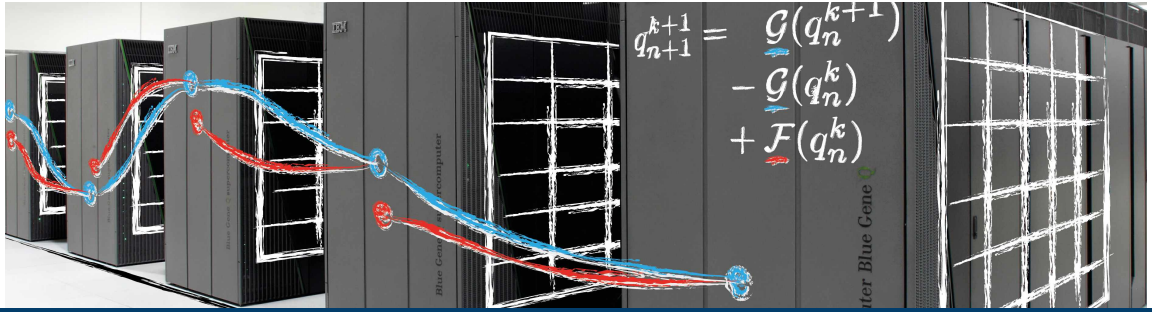
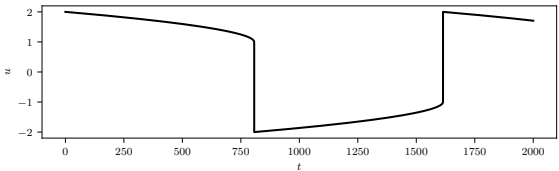


Efficient Massively Space-Time-Parallel Simulations with Adaptive Spectral Deferred Correction

3.12.25 | Thomas Saupe | Jülich Supercomputing Centre

Efficient Massively Space-Time-Parallel Simulations with Adaptive Spectral Deferred Correction



Motivation

- Use **adaptivity** to **efficiently simulate** problems with non-constant global timescale
- Use **spectral deferred correction (SDC)** because of its capabilities for stiff PDEs and parallelisation opportunities
- Use **space-time-parallel** implementations to cater to modern HPC machines

Spectral deferred correction (SDC)

[Dutt et al., 2000]

- SDC numerically approximates solutions to initial value problems (IVP):

$$\partial_t u = f(u,t), \quad u(t=0) = u_0, \quad t \in [0,T]$$

- Integral formulation:

$$u(T) = u(0) + \int_0^T f(u,t)dt$$

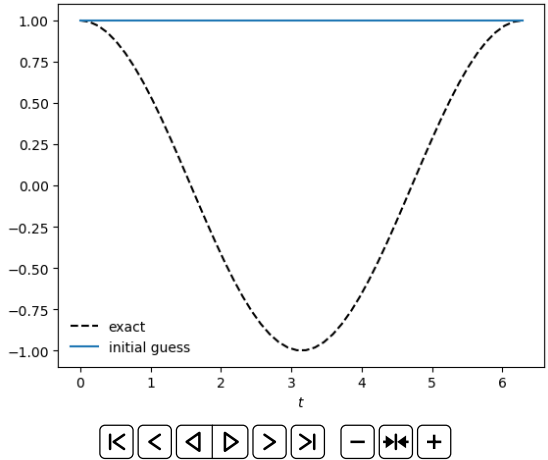
- Discretize the interval with M collocation nodes $\tau_m \in [0,T]$ and define $u_m \approx u(\tau_m)$
- Discretize the integral with quadrature rule Q to arrive at the collocation problem:

$$u_m = u_0 + \sum_{j=1}^{M} Q_{mj} f(u_j,\tau_j), \quad m = 1,\ldots,M$$

SDC iteratively solves collocation problem

- Q is dense, coupling all u_m to each other
- Use lower triangular preconditioner Q_Δ to remove forward coupling between u_m
- "Sweep" through collocation nodes to update u_m^k one by one (k: iteration index)

Example: $\partial_t u = iu,\ u(0) = 1,\ Re(u(t)) = \cos(t)$



Adaptive Algorithm 0: k-adaptivity

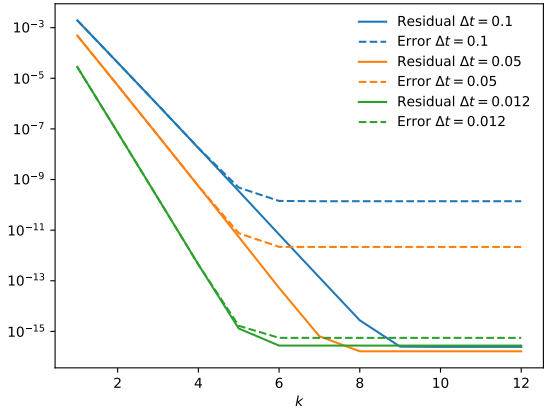
Residual

Subtract both sides of collocation problem

$$r_m^k = u_0 + \sum_{j=1}^{M} Q_{mj} f(u_j^k, \tau_j) - u_m^k$$

Issues with choosing only k adaptively

- Residual indicates how close u_m^k is to the solution of the collocation problem
- Accuracy of the collocation problem itself depends on Δt!



