Multigrid Reduction in Time for Chaotic Dynamical Systems

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Introduction and Motivation

MGRIT

solves the IVP

$$\begin{aligned} \mathbf{u}_0 &= \mathbf{f}_0 \\ \mathbf{u}_{i+1} &= \Phi(\mathbf{u}_i) + \mathbf{f}_{i+1} \qquad\qquad i = 0, 1, 2, \ldots, n \end{aligned}$$

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$$A(\mathbf{u}) = \begin{bmatrix} I & & & & \\ -\Phi & I & & & \\ & -\Phi & I & & \\ & & \ddots & \ddots & \\ & & & -\Phi & I \end{bmatrix} \begin{bmatrix} \mathbf{u}_0 \\ \mathbf{u}_1 \\ \mathbf{u}_2 \\ \vdots \\ \mathbf{u}_n \end{bmatrix} = \begin{bmatrix} \mathbf{f}_0 \\ \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_n \end{bmatrix}$$

The two-level algorithm

- The time-domain is partitioned into C-points and F-points

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- F-relaxation sets the residual to zero at each F-point (block Jacobi)

- the coarse system is solved sequentially

The coarse grid equation

- The "ideal" coarse grid equation applies Φ m-times per interval

$$A_*(\mathbf{u}) = \begin{bmatrix} I & & & & \\ -\Phi^m & I & & & \\ & -\Phi^m & I & & \\ & & \ddots & \ddots & \\ & & & -\Phi^m & I \end{bmatrix} \begin{bmatrix} \mathbf{u}_0 \\ \mathbf{u}_m \\ \mathbf{u}_{2m} \\ \vdots \\ \mathbf{u}_n \end{bmatrix} = \begin{bmatrix} \mathbf{f}_0 \\ \mathbf{f}_m \\ \mathbf{f}_{2m} \\ \vdots \\ \mathbf{f}_n \end{bmatrix}$$

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★ This system is no less expensive to solve

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- A_* is approximated by the coarse operator A_c, where $\Phi_c \approx \Phi^m$ (rediscretization)

The two level algorithm is a nonlinear splitting method

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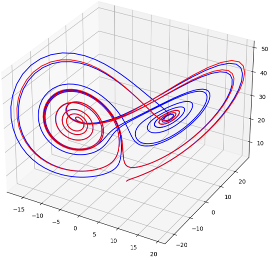
$$[\boldsymbol{\tau}(\mathbf{u})]_i = \Phi^m(\mathbf{u}_{i-m}) - \Phi_c(\mathbf{u}_{i-m})$$

The MGRIT algorithm: overview

- MGRIT extends the two level algorithm to an arbitrary number of levels
  - recursive application of the two-level algorithm
  - the coarsest grid may have as few as two time-points!
- optimal scaling for parabolic problems using FCF relaxation
- becomes more efficient as total number of time-points increases

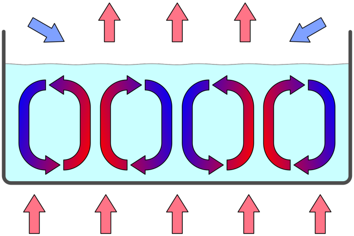
MGRIT does not converge well for chaotic systems



The Lorenz attractor

- Non-linear
- Sensitive to perturbations
- Ill-conditioned

The Lorenz system is a model problem for chaos



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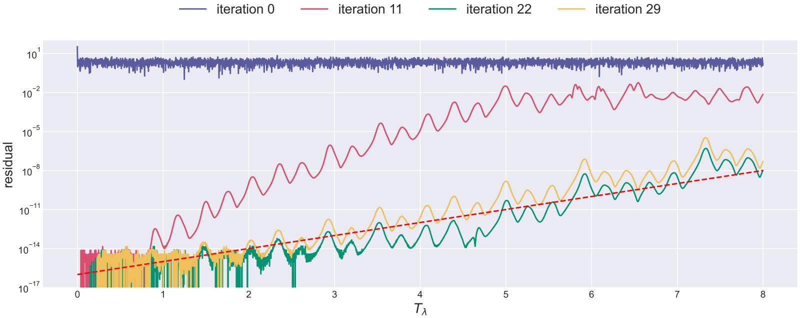
$$\begin{cases} \frac{dx}{dt} = \sigma(y - x), \\ \frac{dy}{dt} = x(\rho - z) - y, \\ \frac{dz}{dt} = xy - \beta z \end{cases}$$

