ML-enhanced Numerics: From Super-resolution to Neural Operators for Parallel-in-Time Methods

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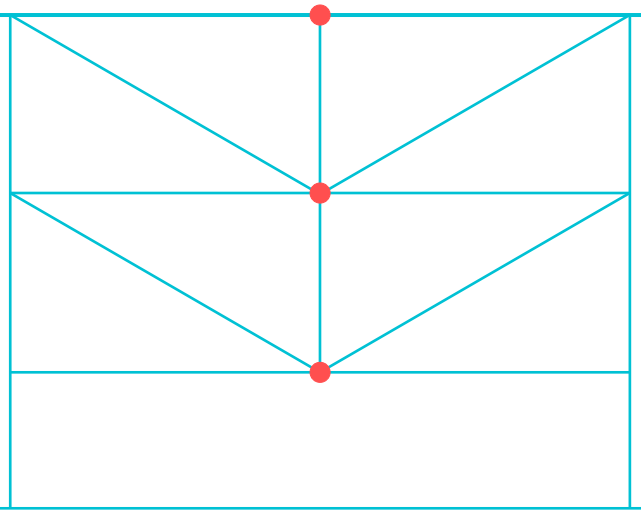

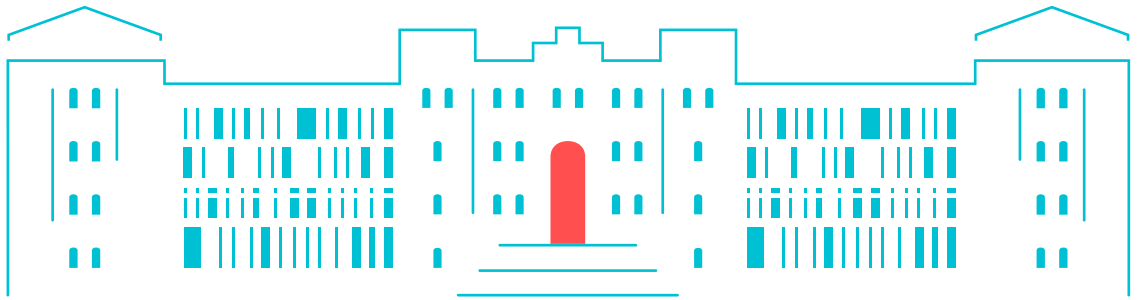

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NeuralPinT

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EuroHPC Joint Undertaking

Sub-mesoscale eddies

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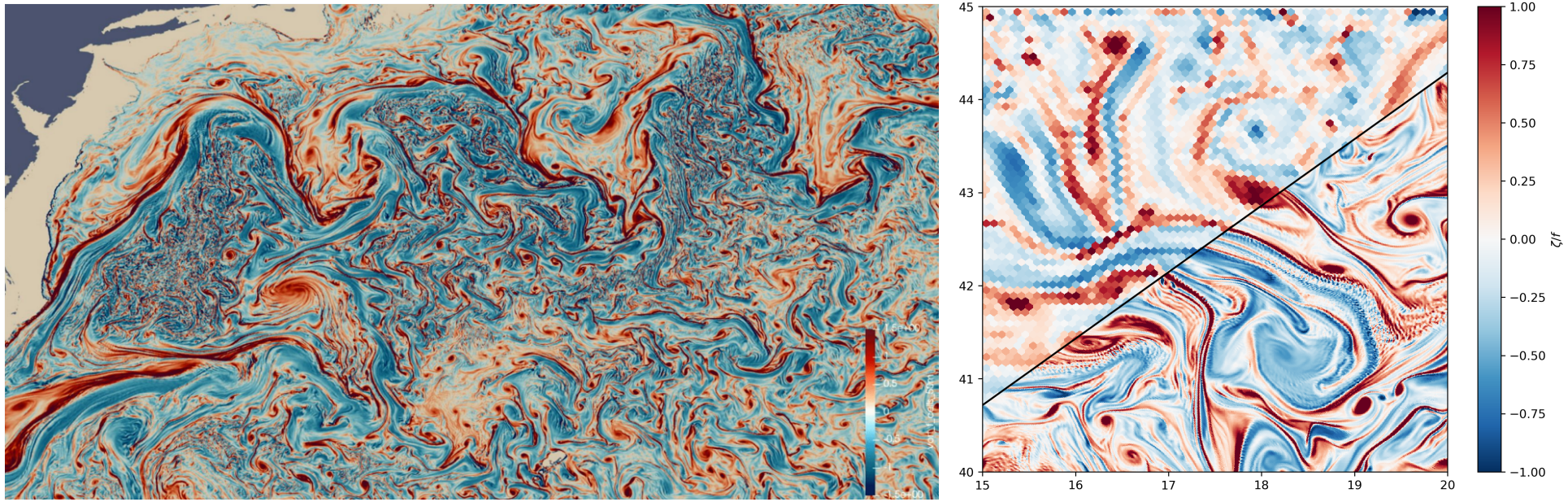

Vorticity in an ICON-O simulation of sub-mesoscale eddies in the North Atlantic (courtesy P. Korn, F. Lapolli, MPI-M)

- resolving sub-mesoscale eddies requires local resolution of $\approx$ 600m
- throughput 64 days per 24h runtime: runs over climatological timescales impractical

➤ solve on coarser grid and correct, add time parallelism

Dynamic deep-learning based superresolution

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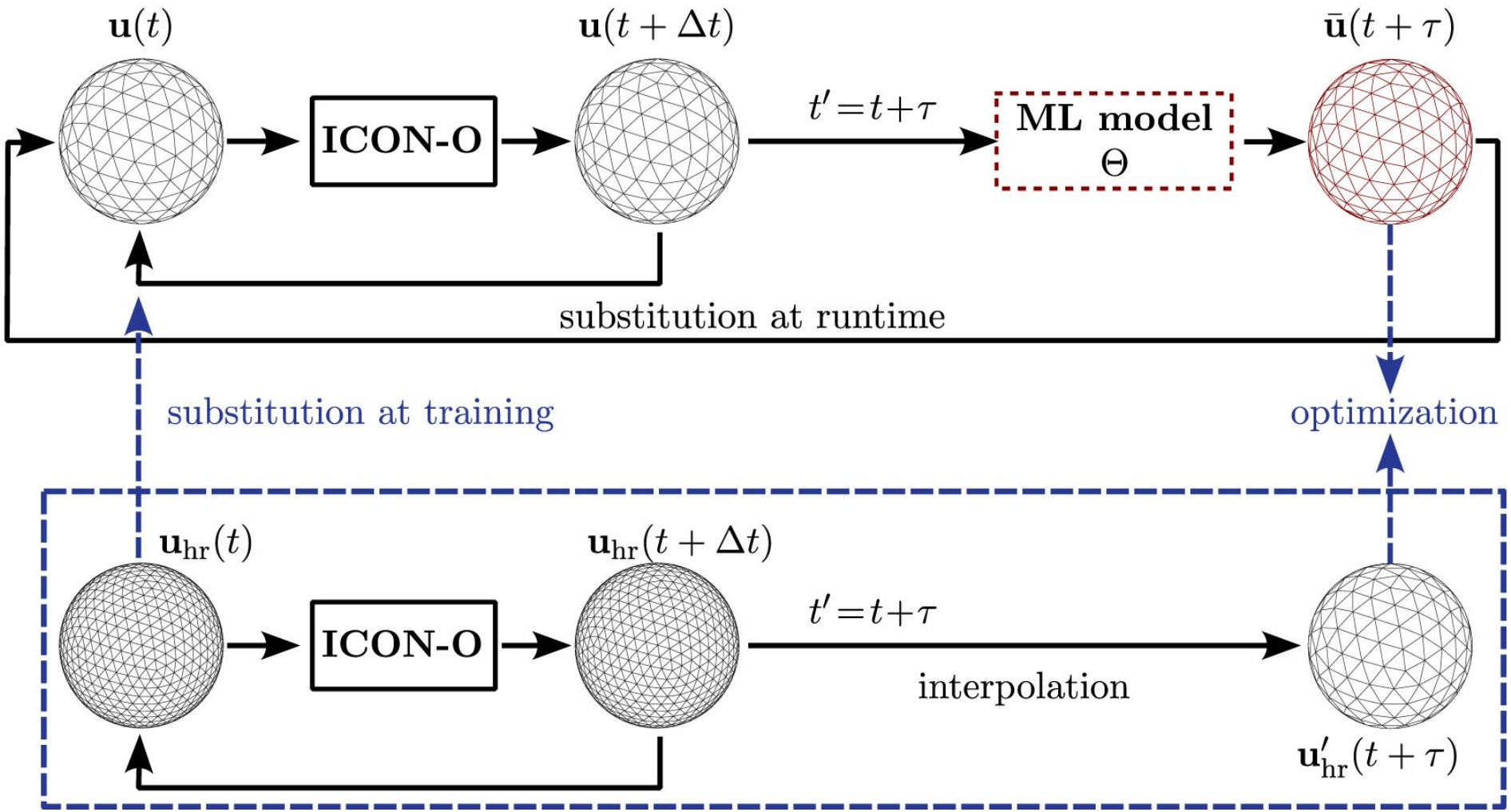

Dynamic deep-learning based superresolution

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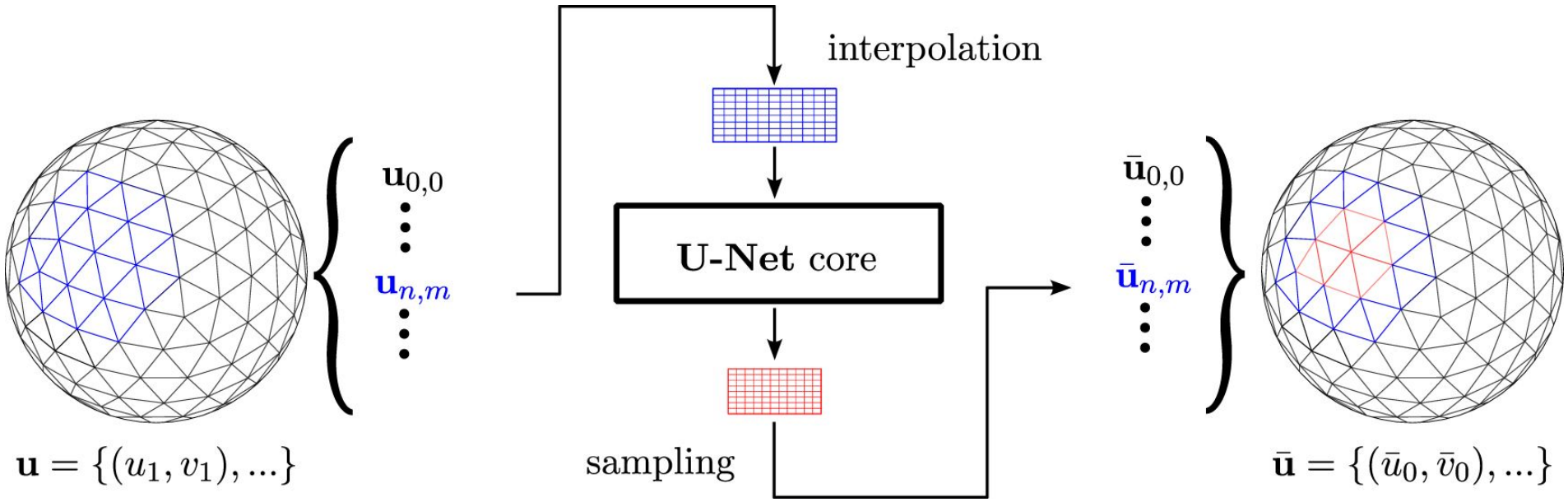