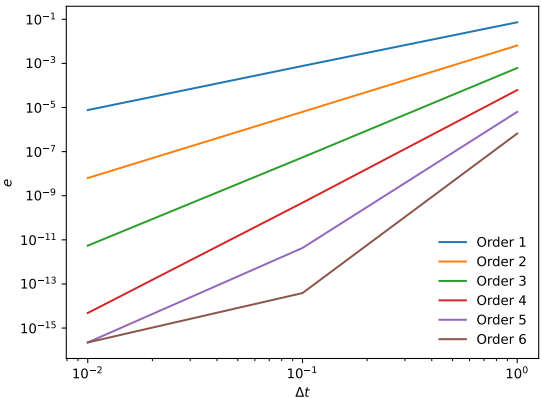
Adaptive selection of Δt in embedded Runge-Kutta

[Hairer et al., 1993, Chapter II.4]

- Order of accuracy p: $e \propto \Delta t^{p+1}$
- Measured error ϵ of order p with Δt, but wanted ϵ_{TOL}? Use

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

- If $\epsilon > \epsilon_{\mathrm{TOL}}$, recompute current step with Δt_{opt}, otherwise move on to next step
- Use $\beta = 0.9$ to prevent restarts



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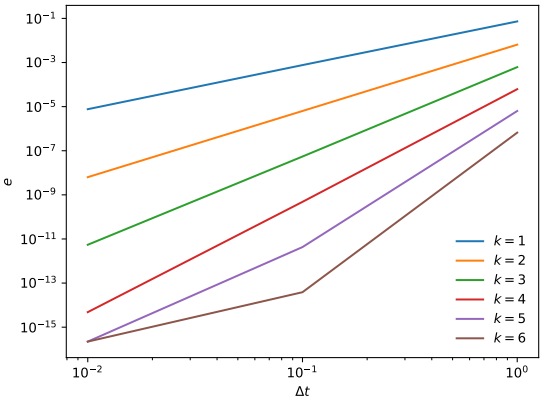
Adaptive Algorithm I: Δt-adaptivity

[Saupe et al., 2024a]

- Order $p = \min(k, 2M - x)$, x depends on Q
- Increment is error estimate of order $k - 1$:

$$\begin{aligned}\epsilon &= \|u_M^k - u_M^{k-1}\|_\infty \\ &= \|u_M^k - u^*(\tau_M) + u^*(\tau_M) - u_M^{k-1}\|_\infty \\ &= \|e_M^k - e_M^{k-1}\|_\infty \\ &\approx \|e_M^{k-1}\|_\infty \propto \Delta t^k\end{aligned}$$

  (embedded Runge-Kutta works very similarly)
- Use fixed number of iterations k
- Plug ϵ and $p = k - 1$ into step size equation from embedded Runge-Kutta



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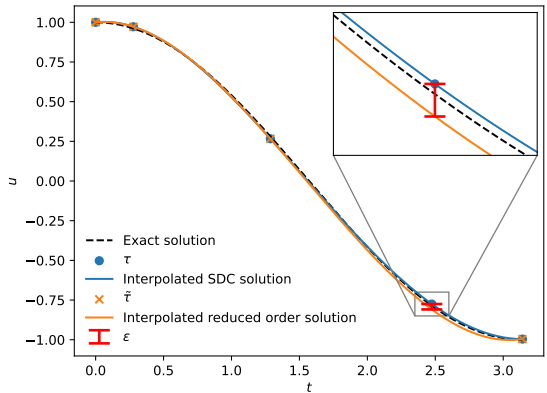
Adaptive Algorithm II: Δt-k-adaptivity

[Saupe et al., 2024a]

- Iterate until SDC iteration is converged
- Choose all nodes but one:
  $\tilde{\tau} = \{\tau_m = 1, \dots M-2, M\}$
- Interpolate u_m^k at $\tilde{\tau}$ to missing node τ_{M-1} to obtain $\tilde{u}_{M-1}^k$ of order $M-1$
- Order $M-1$ error estimate:
  $\epsilon = \|u_{M-1}^k - \tilde{u}_{M-1}^k\| \propto \Delta t^M$
- Plug ϵ and $p = M-1$ into step size equation from embedded Runge-Kutta



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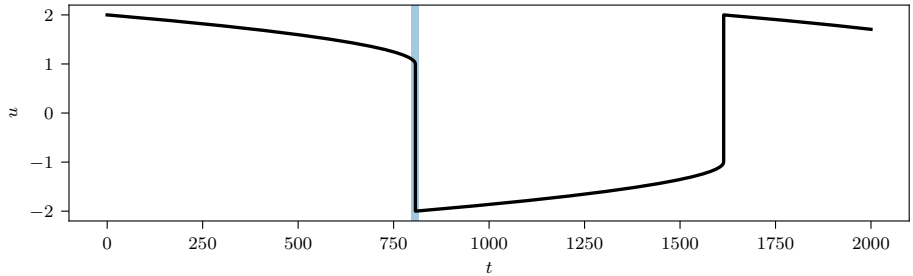
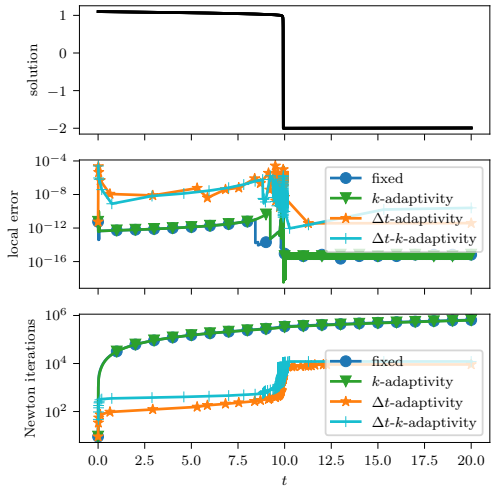
Toy problem: Van der Pol oscillator