- three dimensional
- nonlinear ($-xz$ and xy terms)
- derived by Lorenz as a simplified model of convection
- many chaotic PDEs can be modeled very accurately by finite dimensional ODEs

Classical MGRIT fails to converge for chaotic systems



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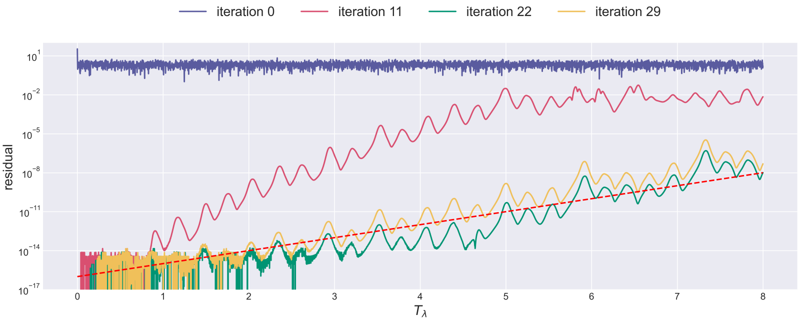


$\lambda \approx 0.9$

$T_\lambda = \frac{\log(10)}{\lambda}$

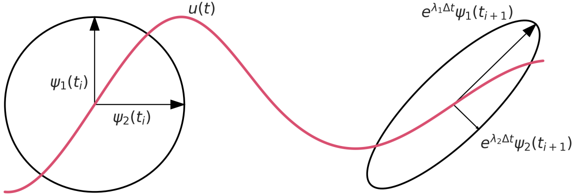
Lyapunov Exponents/Vectors

For the Lorenz system:

λ_1: Unstable- (≈ 0.9) orbits diverge exponentially

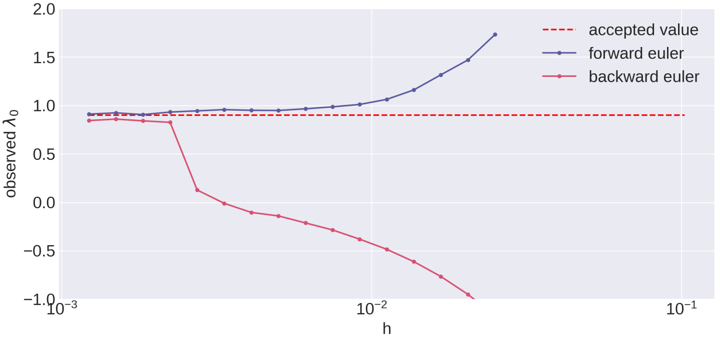
λ_2: Neutral- ($= 0$) phase difference in time

λ_3: Stable- (≈ -14) orbits exponentially approach the strange attractor



The θ Method

Explicit methods too unstable, implicit methods too dissipative



$$\mathbf{u}' = f(\mathbf{u})$$

$$\mathbf{u}_{i+i} = \mathbf{u}_i + hf(\mathbf{u}_i) \qquad \text{Forward Euler}$$

$$\mathbf{u}_{i+i} = \mathbf{u}_i + hf(\mathbf{u}_{i+1}) \qquad \text{Backward Euler}$$

The θ method splits the difference

$$\mathbf{u}' = f(\mathbf{u})$$

$$\mathbf{u}_{i+1} = \mathbf{u}_i + \theta h f(\mathbf{u}_i) + (1-\theta) h f(\mathbf{u}_{i+1}) \qquad \theta \text{ method}$$

- $\theta = 1$: forward Euler
- $\theta = 0$: backward Euler
- $\theta = 1/2$: Crank-Nicolson

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- $\theta = 1/2$: Crank-Nicolson

- What's the best value of θ to use for a given coarsening factor, m?

Asymptotic values of θ

Since the θ method is first order for *any* value of θ, i.e.

$$\phi_\theta(0) = \phi_m(0)$$
$$\phi'_\theta(0) = \phi'_m(0)$$

we can use the extra degree of freedom to find θ such that

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and approximate the fine-grid to *second* order in mh.

