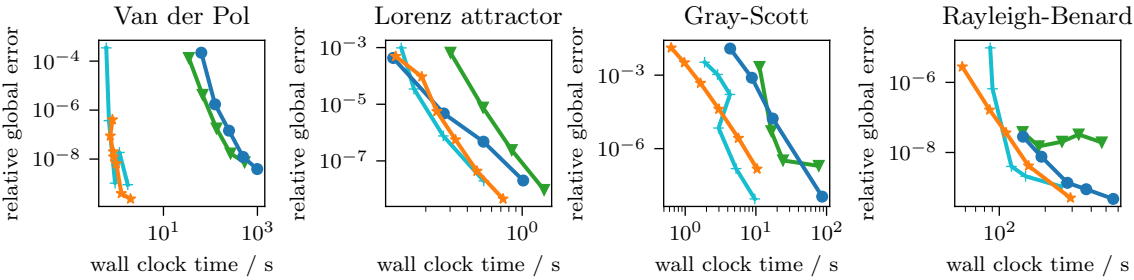
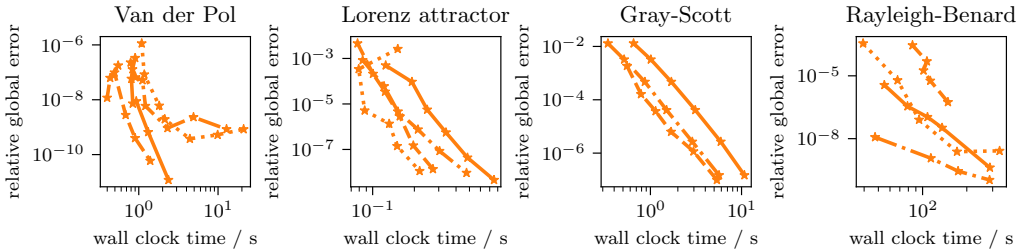
Boosting computational efficiency with adaptivity



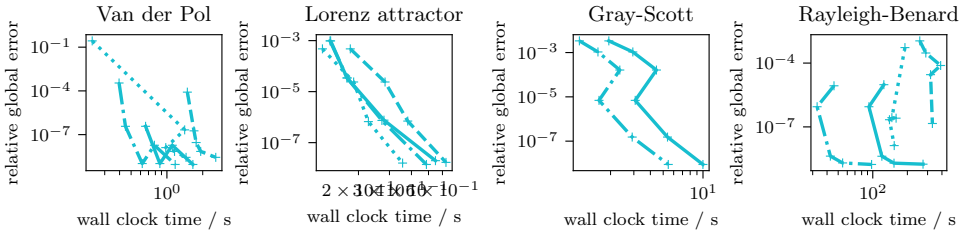
- k-adaptivity: Computing residual is expensive for ODEs
- Δt-adaptivity works well for any accuracy and problem
- Δt-k-adaptivity works best for tight tolerance

Parallel-in-time Δt-adaptivity



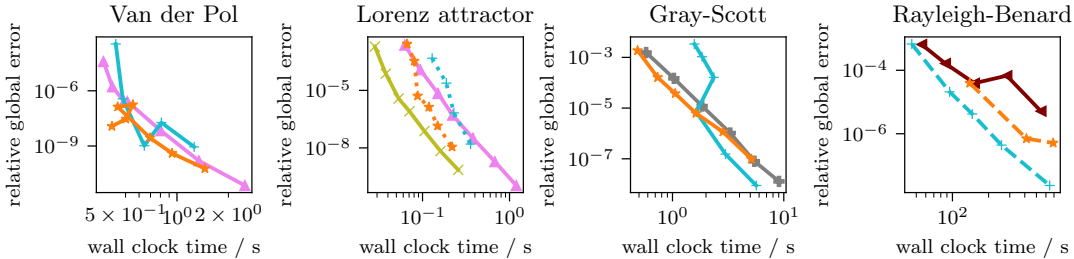
- Performance heavily depends on Q_Δ
- Don't know beforehand if speedup is possible
- At least one parallelization method always gives good speedup
- Combining diagonal SDC and block Gauß-Seidel SDC is seldom worthwhile

Parallel-in-time Δt-k-adaptivity



- Similar poperties w.r.t. parallelisation as Δt-adaptivity
- Here, we often use diagonal Q_Δ in serial as well
  $\rightarrow$ Get same result in diagonal SDC
- Particularly good speedup with diagonal SDC for PDEs