Dynamic deep-learning based superresolution

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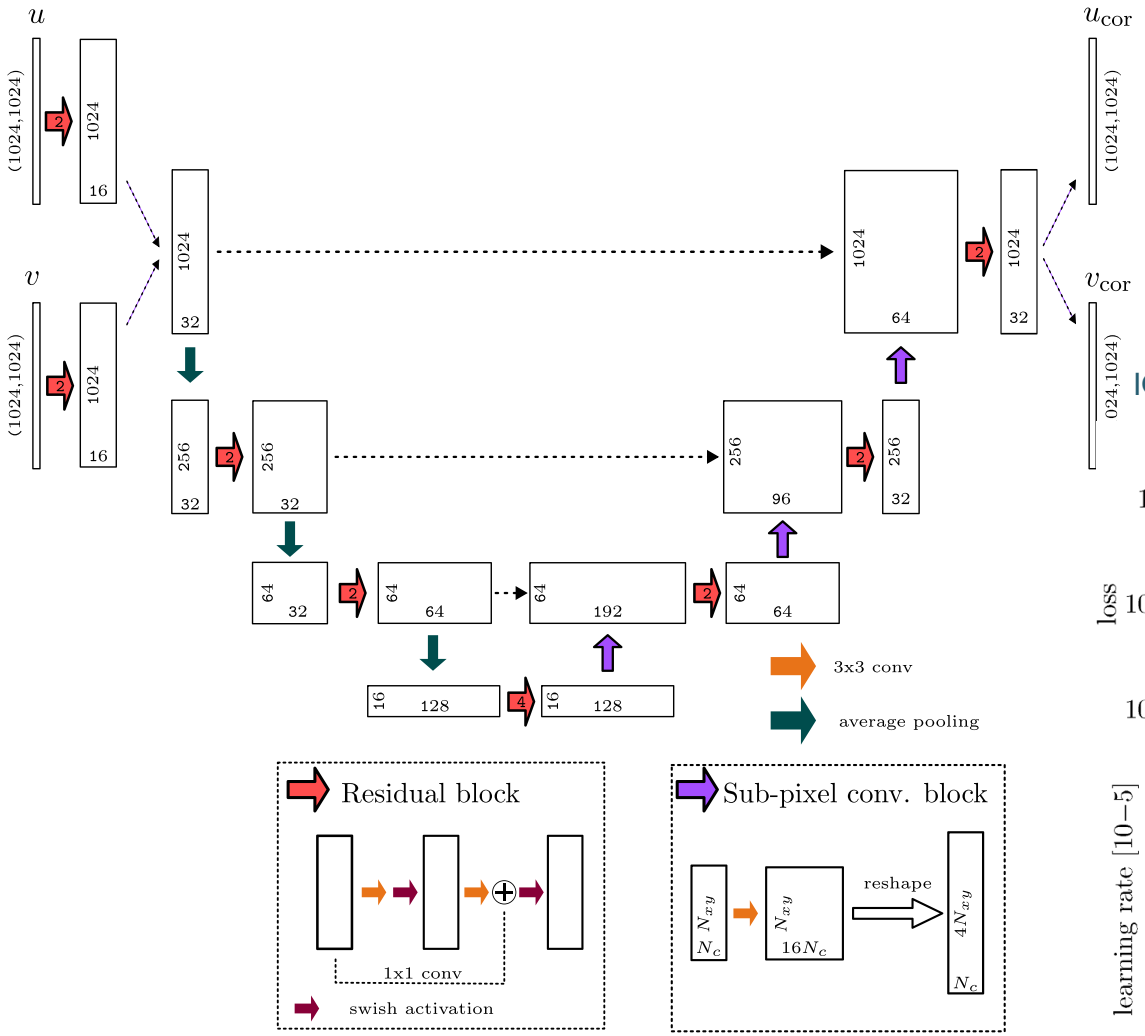
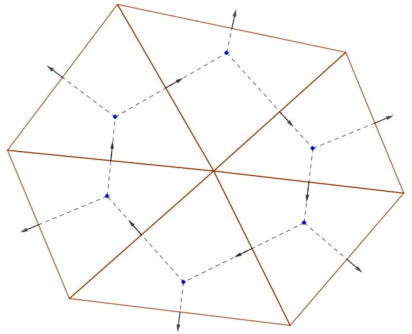
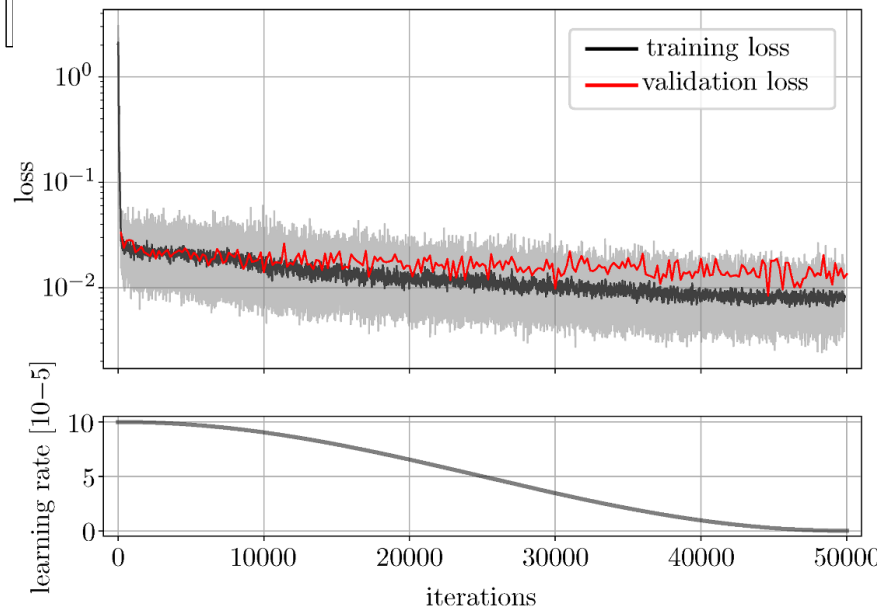




ICON-O grid cell: height in cells, velocity on edges



Dynamic deep-learning based superresolution

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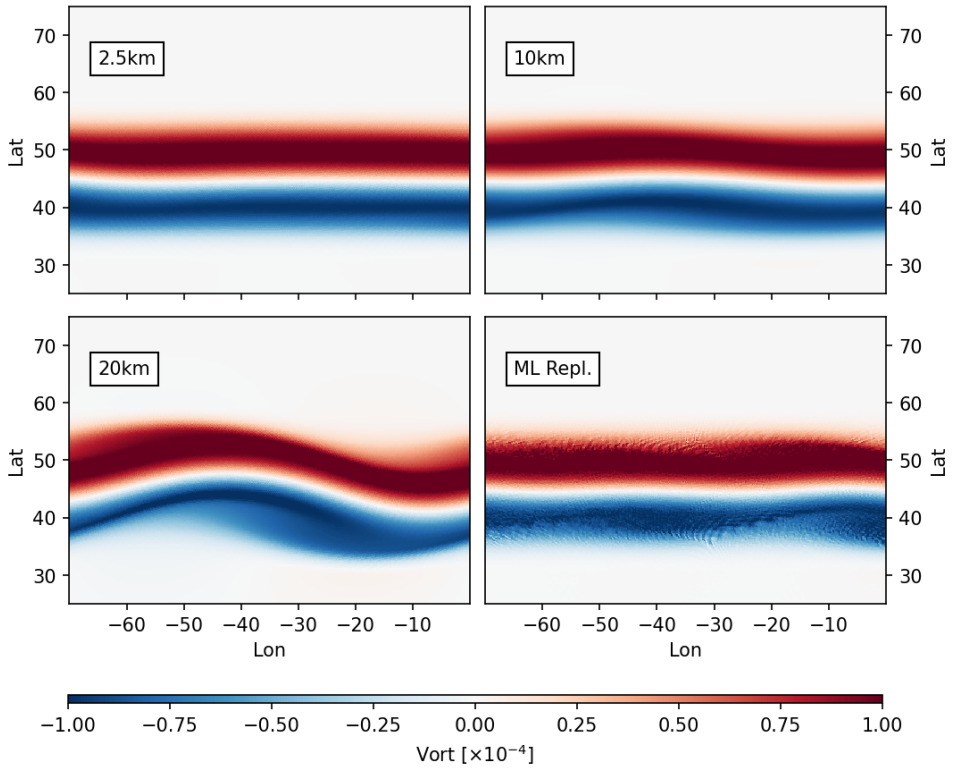
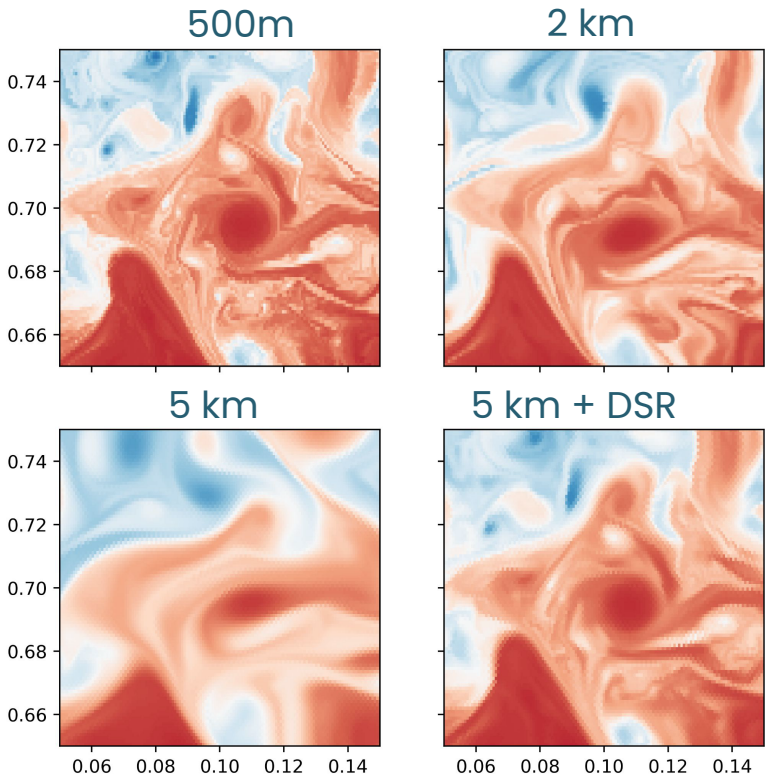
Barotropic instability (SWE, 2D)



- DSR corrects onset of instability on coarse grid

Baroclinic instability (3D)



temperature after 20 days, correction every 6h

(courtesy M. Witte, DKRZ)

Witte, Lapolli, Freese, G., Ruprecht, Korn, Kadow: Dynamic deep learning based super-resolution for the shallow water equations. Machine Learning: Science and Technology 6, 015060. https://dx.doi.org/10.1088/2632-2153/ada19f (2025)

(Physics-informed/Fourier) Neural Operators [Li et al. '21/'23]

