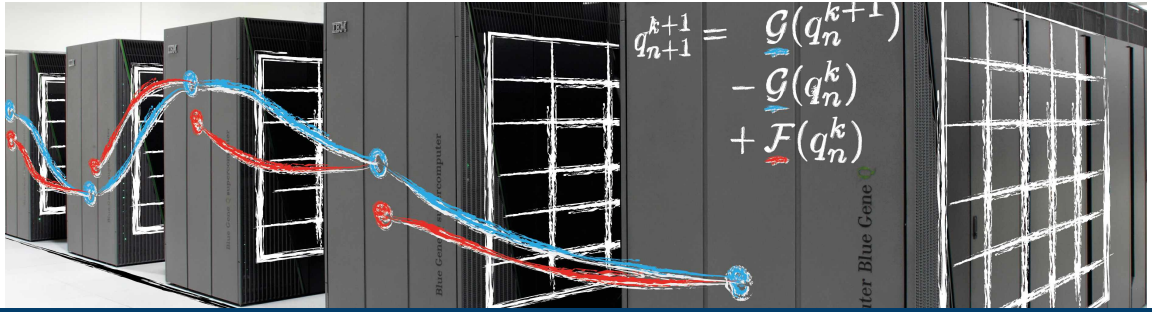


Diagonal spectral deferred correction for 3D Rayleigh-Benard convection

July 8, 2025 | Thomas Saupe, Thibaut Lunet, Sebastian Götschel, Daniel Ruprecht, Robert Speck | JSC & TUHH

Disclaimer: Very much work-in-progress

Rayleigh-Benard convection (RBC)

Equations

$$
\begin{aligned}
T_t - \kappa \Delta T &= -\vec{u} \nabla T \\
\vec{u}_t - \nu \Delta \vec{u} + \nabla p - T \vec{e}_z &= -\vec{u} \nabla \vec{u} \\
\nabla \vec{u} &= 0 \\
\Omega &= [0,1)^2 \times (0,1)
\end{aligned}
$$

Boundary conditions

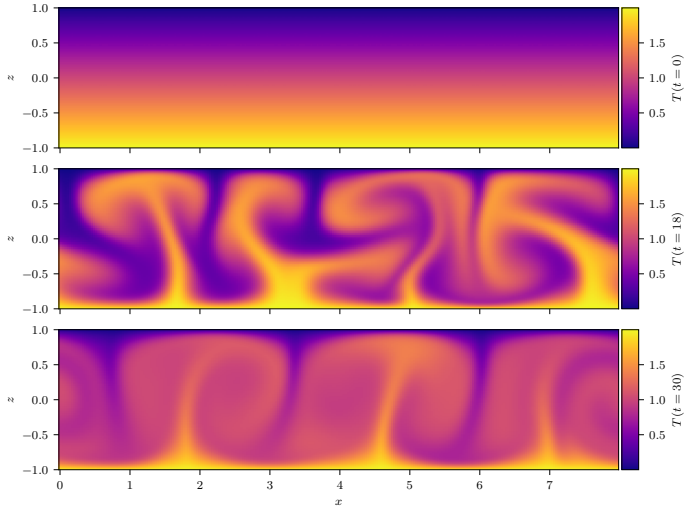
- $\vec{u}(z=0) = \vec{u}(z=1) = 0$
- $T(z=0) = 1,\ T(z=1) = 0$
- periodic in x and y

Dynamics mainly determined by Rayleigh number $Ra = \frac{\alpha g L_z^3 \Delta T}{\kappa \nu}$, turbulence develops from $Ra > 1709$

We pick $Ra > 10^7 \rightarrow$ complicated convection patterns $\rightarrow$ difficult to speed up with PinT

Dynamics in 2D

- Start with stable linear temperature gradient
- Perturb with random noise on the order of 10^{-3}
- Perturbations grow
- Flow settles into quasi-stationary rolling pattern



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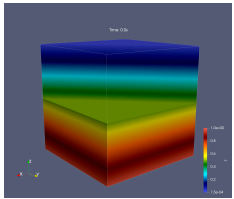
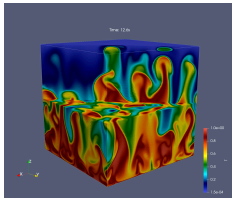
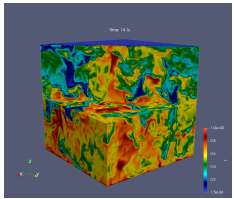
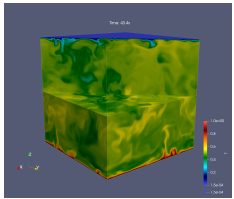
Dynamics in 3D









Same thing, just looks more chaotic!