SDC vs. RKM



- At least mode of adaptive PinT SDC is always competitive with RKM for stiff problems
- In Rayleigh-Benard, no high order comparison RKM available, SDC still better at order 3

Resilience

Tyranny of numbers

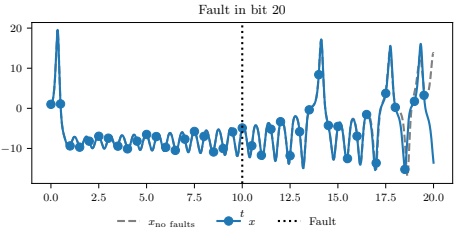
- Insane number of components
- Large chance of failure somewhere
- E.g.: Mariner 8 crashed because of a single faulty diode

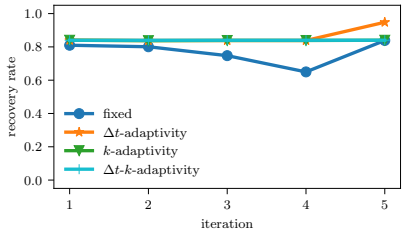
Faults in modern HPC

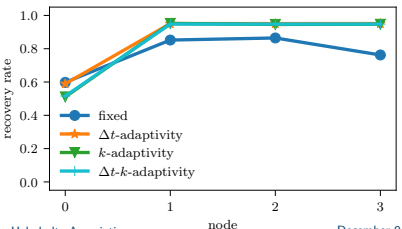
- Sources: Radiation and hardware damage
- Multiple times each day in HPC machines [Glosli et al., 2007, Schroeder et al., 2011]

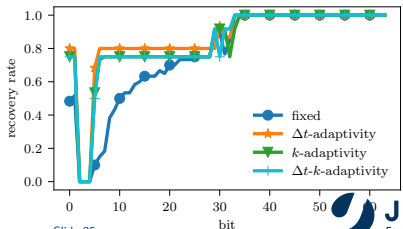
Boosting resilience by adaptivity

Lorenz attractor









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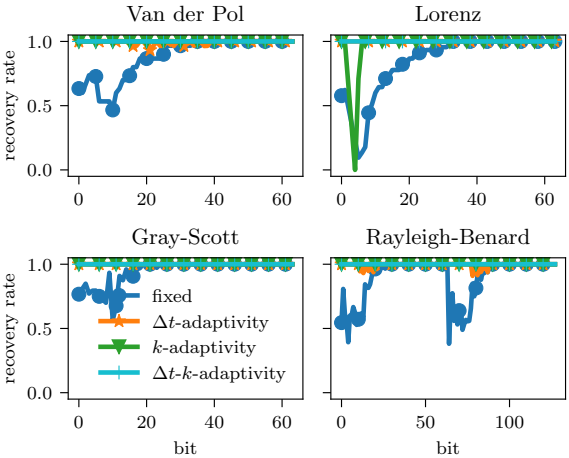
Boosting resilience by adaptivity



- Note: We exclude faults to initial conditions or ones that cause crashes here
- k-adaptivity: Iteration may not converge from faulty initial guess
- Δt-adaptivity: Some faults to intermediate bits don't trigger restart, but show up in the end
- Adaptive step size selection greatly improves resilience!

GPU programming

Analogy: Logging

- CPU: Tiny fast boat arranging logs in stream
- GPU: River that's doing the heavy lifting

Actual programming

- CPU submits operations ("kernels") to stream(s) on GPU
- GPU asynchronously executes operations
- Need to synchronize explicitly if CPU interacts with data on GPU

Porting Python code to GPU

Python philosophy

Perform actual computations within libraries that wrap compiled code

CPU libraries

- NumPy
- mpi4py
- FFTW
- SuperLU

GPU libraries

- CuPy
- NCCL (ships with CuPy)
- cuFFT (ships with CuPy)
- *Hier könnte ihr GPU sparse solver stehen!*

Porting Python code to GPU is mostly easy!

Note that MPI is not stream aware!