- Equation: $u_{tt} - \mu \left(1 - u^2\right) u_t + u = 0$
- Extreme separation of time-scales for $\mu >> 0$
- We focus on the shaded area here

Boosting computational efficiency with adaptivity



SDC strategies

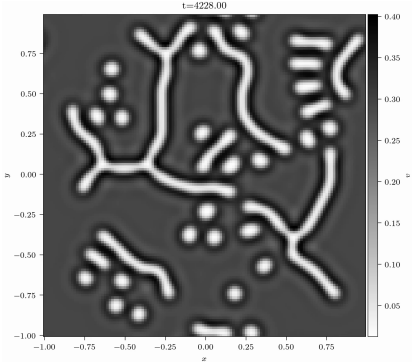
- fixed: fixed iteration number k and step size Δt
- k-adaptivity: adaptive k, fixed Δt
- Δt-adaptivity: adaptive Δt, fixed k
- Δt-k-adaptivity both adaptive

Results

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

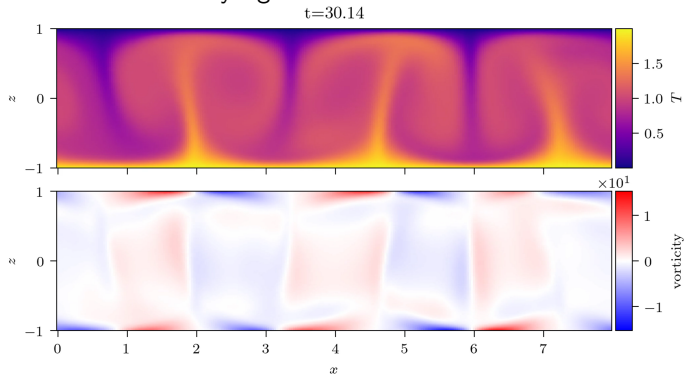
PDE benchmark problems

Gray-Scott



Here: $t \in [0,500]$

Rayleigh-Benard convection



Here: $t \in [10,16]$

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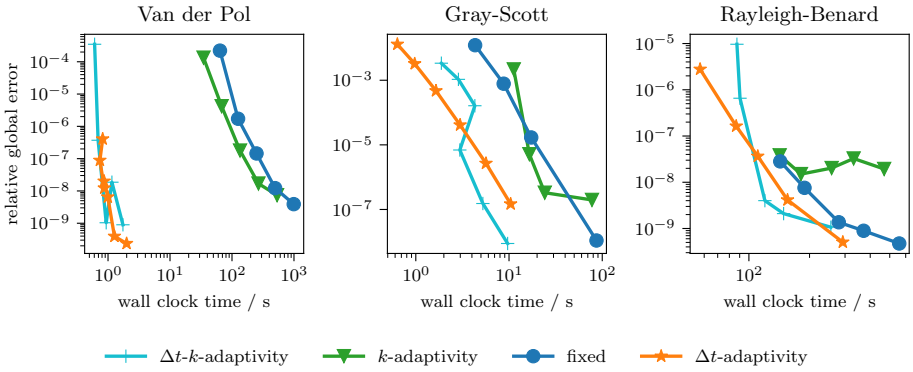
Boosting computational efficiency with adaptivity



- k-adaptivity gives only marginal benefit
- Δt-adaptivity works well for any accuracy and problem
- Δt-k-adaptivity works best for tight tolerance

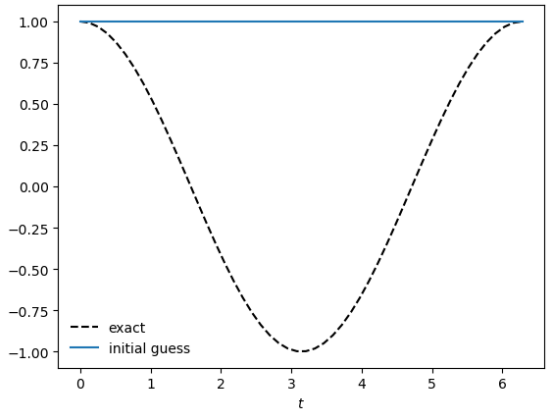
Further speedup by parallelization: Diagonal SDC

[van der Houwen and Sommeijer, 1991, Speck, 2018]

Choose Q_Δ diagonal

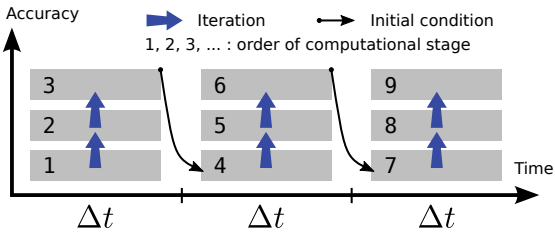
- Diagonal Q_Δ removed forward and backward coupling between u_m
- Update solution at all nodes simultaneously
- "MIN-SR-S" and "MIN-SR-NS" from [Čaklović et al., 2024] yield fast convergence