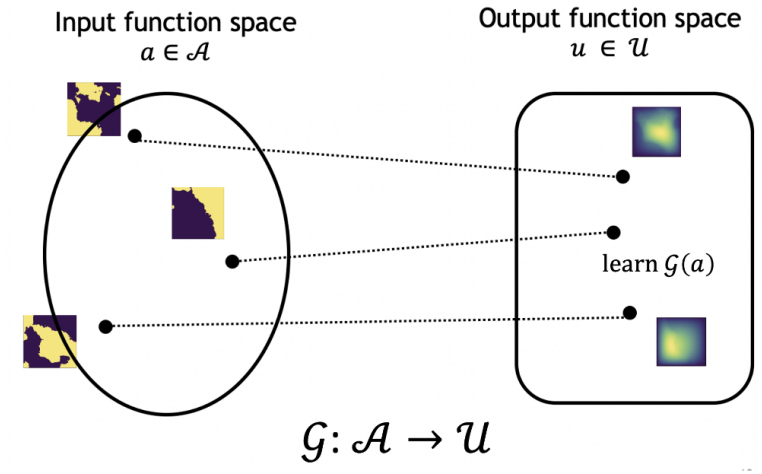


Figure: [Li et al. '21/'23]

- trainable without data (PDE residual as loss)
- fast to evaluate once trained
- leverage heterogeneous architectures

➤ use as fast propagators in Parallel-in-Time (PinT) methods

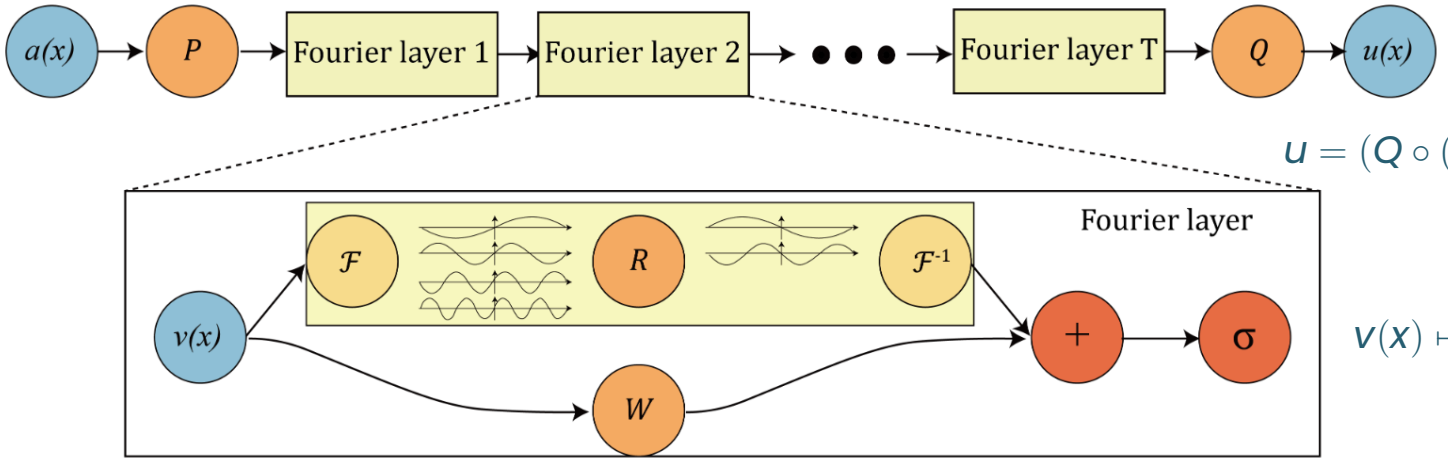


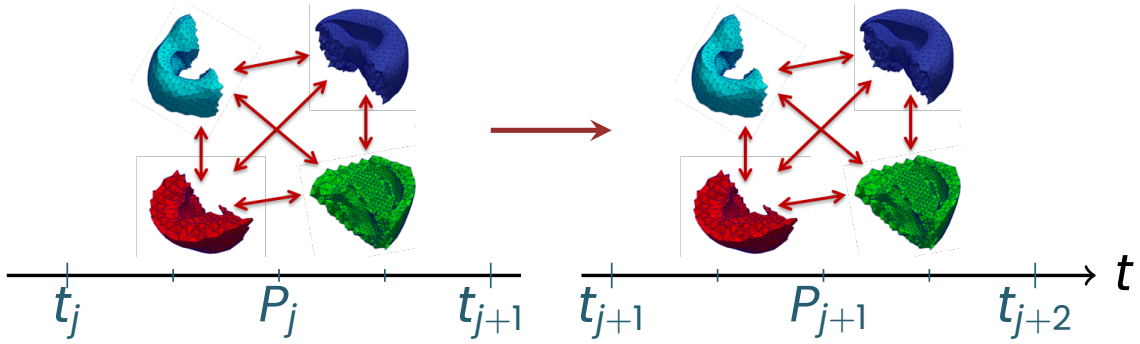
Figure: [Li et al. '21]

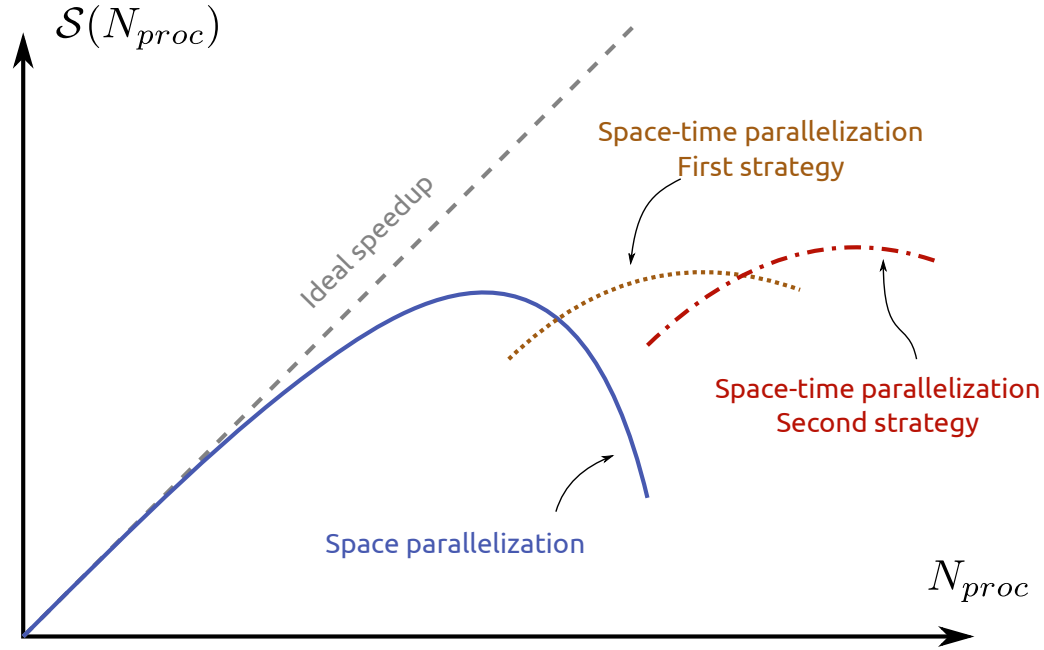
$$u = (Q \circ (K_\ell \circ \sigma_\ell \circ \cdots \circ \sigma_1 \circ K_0) \circ P)(a)$$

K an integral operator:

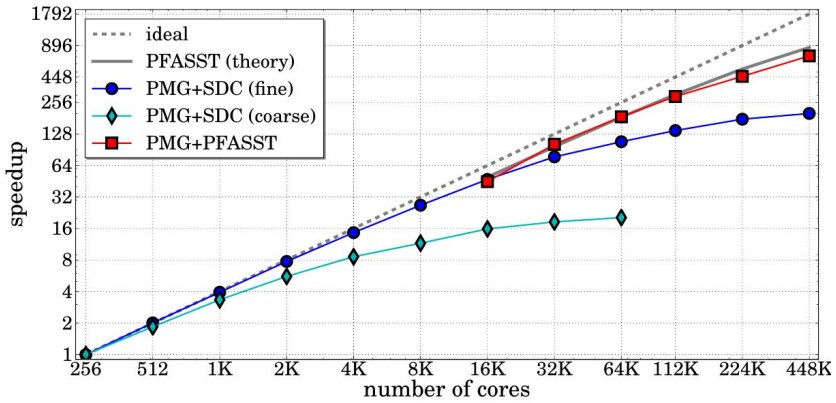
$$v(x) \mapsto \int \kappa(x, y) v(y)\, \mathrm{d}y + W v(v)$$

What PinT promises





[scaling sketch courtesy of Thibaut Lunet]



* D. Ruprecht, R. Speck, M. Emmett, M. Bolten, and R. Krause, "*Poster: Extreme-scale space-time parallelism*," in Proceedings of the 2013 Conference on High Performance Computing Networking, Storage and Analysis Companion, ser. SC '13 Companion, Denver, Colorado, USA, 2013.

Parareal [Lions et al. '01]

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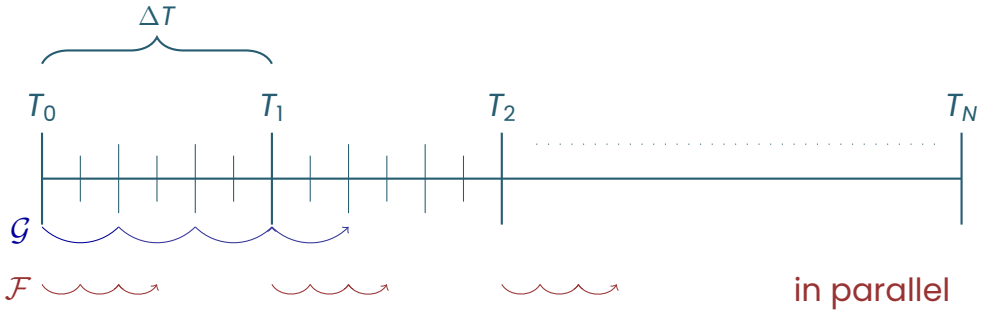
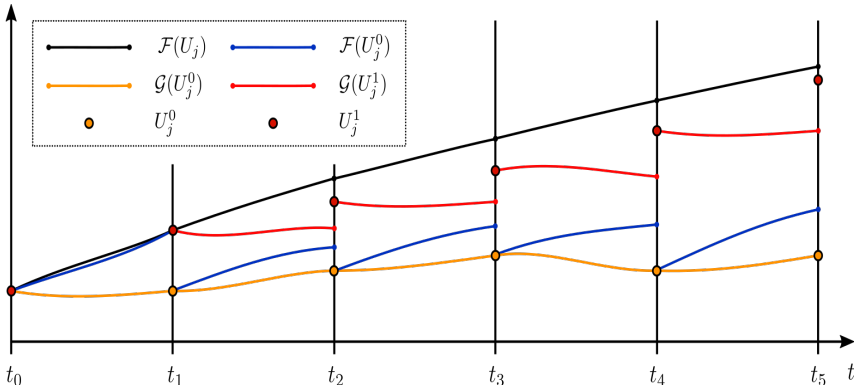
Solve IVPs $y_t = f(y)$



in parallel



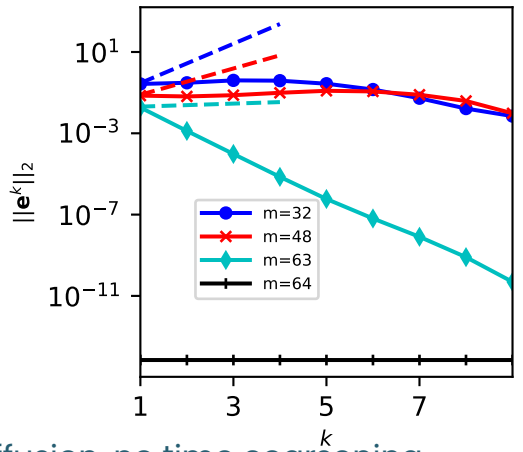
sketch courtesy of Kamran Pentland

In k'th Parareal iteration:

$$Y_n^k = \mathcal{G}(Y_{n-1}^k) + \mathcal{F}(Y_{n-1}^{k-1}) - \mathcal{G}(Y_{n-1}^{k-1}), \quad n = 1, \ldots, N$$

speedup: $S(N_p) \leq \min\left(\frac{N_p}{N_{\text{it}}}, \frac{\text{runtime fine}}{\text{runtime coarse}}\right)$