Porting Gray-Scott implementation to GPU

Fourier pseudo-spectral method

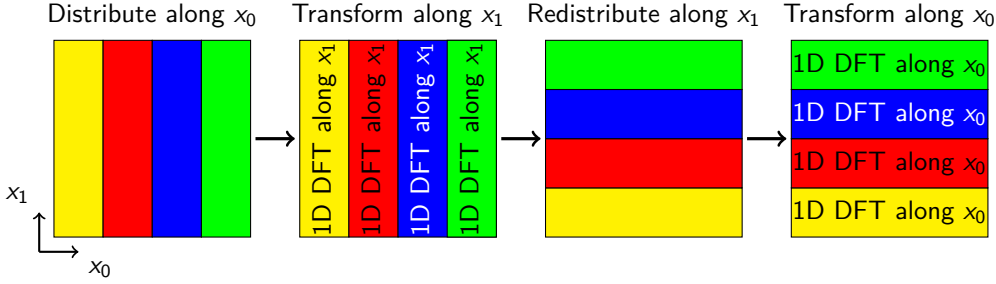
- Laplacian is diagonal $\rightarrow$ invert by division
- Right hand side evaluations: Need only multiplication and addition
- Need library for distributed FFTs! $\rightarrow$ mpi4py-fft

GPU porting

- Swap NumPy for CuPy
- Port mpi4py-fft to GPUs

Port mpi4py-fft to GPU

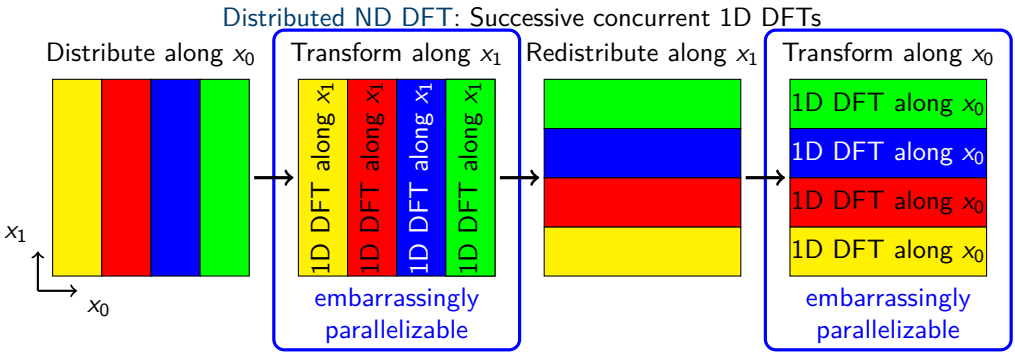
Distributed ND DFT: Successive concurrent 1D DFTs



Port to GPU

- Implement CuPy array interface
- Replace FFTW with cuFFT
- Implement Alltoall in NCCL
- Add NCCL as communication back-end

Port mpi4py-fft to GPU



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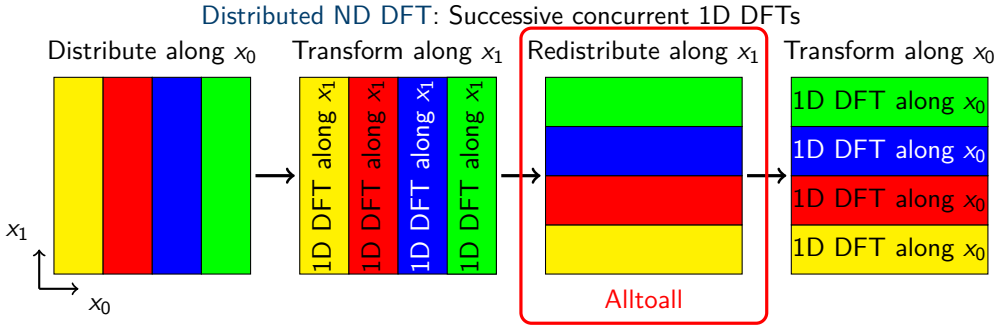

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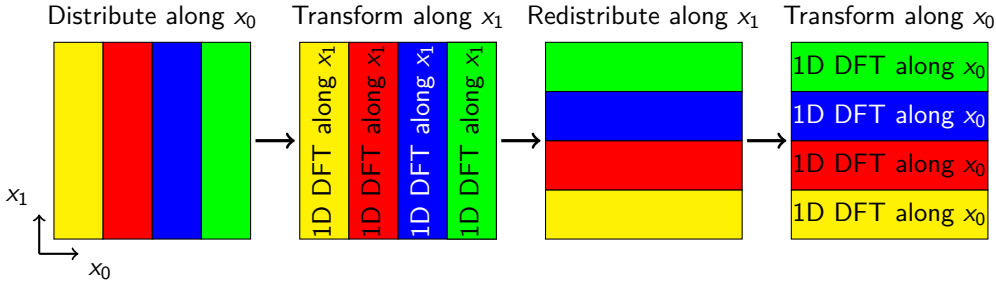