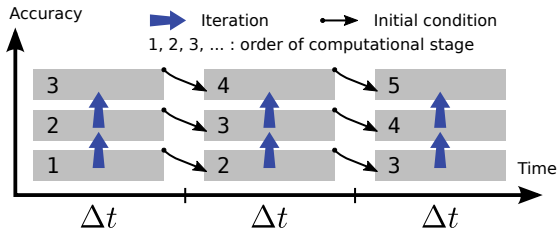
Example: $\partial_t u = iu,\ u(0) = 1,\ Re(u(t)) = \cos(t)$



Further speedup by parallelization: Pipelining

SDC 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

Figure provided by Thibaut Lunet

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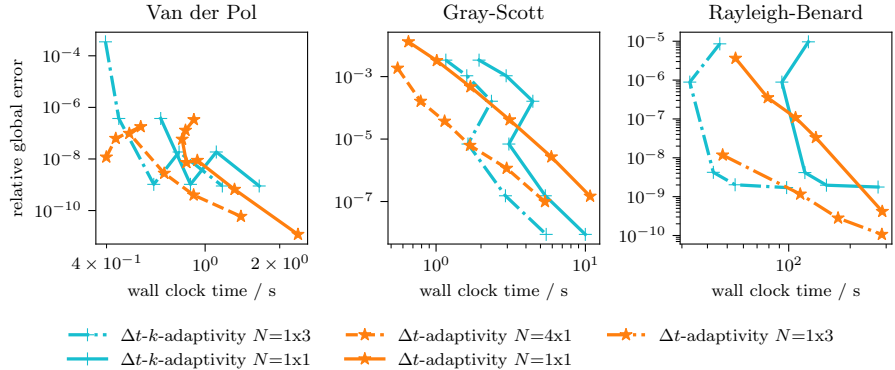
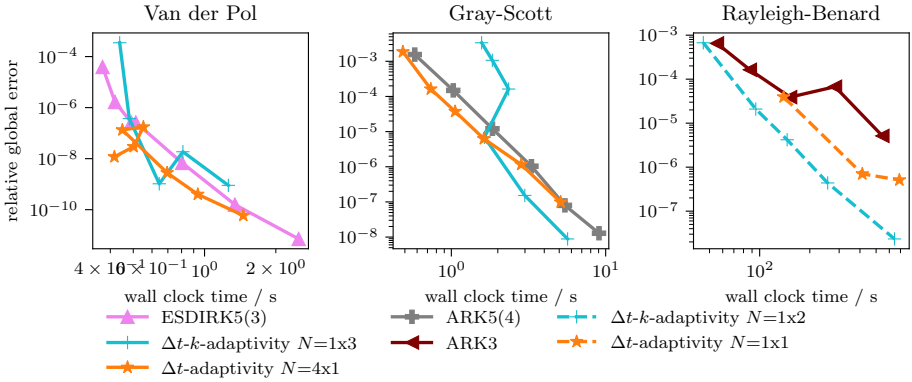
Parallel-in-time speedup



- Number of tasks: N = [tasks in block-Gauß-Seidel]x[tasks in diagonal SDC]
- Diagonal SDC gives decent speedup most of the time
- Speedup by pipelining only for some problems
- Combination of both rarely gives speedup

Time-parallel SDC vs. reference Runge-Kutta method

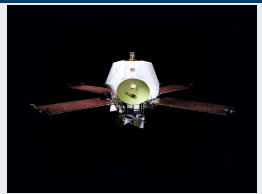


- At least mode of adaptive PinT SDC is always competitive with RKM for stiff problems
- In Rayleigh-Benard, no high order comparison RKM available, SDC still better at low order

Resilience

Tyranny of numbers

- Insane number of components
- Large chance of failure somewhere
- E.g.: Mariner 8 crashed because of a single faulty diode [JOHNSON, 2021]

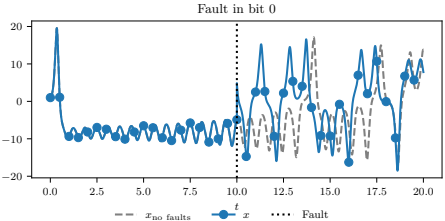


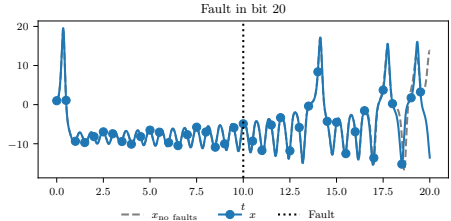
Faults in modern HPC

- Sources: Radiation [Lapinsky and Easty, 2006] and hardware damage [Schroeder et al., 2011]
- Multiple times each day in HPC machines [Glosli et al., 2007, Schroeder et al., 2011]