Spatial discretization and solver

- Use global spectral method with Fourier $\times$ Fourier $\times$ ultraspherical discretization
  $\rightarrow$ ultraspherical discretization from [Olver and Townsend, 2013] is fancy Chebychev discretization
- Treat convection ($F(\vec{u})$) explicitly and only linear terms implicitly:

$$\underbrace{\begin{pmatrix} I & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & I & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}}_{M} \begin{pmatrix} u \\ v \\ w \\ T \\ p \end{pmatrix}_t + \underbrace{\begin{pmatrix} -\nu\Delta & 0 & 0 & 0 & \partial_x \\ 0 & -\nu\Delta & 0 & 0 & \partial_y \\ 0 & 0 & -\nu\Delta & -I & \partial_z \\ 0 & 0 & 0 & -\kappa\Delta & 0 \\ \partial_x & \partial_y & \partial_z & 0 & 0 \end{pmatrix}}_{L} \begin{pmatrix} u \\ v \\ w \\ T \\ p \end{pmatrix} = F\left(\begin{pmatrix} u \\ v \\ w \\ T \\ p \end{pmatrix}\right)$$

- M is not invertible $\rightarrow$ differential algebraic equation (DAE)
- No worries: $M + \Delta t L$ is invertible $\rightarrow$ no DAE-specific method needed

Space-parallelism

Parallelize Fourier spectral methods

- Need distributed FFT $\rightarrow$ very common, no problem
- Differentiation matrices are diagonal $\rightarrow$ easily distributed

Parallelize ultraspherical spectral methods

- Need distributed DCT $\rightarrow$ express via FFTs, no problem
- Differentiation matrices are not diagonal $\rightarrow$ can't easily distribute inversion

Parallelize RBC

- Matrices are built from 1D matrices using Kronecker product
- Use pencil decomposition, aligned in z for matrix application
- FFTs require expensive all-to-all communication

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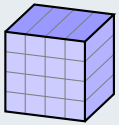

Time discretization: Spectral deferred correction (SDC)

[Dutt et al., 2000, Weiser, 2015]

- Start with initial value problem

$$u(\Delta t) = \int_0^{\Delta t} f(u)dt + u(0)$$

- Choose M collocation nodes τ_m and discretize the integral with spectral quadrature rule Q

$$(I - \Delta t Q f)(\vec{u}) = \vec{u}_0,$$

  where $\vec{u} = (u(\tau_1), \dots u(\tau_M))$

- Solve iteratively with preconditioner Q_Δ

$$(I - \Delta t Q_\Delta f)(\vec{u}^{k+1}) = \vec{u}_0 + \Delta t(Q - Q_\Delta) f(\vec{u}^k)$$

See Thibaut's talk tomorrow morning for loads more detail!

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Time parallelisation: Diagonal SDC

[van der Houwen and Sommeijer, 1991, Speck, 2018, Čaklović et al., 2024]

Q_Δ lower triangular

- Solve SDC iteration with forward substitution
- Can write as kM stage DIRK method

Q_Δ diagonal

- Removes coupling within SDC iteration
- Perform implicit solves and f evaluations in parallel
- Looks like k stage (S)DIRK method on each task

Butcher tableau for third order SDC

τ_1	$\tilde{q}_{11}$								
τ_2	$\tilde{q}_{21}$	$\tilde{q}_{22}$							
τ_3	$\tilde{q}_{31}$	$\tilde{q}_{32}$	$\tilde{q}_{33}$						
τ_1	a_{11}	a_{12}	a_{13}	$\tilde{q}_{11}$					
τ_2	a_{21}	a_{22}	a_{23}	$\tilde{q}_{21}$	$\tilde{q}_{22}$				
τ_3	a_{31}	a_{32}	a_{33}	$\tilde{q}_{31}$	$\tilde{q}_{32}$	$\tilde{q}_{33}$			
τ_1				a_{11}	a_{12}	a_{13}	$\tilde{q}_{11}$		
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τ_3				a_{31}	a_{32}	a_{33}	$\tilde{q}_{31}$	$\tilde{q}_{32}$	$\tilde{q}_{33}$
	0	0	0	0	0	0	0	0	1

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Butcher tableau for third order diagonal SDC on three tasks