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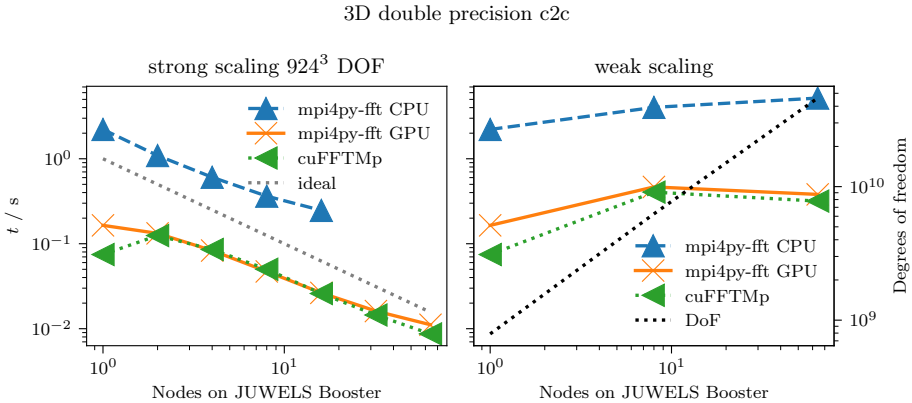
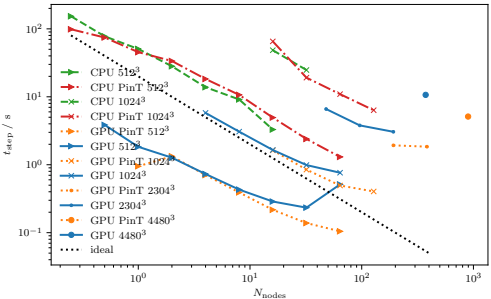
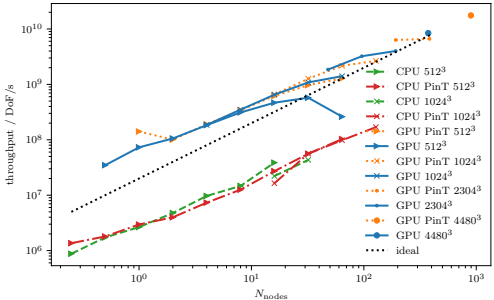
Parallel scaling of mpi4py-fft GPU port



Remarkably competitive with optimized NVIDIA competition cuFFTMp

Parallel scaling of Gray-Scott implementation





GPUs significantly outperform CPUs

- 16 tasks per node on CPU cluster
- 4 tasks per node on GPU cluster
- $\approx$ 10x speedup at same number of nodes

Use diagonal SDC to extend scaling

- Shifts from all-to-all to reduce
- Improves strong scaling
- Enables scaling up to 3584 GPUs

Porting RBC implementation to GPU

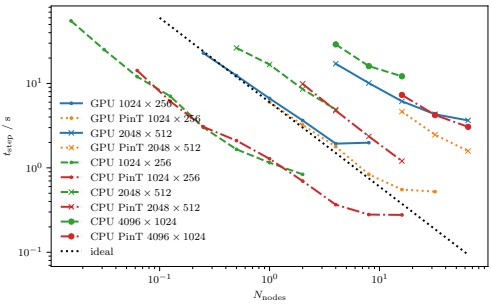
Fourier and ultraspherical pseudo-spectral method

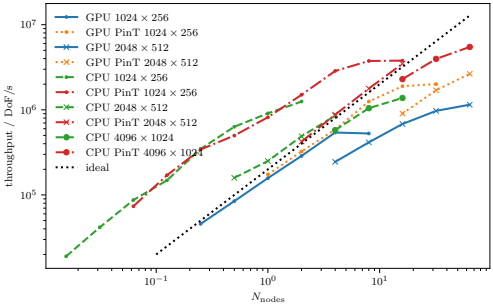
- System matrix is non-diagonal $\rightarrow$ solve by LU decomposition using SuperLU
- Right hand side evaluations: Need only multiplication and addition
- Need library for distributed FFTs and DCTs $\rightarrow$ mpi4py-fft

GPU porting

- Swap NumPy for CuPy
- Use port of mpi4py-fft to GPUs
- ↯No suitable replacement for SuperLU available at the moment $\rightarrow$ LU decompositions stay on CPU