Aim : Make $\mathcal{G}$ cheaper while keeping K constant



1d adv., no num. diffusion, no time coarsening

Test problem: Black-Scholes equation

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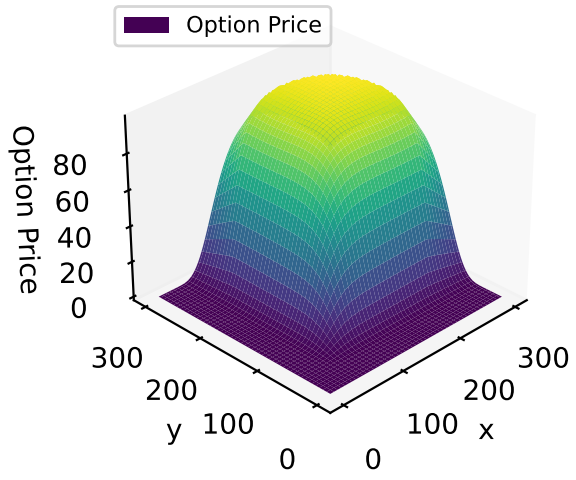
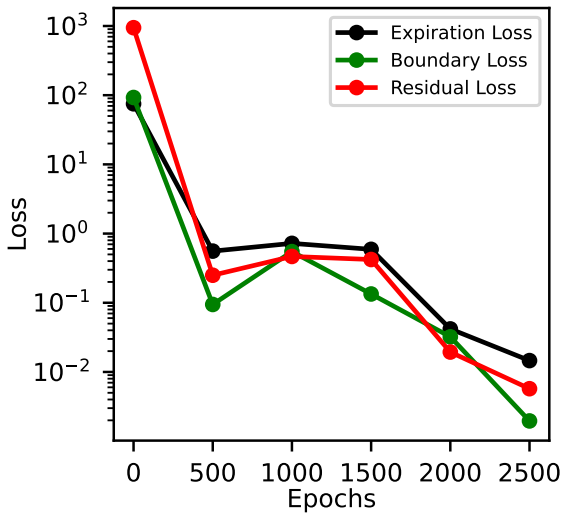
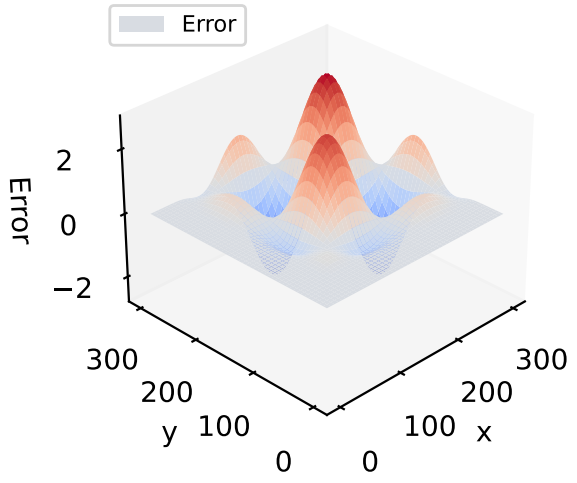
$$\frac{\partial u}{\partial t} + \frac{1}{2}\sigma_1^2 x^2 \frac{\partial^2 u}{\partial x^2} + \frac{1}{2}\sigma_2^2 y^2 \frac{\partial^2 u}{\partial y^2}$$
$$+ \rho\sigma_1\sigma_2 xy \frac{\partial^2 u}{\partial x \partial y} + rx\frac{\partial u}{\partial x} + ry\frac{\partial u}{\partial y} - ru = 0$$

+ Dirichlet boundary conditions, terminal condition







Neural operators for Parareal

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Train ML model to predict $y(t_n) \mapsto y(t_{n+1})$

1. feedforward neural network (fully connected) PINN-P
2. Fourier neural operator PINO

Loss function:

- PDE residual $f(V)$: $\text{MSE}_\text{f} = \frac{1}{N_f} \sum_{i=1}^{N_f} \|f(\tilde{V}(t_i, S_i))\|^2$
- boundary loss term: $\text{MSE}_\text{b} = \frac{1}{N_b} \sum_{i=1}^{N_b} \left\|\tilde{V}(t_i, S_i) - V(t_i, S_i)\right\|^2$

  (better use hard constraints)
- loss at expiration: $\text{MSE}_\text{exp} = \frac{1}{N_\text{exp}} \sum_{i=1}^{N_\text{exp}} \left\|\tilde{V}(T, S_i) - \max(S_i - K, 0)\right\|^2$
- total loss: $\text{MSE}_\text{total} = \text{MSE}_f + \text{MSE}_\text{exp} + \text{MSE}_b$ (no data loss!)

Parareal performance

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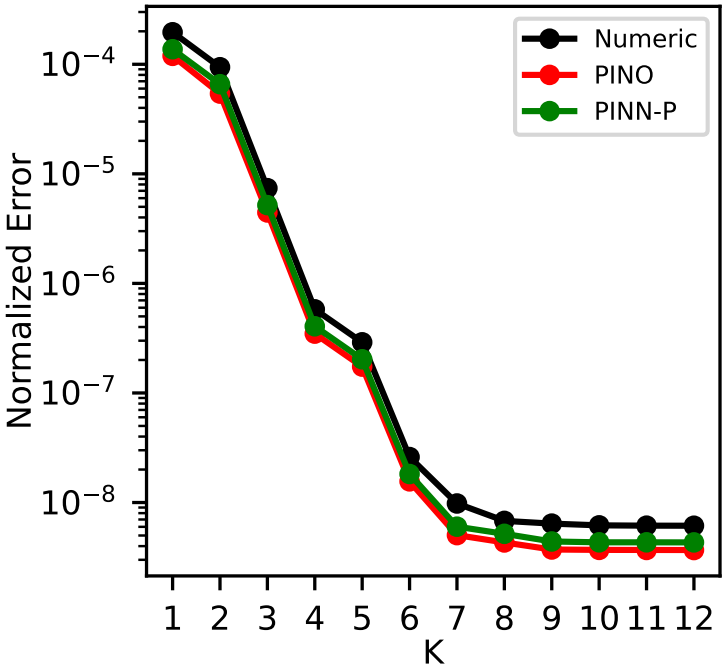
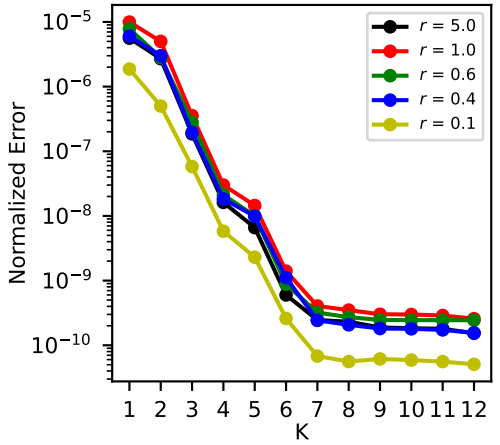
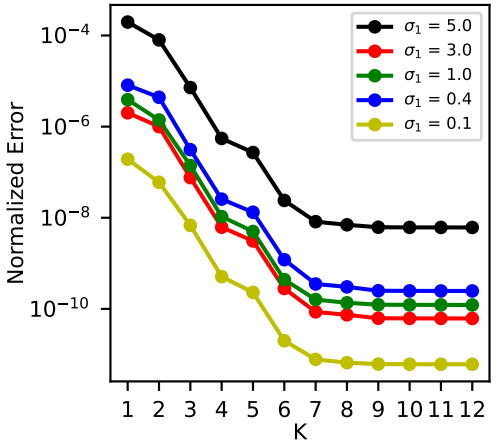
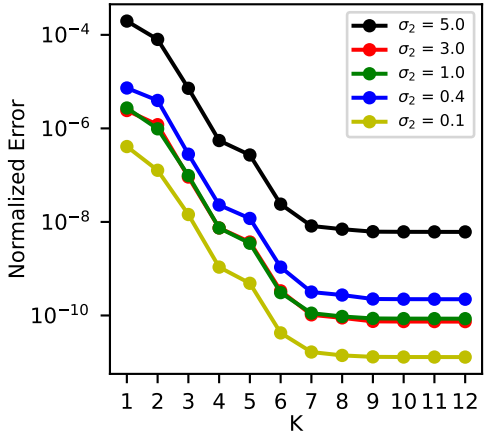
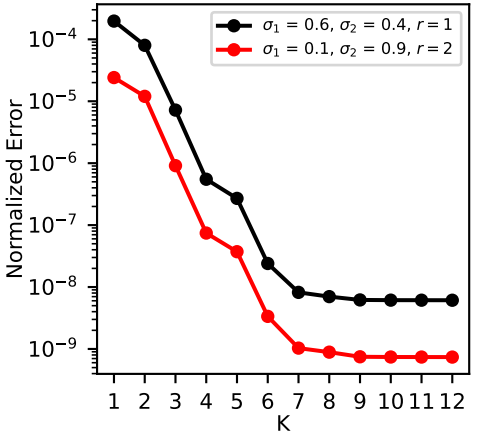