Boosting resilience by adaptivity

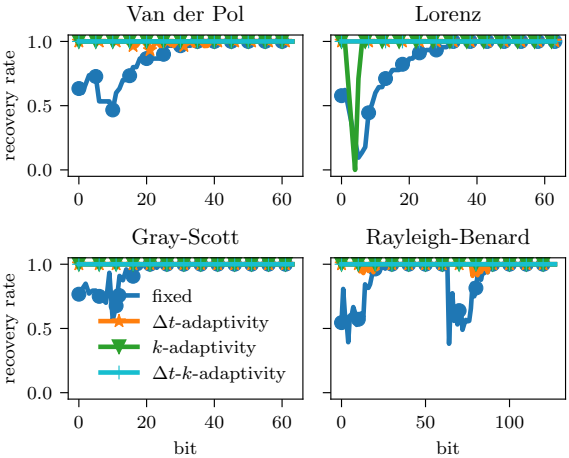
Lorenz attractor





- Flipping individual bits can silently corrupt simulation result
- Adaptive Runge-Kutta methods are naturally resilient [Benson et al., 2015]
- The same is true for adaptive SDC [Saupe et al., 2024b]

Boosting resilience by adaptivity



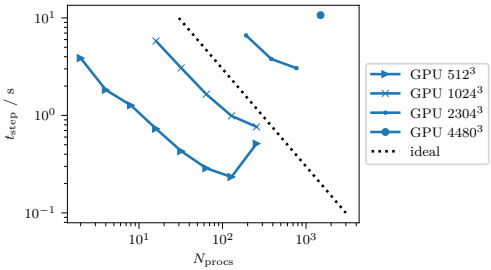
- Bits 0: sign, 1-12: exponent, 13-64: mantissa
- Note: We exclude faults to initial conditions or ones that cause crashes here
- k-adaptivity: Iteration may not converge from faulty initial guess
- Adaptivity greatly improves resilience

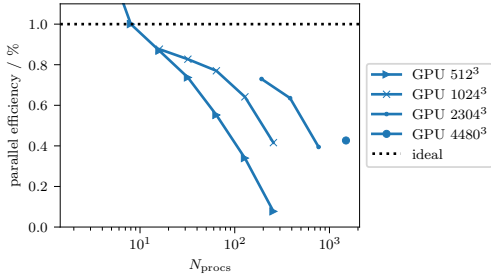
High performance computing (HPC)

Figure: The JUWELS booster module (left) and cluster module (right) at Jülich Supercomputing Centre. Image taken from [Alvarez, 2021, Figure 1] under CC BY 4.0 licence. Copyright: Forschungszentrum Jülich GmbH.

- Modern supercomputers are networks of compute nodes
- GPUs supply most of the compute power in current machines

Parallel scaling of 3D Gray-Scott implementation on GPUs

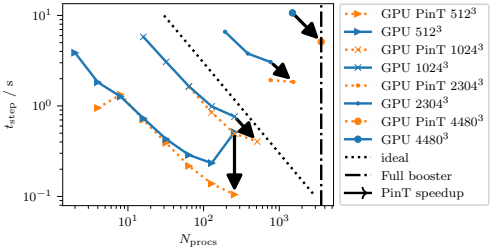


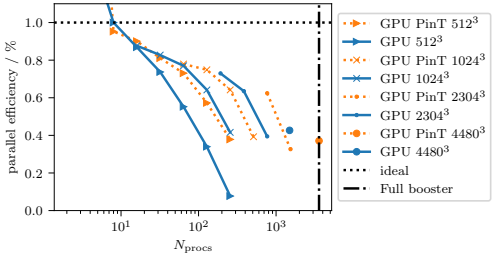


Use diagonal SDC to extend scaling

- Diagonal SDC is not too demanding of the network
- Improves strong scaling
- Enables scaling up to 3584 GPUs ($\approx 95\,\%$ of JUWELS booster)

Parallel scaling of 3D Gray-Scott implementation on GPUs





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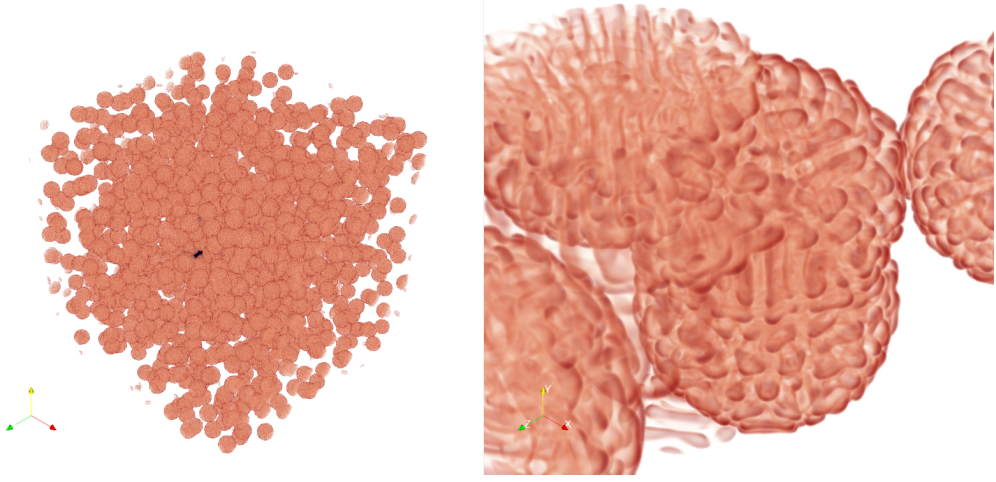
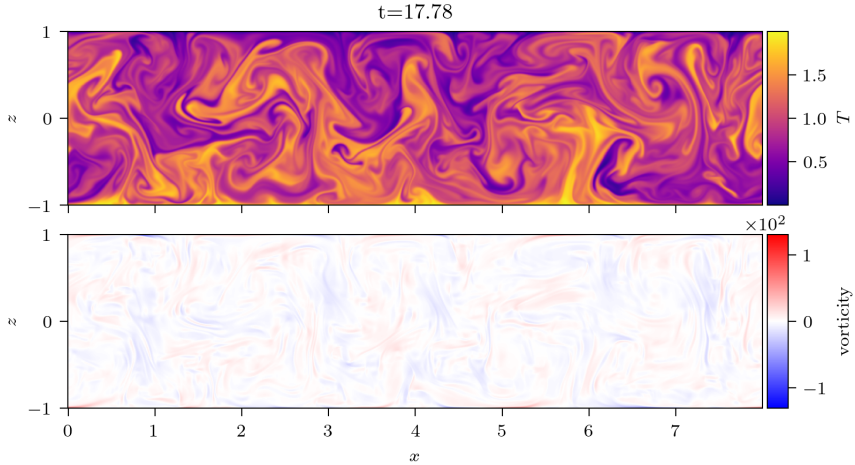
Large space-time parallel Gray-Scott simulation