τ_1	$\tilde{q}_1$								
τ_2		$\tilde{q}_2$							
τ_3			$\tilde{q}_3$						
τ_1	a_{11}	a_{12}	a_{13}	$\tilde{q}_1$					
τ_2	a_{21}	a_{22}	a_{23}		$\tilde{q}_2$				
τ_3	a_{31}	a_{32}	a_{33}			$\tilde{q}_3$			
τ_1				a_{11}	a_{12}	a_{13}	$\tilde{q}_1$		
τ_2				a_{21}	a_{22}	a_{23}		$\tilde{q}_2$	
τ_3				a_{31}	a_{32}	a_{33}			$\tilde{q}_3$
	0	0	0	0	0	0	0	0	1

Measure PinT speedup

1. Establish that SDC is faster than time-serial reference method
2. Demonstrate that space-time-parallel scaling is better than space-only scaling
3. Implement in "production" code

Implement RBC in pySDC

- pySDC: Prototyping library for SDC and PFASST
- Demonstrate good performance of SDC for RBC
- Supports GPUs
- See [Speck, 2019]

Implement SDC in Dedalus

- Framework for spatial discretization with pseudo-spectral methods
- Demonstrate SDC implementation in existing code
- Is somewhat optimized
- See [Burns et al., 2020]

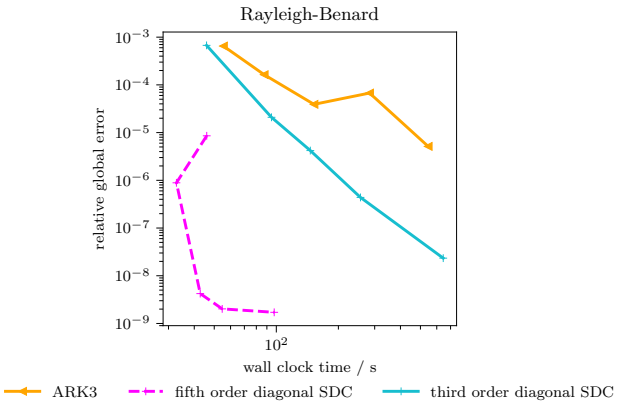
Comparison against DIRK-type method for 2D RBC

Reference method

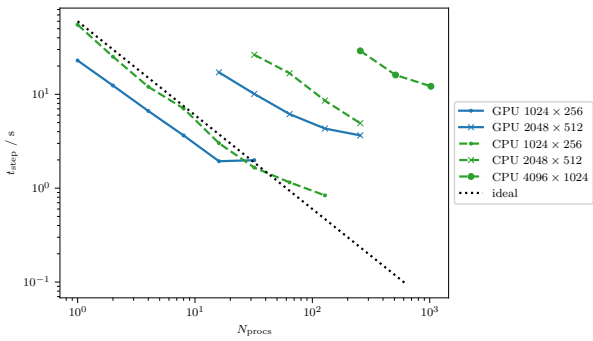
- Need stiffly accurate IMEX method to deal with algebraic constraint
- Best high-order method we could find: Four-stage, third order method ARK3 [Ascher et al., 1997, Section 2.8]

Comparison results

- Third order diagonal SDC on 2 tasks is faster than ARK3
- Increase order of SDC to 5 simply by adding one collocation node
- Fifth-order diagonal SDC on 3 tasks is much faster



3D scaling with pySDC on JURECA / JUWELS booster



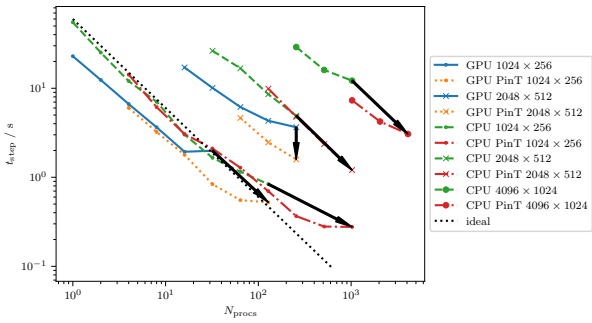
CPUs vs GPUs

- Sparse linear solves not accelerated on GPU
- FFTs faster on GPU

Use diagonal SDC to extend scaling

- Uses 4 tasks in time
- Circumvents space-decomposition limit
- Improves strong scaling
- Enables scaling up to 4096 CPUs