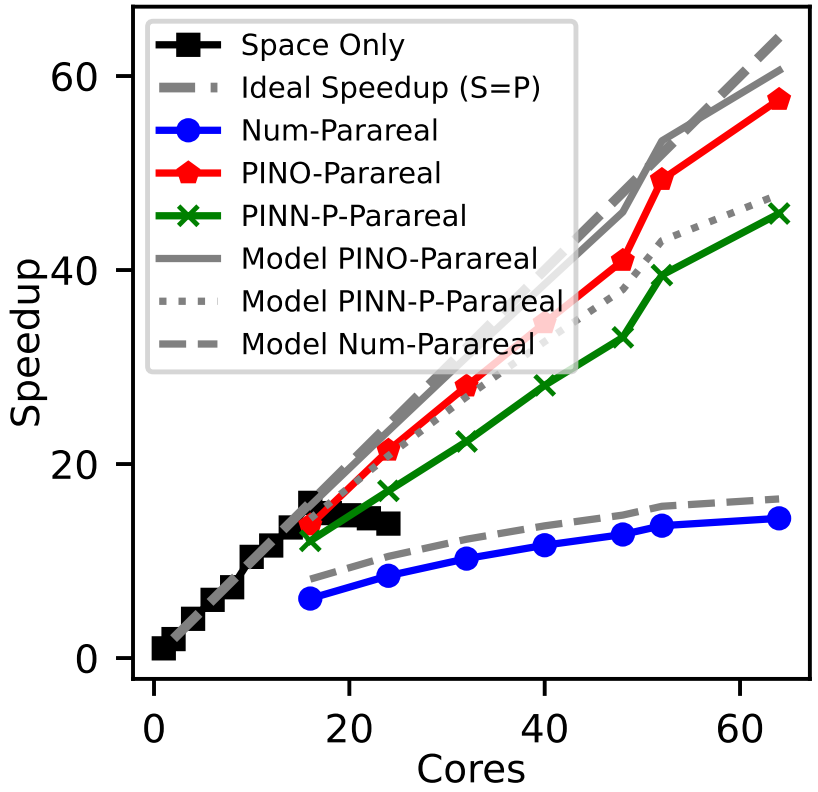


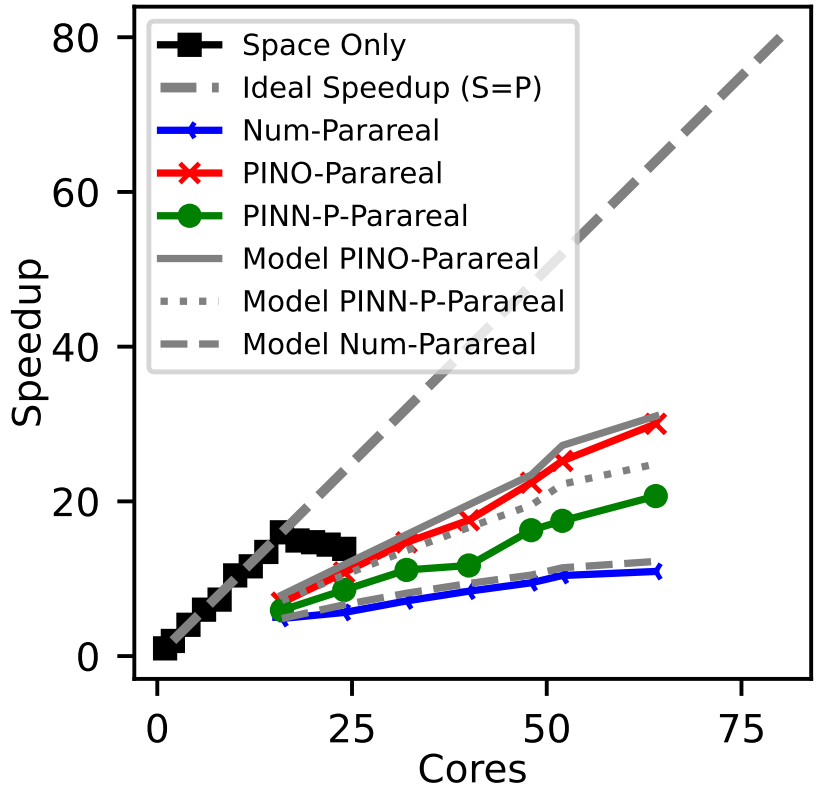






Parareal performance





- Ibrahim, G., Ruprecht: Parareal with a physics-informed neural network as coarse propagator, Parallel Processing. Euro-Par 2023. Lecture Notes in Computer Science, vol 14100. Springer (2023) https://doi.org/10.1007/978-3-031-39698-4_44
- Ibrahim, G., Ruprecht: Space-time parallel scaling of Parareal with a Fourier Neural Operator as coarse propagator, arXiv:2404.02521 (accepted at PASC 2025)

Rayleigh-Bénard Convection

Convective motion in fluids due to temperature gradient

$$\frac{\partial U}{\partial t} + U \cdot \nabla U = -\frac{1}{\rho}\nabla p + \mu \nabla^2 U + g e_z T$$

$$\frac{\partial T}{\partial t} + U \cdot \nabla T = \alpha \nabla^2 T$$

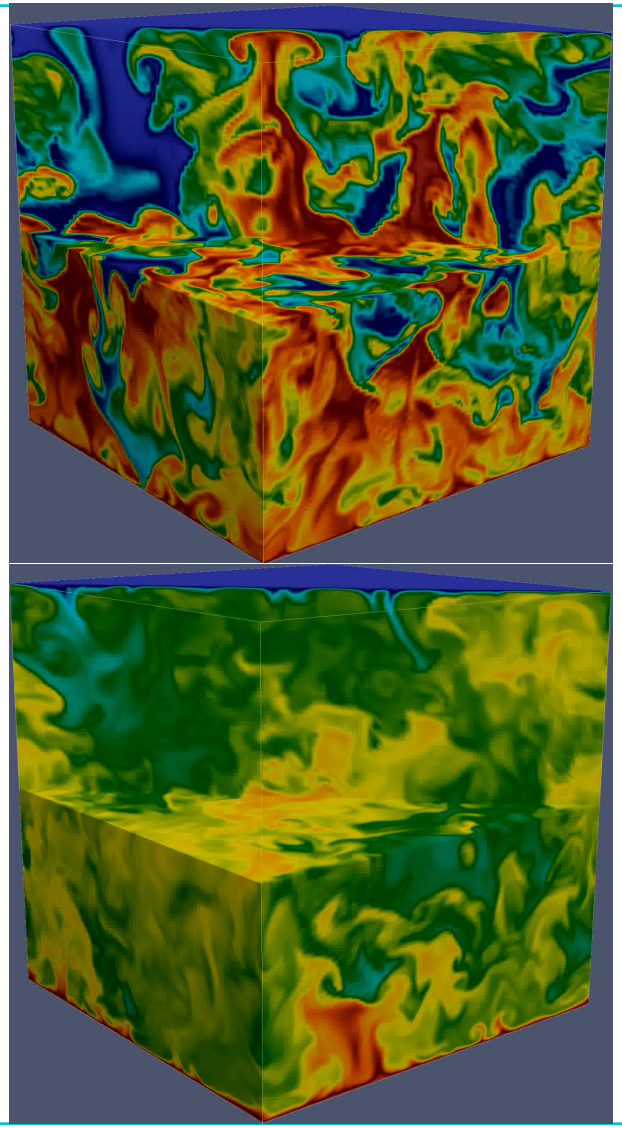
$$\operatorname{div}(U) = 0$$

$$\int_\Omega p \, dx = 0$$

$$\mathrm{Ra} = \frac{\rho \beta \Delta T L^3 g}{\mu \alpha}$$

Parareal: moderate speedup, performance degrades for high Ra

[Clarke et al. '20]



Spectral Deferred Corrections (SDC) [Dutt et al. '00]

Fully implicit RKM/Collocation: dense matrix in Butcher tableau

$$\begin{array}{c|c} c & Q \\ \hline & b^T \end{array} \qquad k_i = f\left(t_n + c_i h, y_n + h\sum_{j=1}^{s} q_{ij} k_j\right) \qquad y_{n+1} = y_n + h\sum_{i=1}^{s} b_i k_i$$

- expensive to solve $Y - \Delta t Q F(Y) = Y_0$

➤ use preconditioned fixed-point iteration

- find suitable preconditioner (lower triangular)
- iterate

$$Y^{k+1} - \Delta t Q_\Delta F(Y^{k+1}) = Y_0 + \Delta t (Q - Q_\Delta) F(Y^k)$$

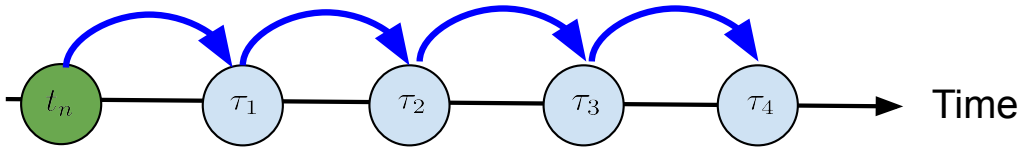
- preconditioner inversion by forward substitution ("sweep")

Preconditioners, e.g., based on Euler

$$Q_\Delta^{\text{EE}} = \begin{bmatrix} 0 & 0 & \dots & 0 & 0 \\ \Delta\tau_2 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \Delta\tau_2 & \Delta\tau_3 & \dots & \Delta\tau_M & 0 \end{bmatrix} \quad Q_\Delta^{\text{IE}} = \begin{bmatrix} \Delta\tau_1 & 0 & \dots & 0 \\ \Delta\tau_1 & \Delta\tau_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \Delta\tau_1 & \Delta\tau_2 & \dots & \Delta\tau_M \end{bmatrix}$$

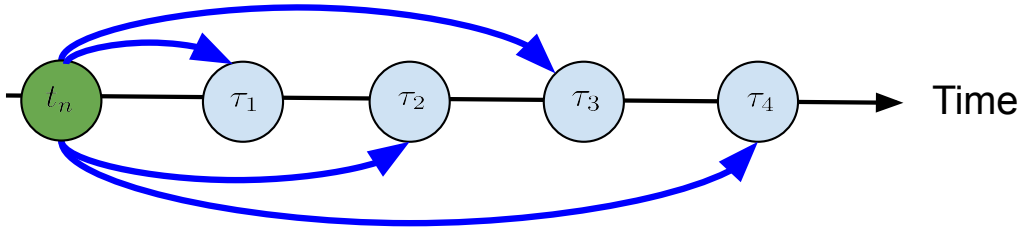
or St. Martin's LU trick [Weiser '14]

$$Q_\Delta^{\text{LU}} = U^T \text{ for } Q^T = LU$$



$$y_m^{k+1} = y_n + \Delta t \sum_{j=1}^{M} q_{m,j} f(y_j^k) + \Delta t \sum_{j=1}^{m} \alpha_j \left(f(\tau_j, y_j^{k+1}) - f(\tau_j, y_j^k) \right)$$

Choose diagonal Q_Δ



$$y_m^{k+1} = y_n + \Delta t \sum_{j=1}^{M} q_{m,j} f(y_j^k) + \Delta t \alpha_m \left(f(\tau_m, y_m^{k+1}) - f(\tau_m, y_m^k) \right)$$

Simple choices, e.g.,

$$Q_\Delta^{\text{Qpar}} = \text{diag}(q_{ii}), \qquad Q_\Delta^{\text{IEpar}} = \text{diag}(\tau_1, \ldots, \tau_m)$$

but: slow convergence [van der Houwen/ Sommeijer 1991, Speck '18]

Alternative: optimize coefficients (e.g., [Speck '18, pySDC])

Parallel SDC – optimize coefficients

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Dahlquist's test equation:

$$y' = \lambda y,\ y(0) = 1 \quad \lambda \in \mathbb{C}, t \in [0,1]$$

SDC sweep:

$$(I - \Delta t Q_\Delta) y^{k+1} = \Delta t \lambda (Q - Q_\Delta) y^k + y_0$$

error propagation matrix:

$$e^{k+1} = K(z) e^k, \quad K(z) = z(I - zQ_\Delta)^{-1}(Q - Q_\Delta)$$

with $z = \Delta t \lambda$, e^k error to collocation solution

➤ minimize spectral radius $\rho(K)$

non-stiff limit: $K_{\text{NS}} = \lim_{|z| \to 0} \frac{K(z)}{z} = Q - Q_\Delta$

stiff limit: $K_{\text{S}} = \lim_{|z| \to \infty} K(z) = I - Q_\Delta^{-1} Q$

optimization problems difficult to solve (already for moderate M)