$N = 2304^3$ on $4 \times 192 = 768$ GPUs on JUWELS booster

Large space-time parallel Rayleigh-Benard simulation



$N = 4096 \times 1024$ on $4 \times 1024 = 4096$ CPUs on JURECA DC

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Conclusion

Summary

- Developed two algorithms for Δt-adaptivity in SDC
  - Demonstrated improved computational efficiency
  - Demonstrated speedup via time-parallelism
  - Showed that time-parallel adaptive SDC can outperform reference Runge-Kutta methods for PDEs
  - Demonstrated increased resilience against soft faults
- Developed space-time parallel implementation of Gray-Scott that scaled up to all of Juwels booster

Collaborators

- Sebastian Götschel
- Thibaut Lunet
- Daniel Ruprecht
- Robert Speck

Codes used / developed

pySDC

GPU port of mpi4py-fft

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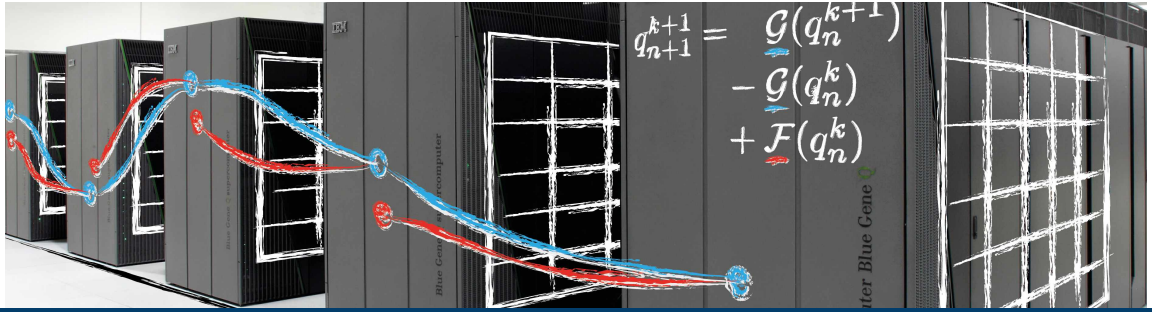

Efficient Massively Space-Time-Parallel Simulations with Adaptive Spectral Deferred Correction

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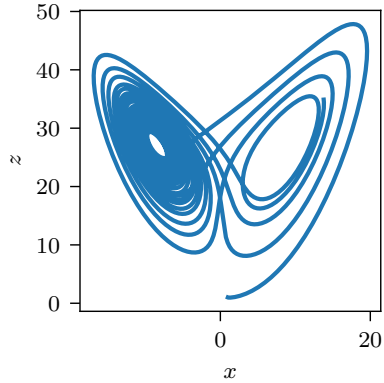
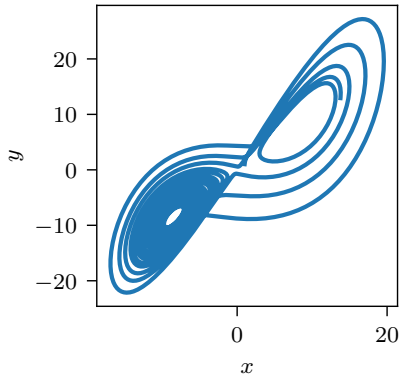
Benchmark problem II: Lorenz attractor [Lorenz, 1963]

- Equation:

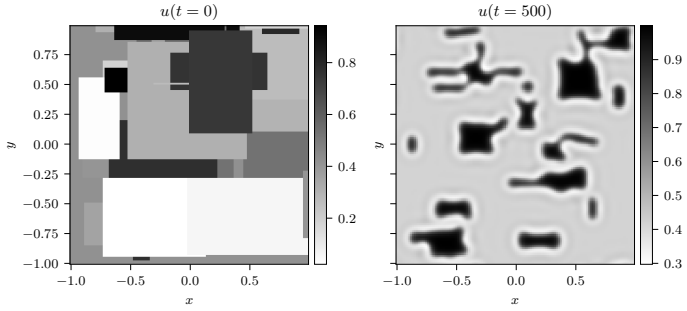
$$x_t = \sigma(y - x)$$
$$y_t = \rho x - y - xz$$
$$z_t = xy - \beta z$$