Parallel scaling of RBC implementation





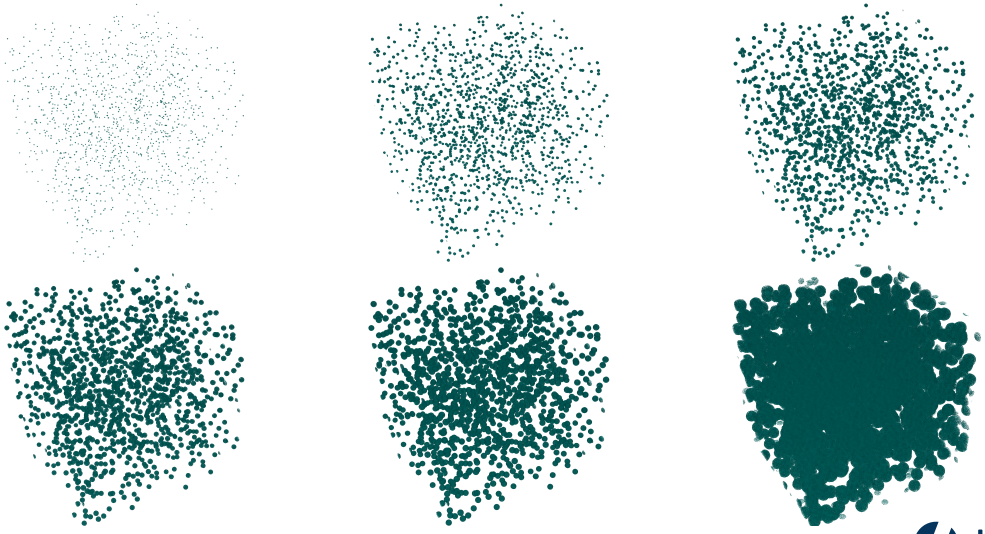
CPUs outperform GPUs

- 64 tasks per node on CPU cluster
- 4 tasks per node on GPU cluster
- LU takes most of the time!

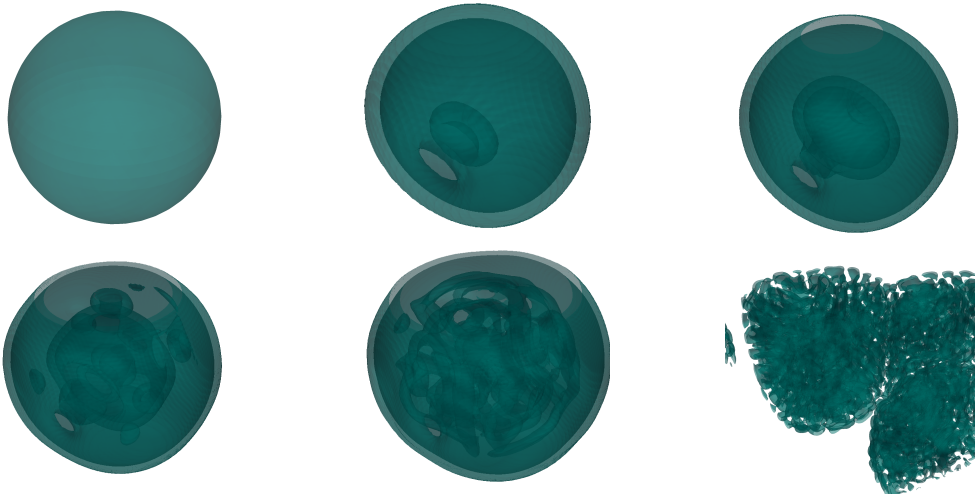
Use diagonal SDC to extend scaling

- Circumvents space-decomposition limit
- Improves strong scaling
- Enables scaling up to 4096 CPUs

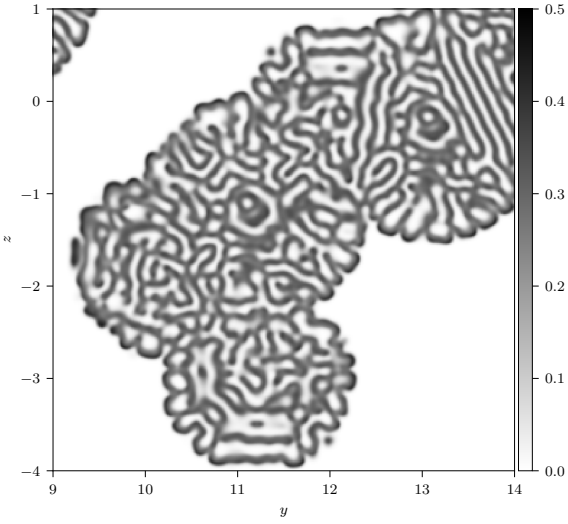
Large space-time parallel Gray-Scott simulation