Optimized parallel SDC – non-stiff limit

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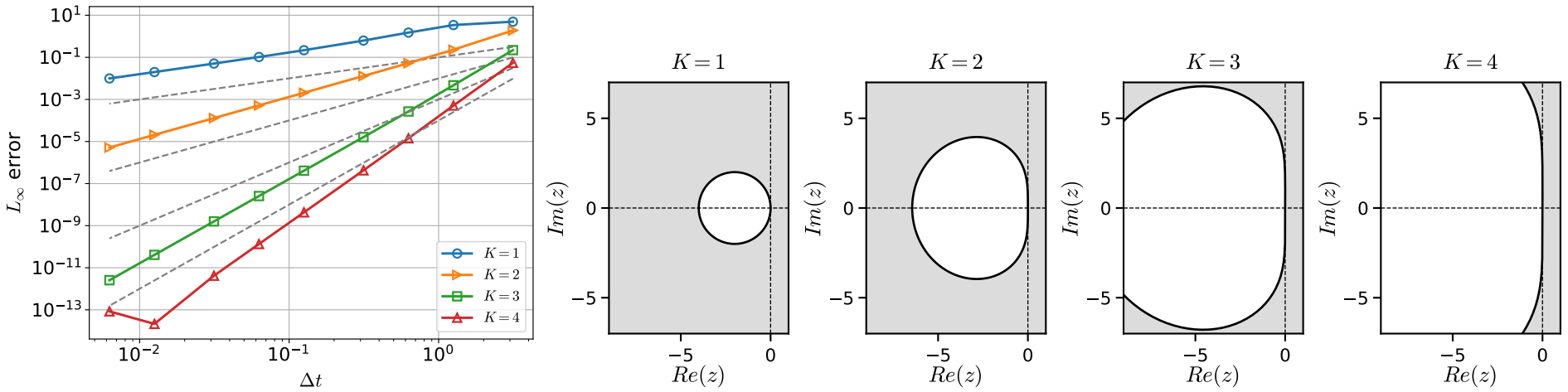
Aim for nilpotency of $K(z)$: $\rho(K_{\text{NS}}) = 0$ for

$$Q_\Delta^{\text{MIN-SR-NS}} = \text{diag}\left(\frac{\tau_1}{M}, \ldots, \frac{\tau_M}{M}\right)$$

➤ each SDC iteration with $Q_\Delta^{\text{MIN-SR-NS}}$ preconditioning removes the respective lowest order term in the error



convergence and stability MIN-SR-NS (4 Radau-II nodes), gray: unstable

Optimized parallel SDC – stiff limit

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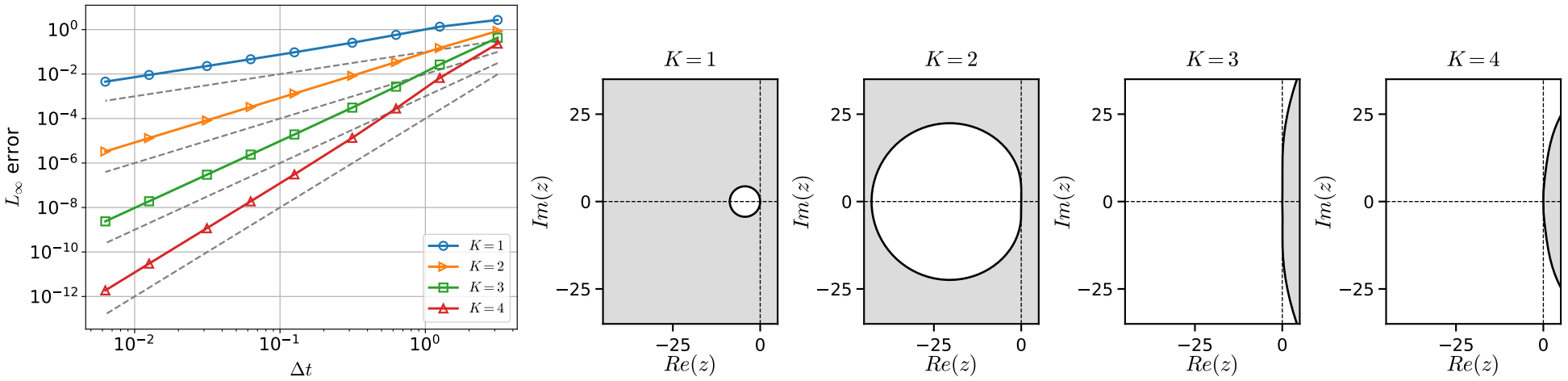
$Q_\Delta^{\text{MIN-SR-S}}$ obtained by numerically minimizing

$$\left|\det\left[(1-t)I + tQ_\Delta^{-1}Q\right] - 1\right|, \quad \forall t \in \{\tau_1, \ldots, \tau_M\}$$

obtains a local minimum of $\rho(K_S)$

- but: no guarantee for existence or uniqueness of solutions
- numerical experiments: increasingly ordered coefficients in Q_Δ lead to better stability



convergence and stability MIN-SR-S (4 Radau-II nodes), gray: unstable

Optimized parallel SDC – stiff limit

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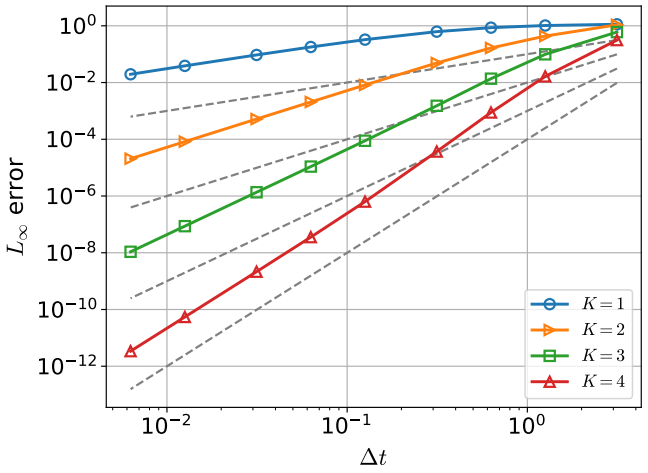
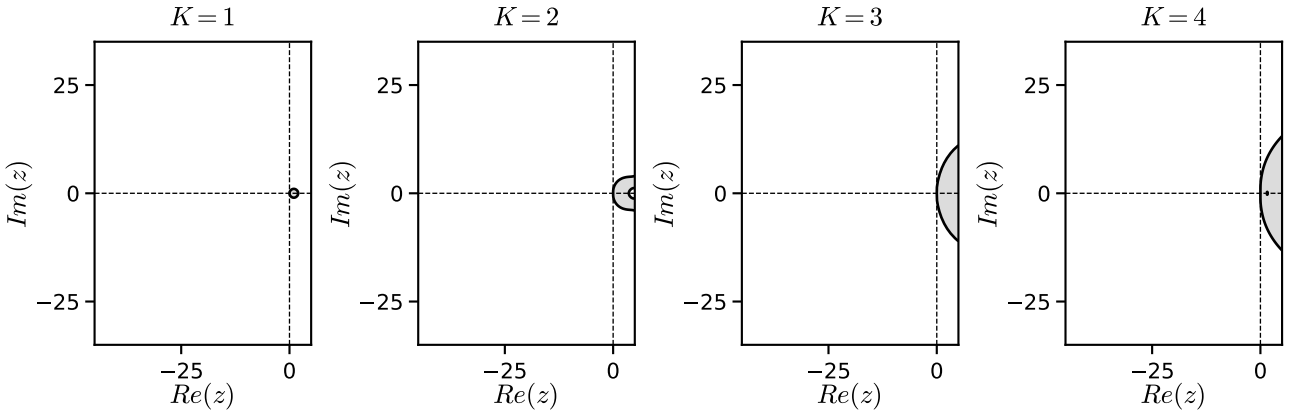
Alternative: iteration-dependent preconditoner $Q_\Delta^{(k)}$
error propagation matrix $K^{(k)}(z) = z(I - zQ_\Delta^{(k)})^{-1}(Q - Q_\Delta^{(k)})$

$$\lim_{|z|\to\infty} e^k = K_S^{(k)} \cdots K_S^{(1)} e^0 \text{ with } K_S^{(k)} = \lim_{|z|\to\infty} K^{(k)}(z) = I - (Q_\Delta^k)^{-1} Q$$

Then:

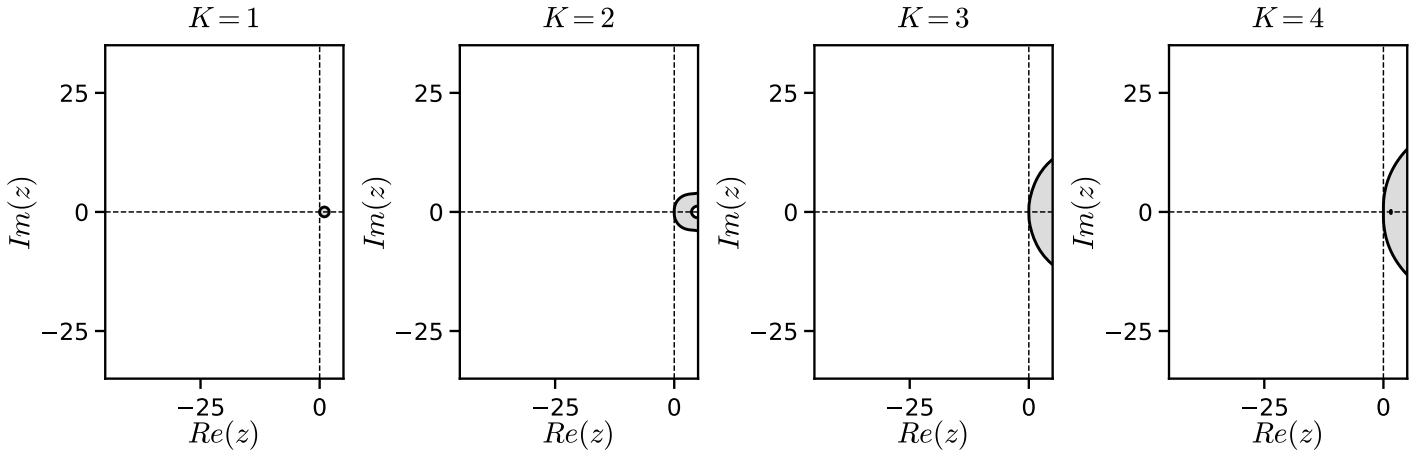
$$Q_\Delta^{\text{MIN-SR-FLEX},(k)} = \text{diag}(\frac{\tau_1}{k}, \ldots, \frac{\tau_M}{k}) \text{ has } K_S^{(M)} \cdot \cdots \cdot K_S^{(1)} = 0$$