- Chaotic behavior (Butterfly effect)





Benchmark problem III: Gray-Scott



- Equation:

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

- Turing instability: Perturbations + diffusion = complex shapes

Benchmark problem III

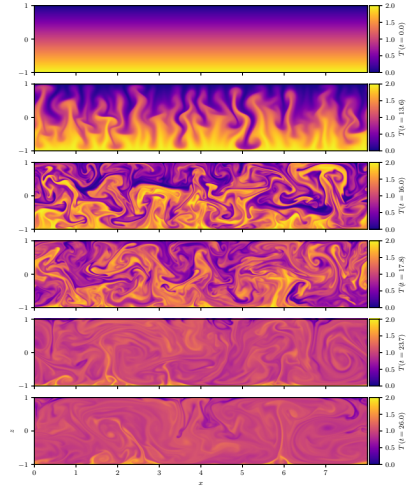
Rayleigh-Benard convection

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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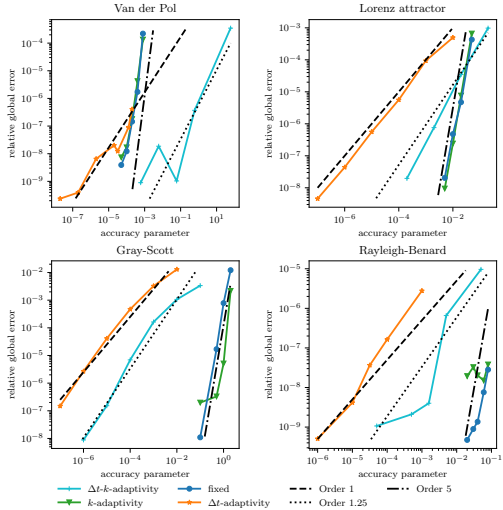
“Order” of adaptive schemes



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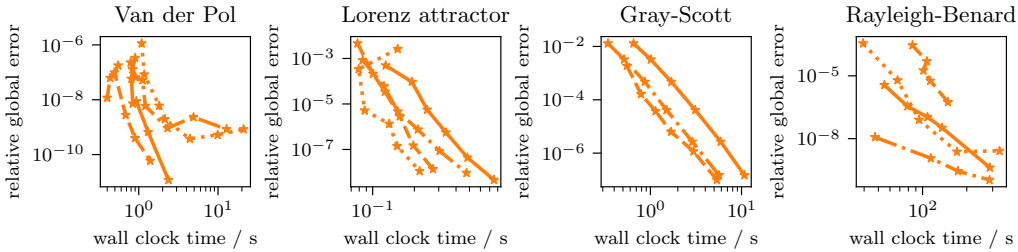
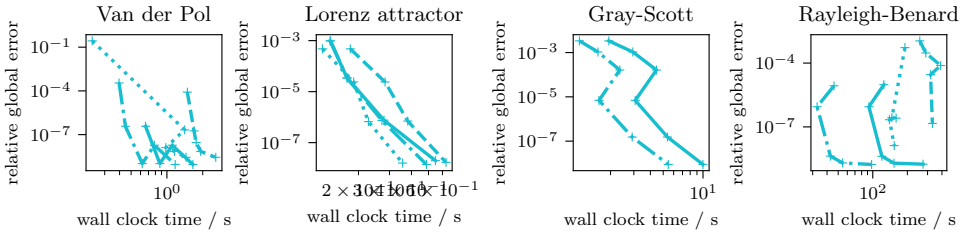
Parallel-in-time Δt-adaptivity



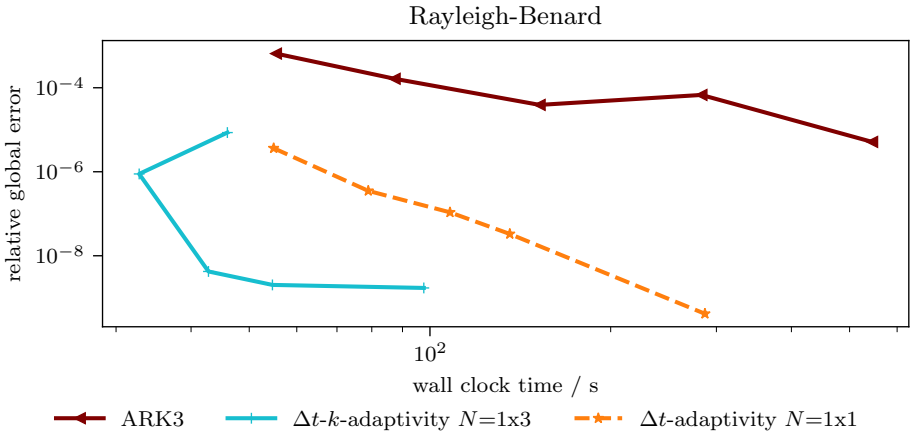
- Performance heavily depends on Q_Δ
- Don't know beforehand if speedup is possible
- At least one parallelization method always gives good speedup
- Combining diagonal SDC and block Gauß-Seidel SDC is seldom worthwhile