3D scaling with pySDC on JURECA / JUWELS booster



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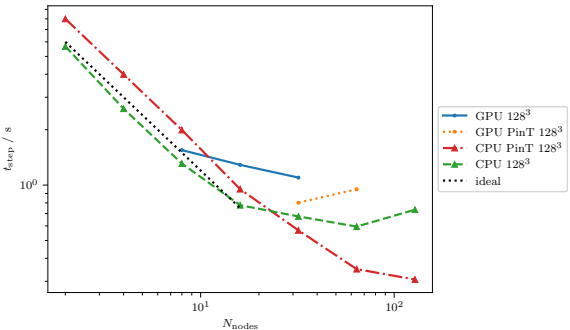
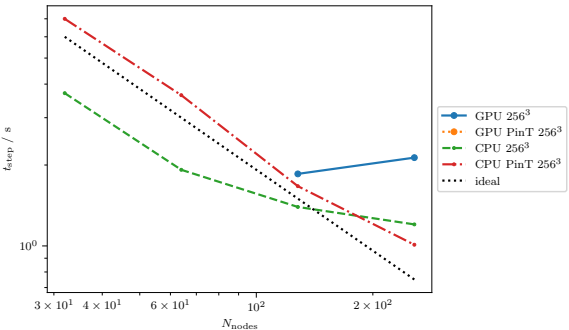
3D scaling with pySDC on JURECA / JUWELS booster

$N = 128^3$



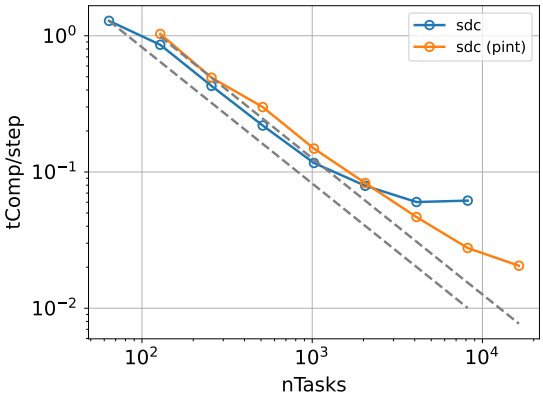
$N = 256^3$



- PinT can again be used to extend scaling limits
- Don't yet know why PinT is slower for few tasks
- GPU implementation suffers from huge memory footprint

3D parallel scaling with Dedalus on JUWELS cluster

$N = 128^3$



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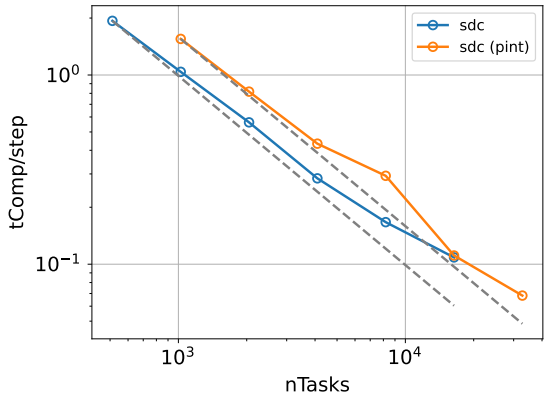

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Next stop: Jupiter

Implementation

- Reduce memory footprint
- Improve GPU performance

Measurements

- Measure performance for $N = 512^3$
- Measure performance on JUPITER

Conclusions

- Diagonal preconditioners from Gaya and Thibaut ([Čaklović et al., 2024]) are excellent
- Diagonal SDC can extend parallel scaling limits
- No coarsening involved
- Works even for complicated benchmark with heavy convection

pySDC

SCAN ME

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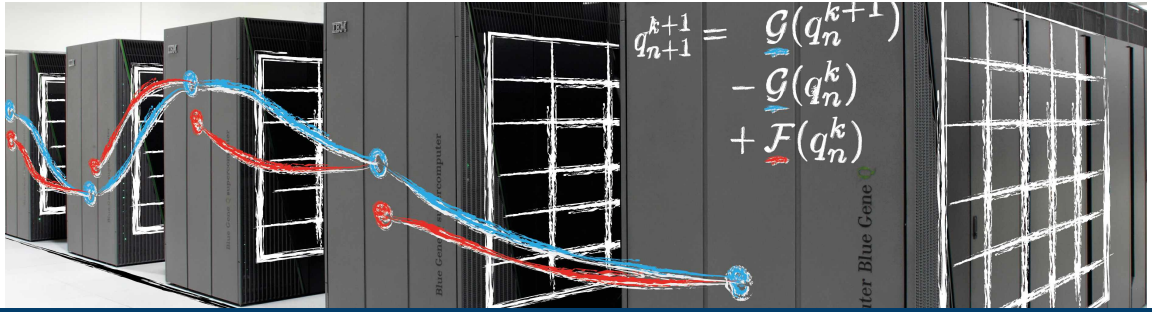

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