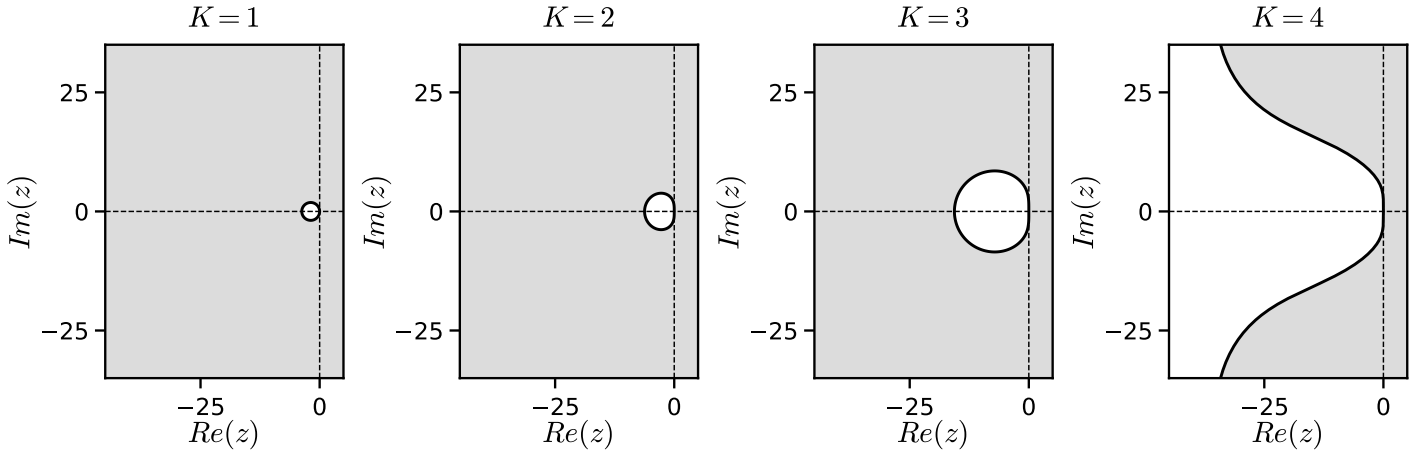


convergence and stability MIN-SR-FLEX (4 Radau-II nodes), gray: unstable

Optimized parallel SDC – stability

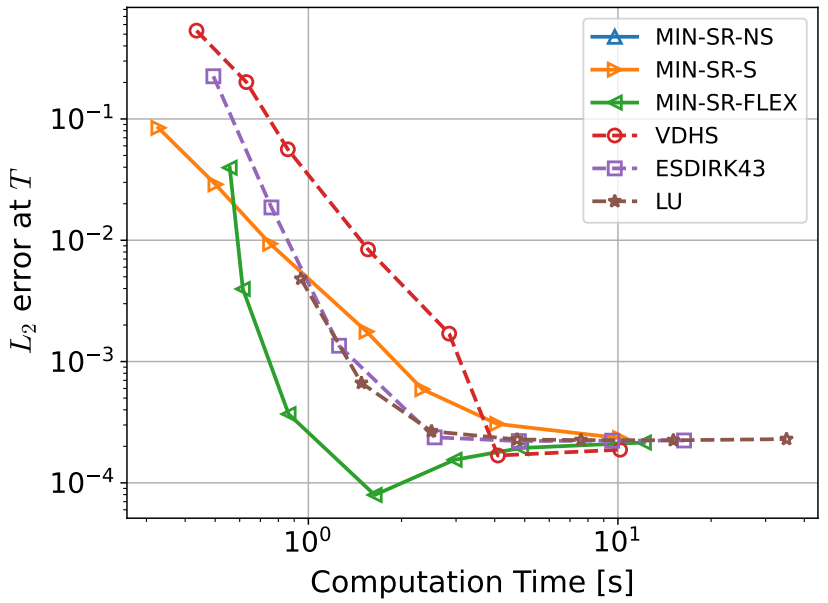


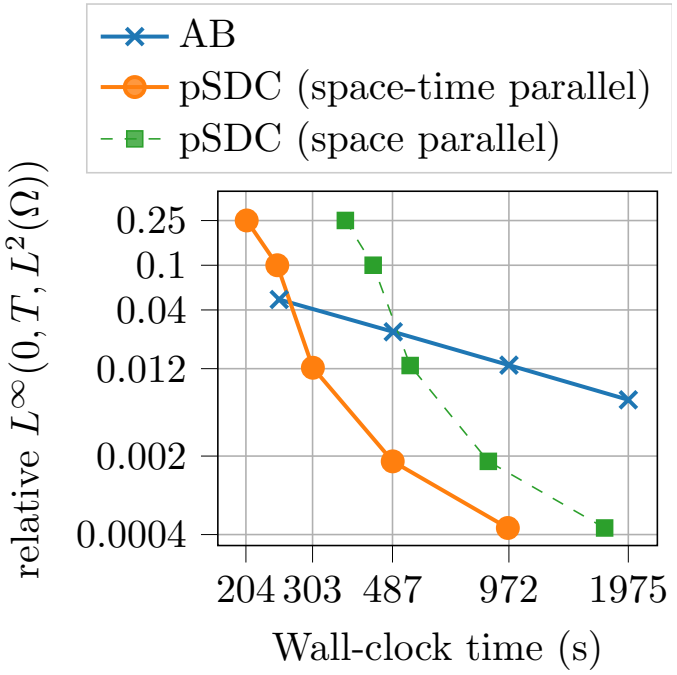
MIN-SR-FLEX (4 Radau-II nodes), similar to LU preconditioner, gray: unstable



[van der Houwen/ Sommeijer 1991] by minimizing $\rho(I - Q_\Delta^{-1}Q)$, gray: unstable

Parallel SDC: Performance





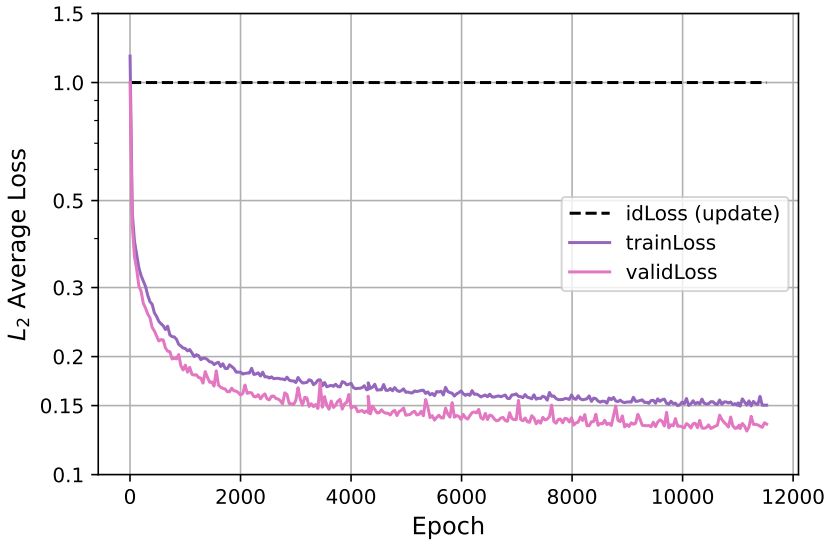
Left: Allen-Cahn equation (pySDC); Right: SWE in ICON-O with MIN-SR-FLEX, 48 cores (4 time, 12 space/48 space)

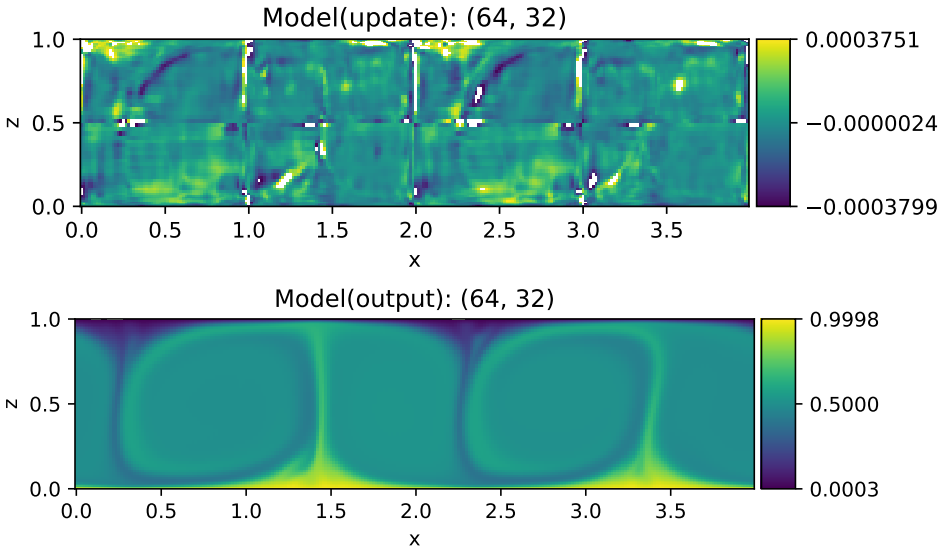
- Čaklović, Lunet, G., Ruprecht: Improving Efficiency of Parallel Across the Method Spectral Deferred Corrections, SIAM J. Sci. Comput. 47(1), 2025
- Freese, G., Lunet, Ruprecht, Schreiber: Parallel performance of shared memory parallel spectral deferred corrections, arXiv 2403.20135, 2024 (under revision in IJHPCA)

FNO for RBC

TUHH

FNO to predict $y(t_n) \mapsto \Delta y = y(t_{n+1}) - y(t_n)$





Variable	Δ**t** $= 1e^{-3}$	Δ**t** $= 1e^{-2}$	Δ**t** $= 1e^{-1}$	Δ**t** $= 1e^{0}$
velocity$_x$	2.4e-05	1.8e-03	1.9e-02	1.6e-01
velocity$_z$	3.2e-05	1.8e-03	1.9e-02	1.4e-01
buoyancy	1.8e-05	9.5e-04	1.0e-02	7.5e-02
pressure	8.5e-06	6.5e-04	7.1e-03	6.0e-02
average	**2.1e-05**	1.3e-03	1.4e-02	1.1e-01

PINO to improve parallel SDC?

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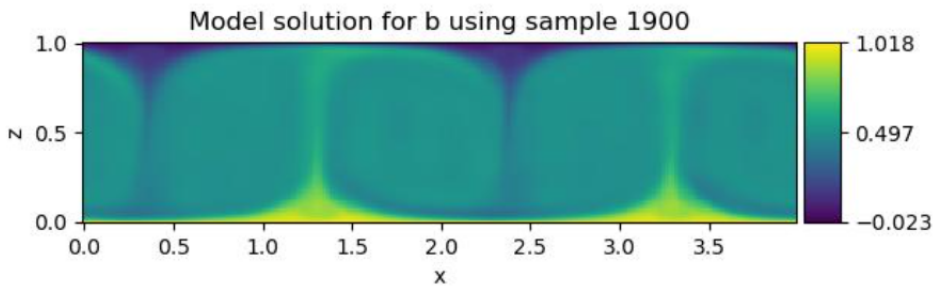
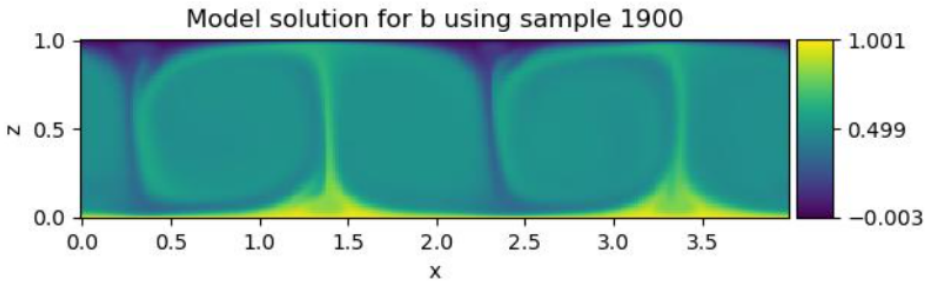
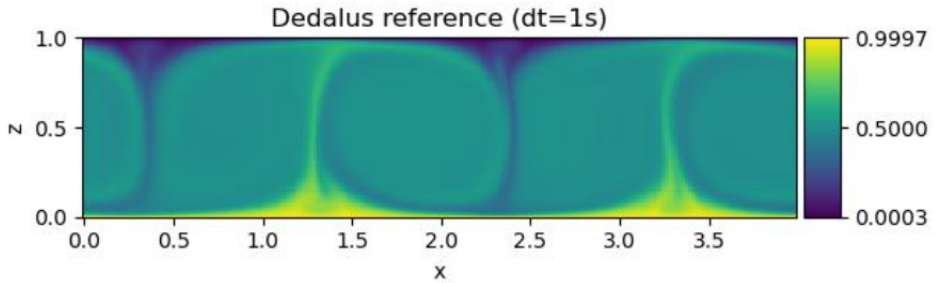
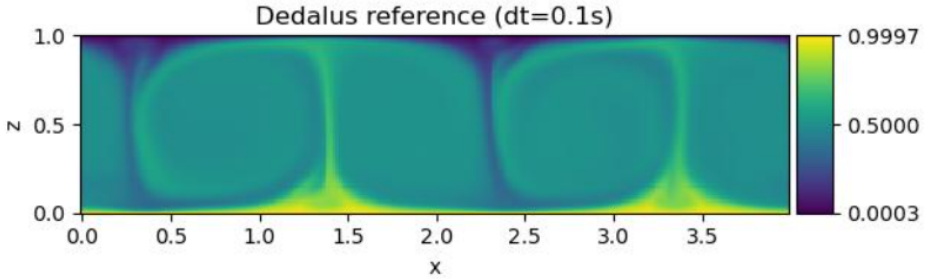
Use a PINO to build an initial guess for the next time-step in SDC:

- potentially very cheap, can be run on GPU
- hopefully more accurate than a simple identity operator (i.e copy)









PINO to improve parallel SDC?