Large space-time parallel Gray-Scott simulation: Zoom

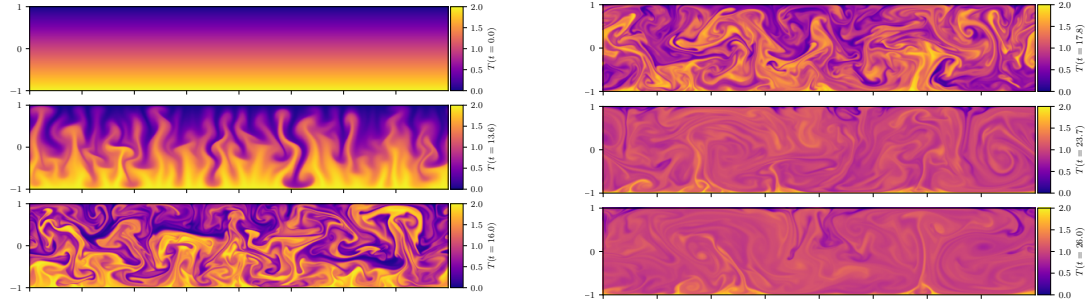


Large space-time parallel Gray-Scott simulation: 2D slice



- Turing instability: Small perturbations + diffusion = complex patterns
- Turing patterns in Gray-Scott in 3D not widely studied
- Use simulations such as this one with Δt-adaptivity and $N = 2304^3$ on $4 \times 192 = 768$ GPUs on JUWELS booster to change that

Large space-time parallel Rayleigh-Benard simulation



- Use Rayleigh number 2×10^7 on $N = 4096 \times 1024$ grid
- Use Δt-k-adaptivity with four Gauß-Radau nodes for step size selection
- Use $4 \times 1024 = 4096$ CPUs on JURECA DC (32 nodes)
- Use approx. 140k CPU hours to reach $t = 26$ because IMEX stability limit requires $\Delta t \approx 10^{-3}$

Sources I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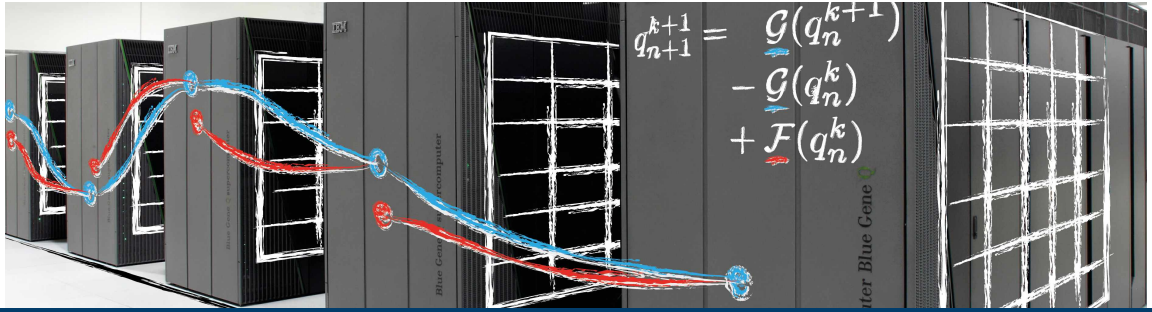

Massively parallel adaptive spectral deferred correction in Python

December 9, 2024 | Thomas Baumann | Jülich Supercomputing Centre

Porting mpi4py-fft to GPU: Alltoall in NCCL

N,r ← Number of GPUs, MPI rank ▷ Initialize variables
sendbufs, sendbufs ← {}, {}

NCCL group start ▷ Launch all communications in a single kernel
for i in 0, 1, ..., N: **do**
    send_to ← (r + i) % N
    recv_from ← (r - i + N) % N
    sendbufs[i] ← contiguous copy of data to send
    recvbufs[i] ← contiguous empty array
    NCCL receive from recv_from
    NCCL send to send_to
end for
NCCL group end ▷ Wait for all communication to finish before unpacking

copy recvbufs to destination array

Record all of this to CUDA graph!

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