Parallel-in-time Δt-k-adaptivity



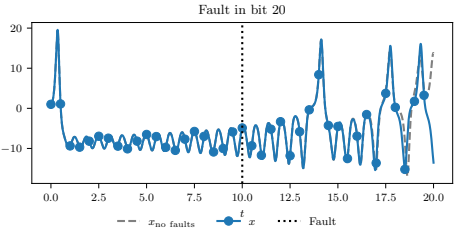
- Similar poperties w.r.t. parallelisation as Δt-adaptivity
- Here, we often use diagonal Q_Δ in serial as well
  $\rightarrow$ Get same result in diagonal SDC
- Particularly good speedup with diagonal SDC for PDEs

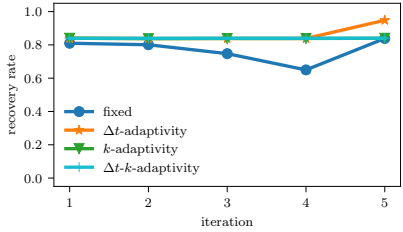
Order 5 SDC vs. order 3 RK for RBC

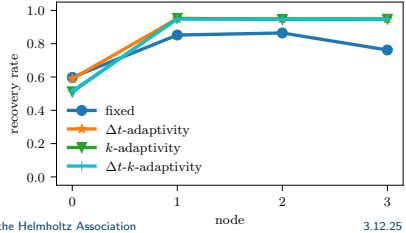


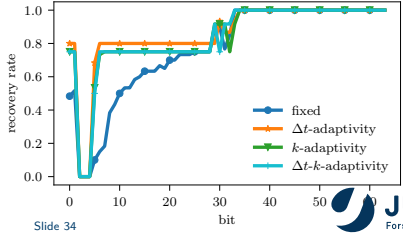
Boosting resilience by adaptivity

Lorenz attractor









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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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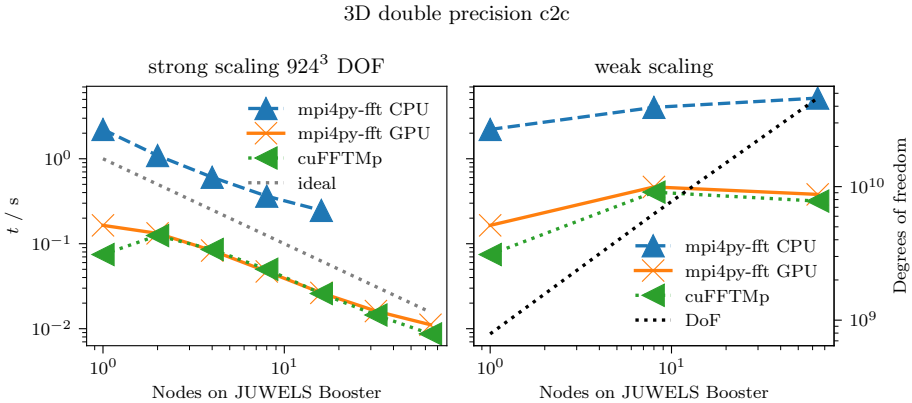
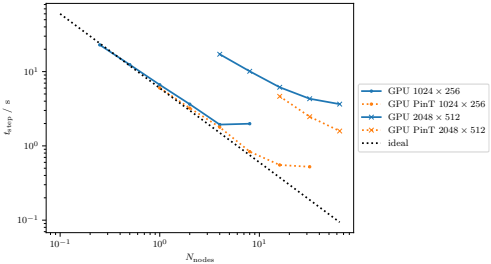
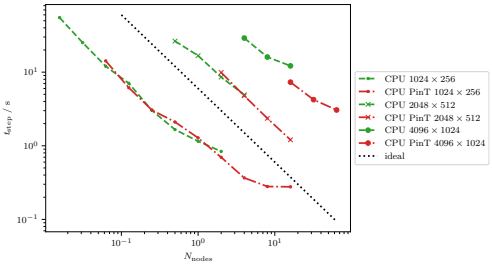
Parallel scaling of mpi4py-fft GPU port



Remarkably competitive with optimized NVIDIA competition cuFFTMp

Parallel scaling of RBC implementation





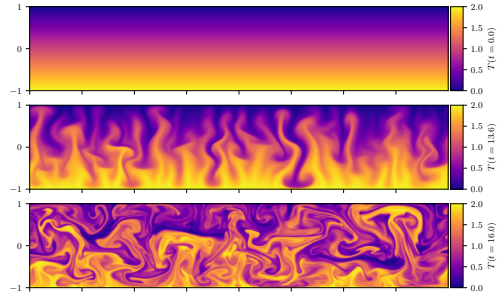
Open issues on GPUs

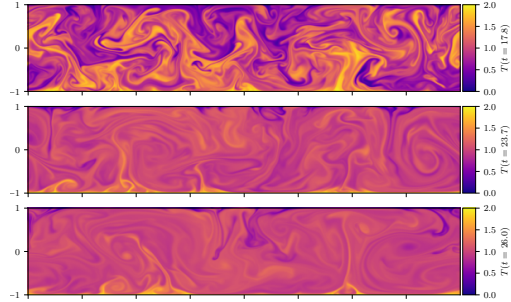
- linear solver is not available on GPU
- current implementation is faster on CPUs

Use diagonal SDC to extend scaling

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

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 $\Delta t \approx 10^{-3}$