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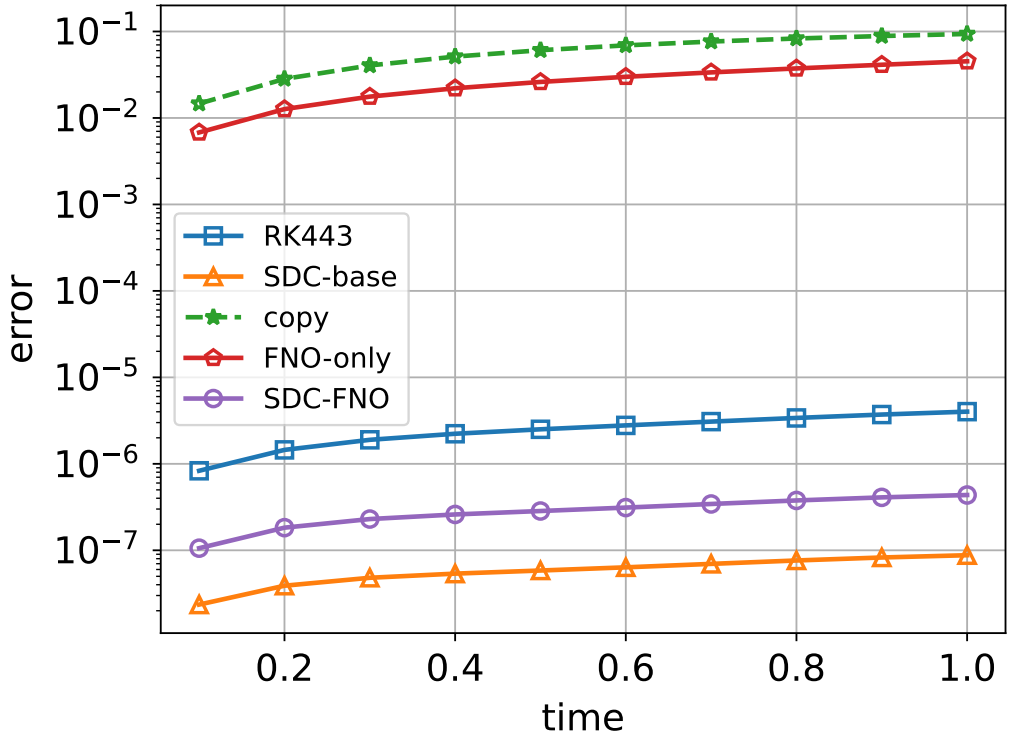
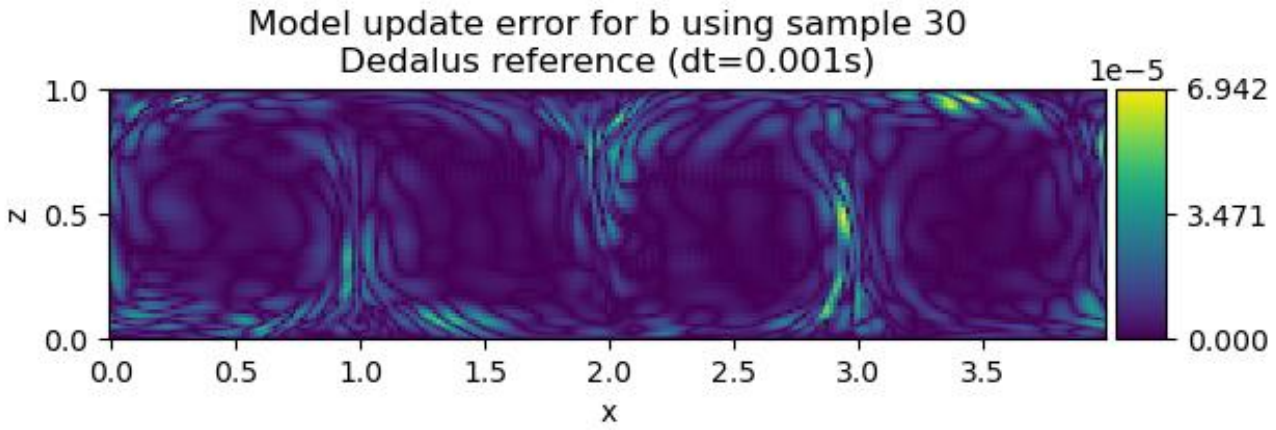
- $\Omega = [0, 4] \times [0, 1], N_x = 256, N_z = 64$
- $T = [0, 1], \Delta t = 0.01$ (stability limit), 4 nodes pSDC (MIN-SR-FLEX)
- pSDC + `dedalus` (pseudo-spectral solver)





PINO to improve parallel SDC?

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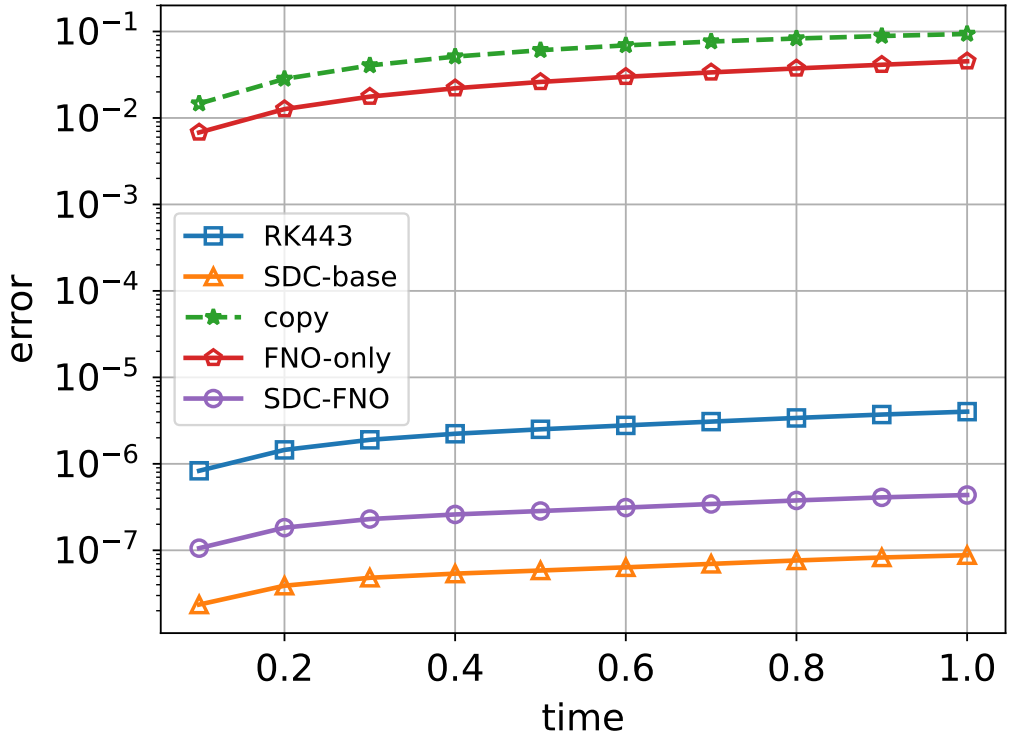

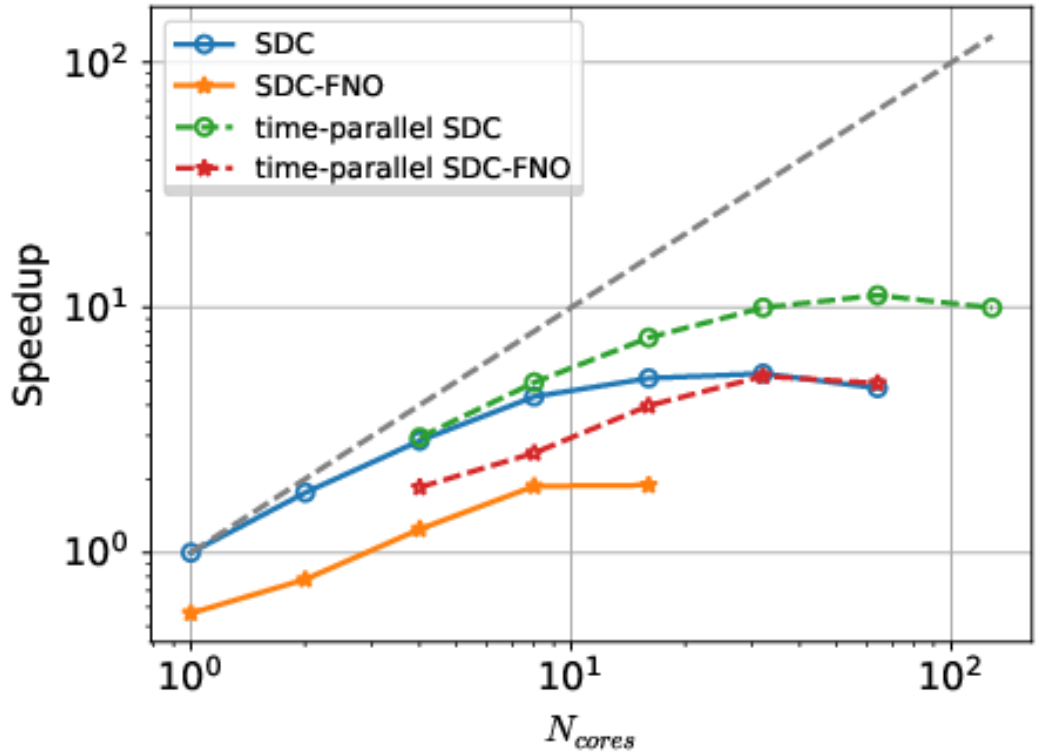

Conclusion

TUHH

- Dynamic deep learning-based superresolution can improve challenging simulations
- Neural operators can make for good coarse propagators in Parareal
- ML models allow leveraging GPU architectures for enhanced inference performance
- …but numerical methods don't always benefit from ML
- Parallel SDC can give good speedups for challenging problems

Thanks!

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