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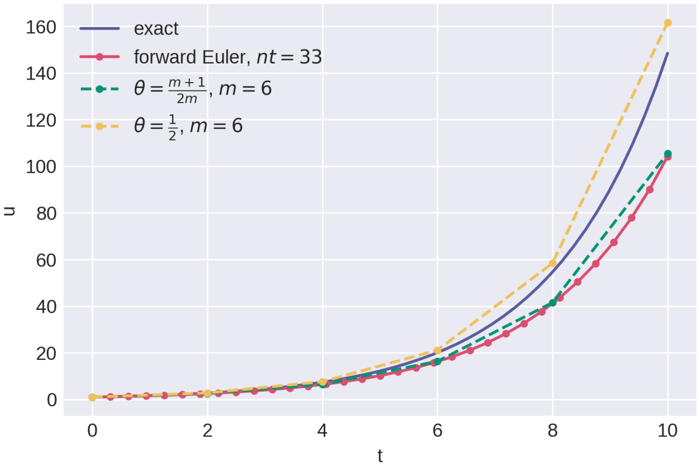
Forward Euler:

$$\theta_m = \frac{m+1}{2m}$$

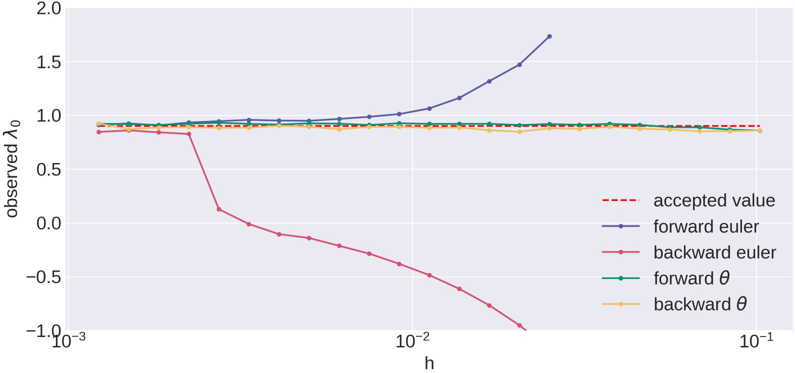
Backward Euler:

$$\theta_m = \frac{m-1}{2m}$$

The θ method approximates the fine-grid to second order, and the continuous equation to first order

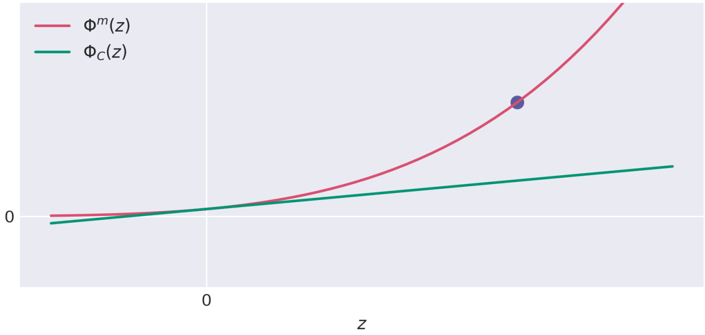


The asymptotic values of θ better preserve Lyapunov exponents on coarse grids



Δ correction

τ correction is a constant correction



$$A_c(\mathbf{v}^{k+1}) = \mathbf{f}$$

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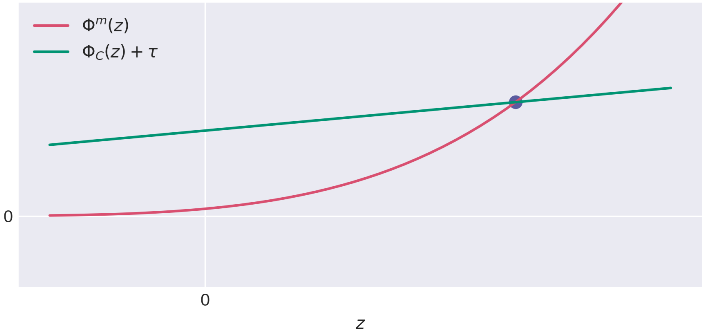
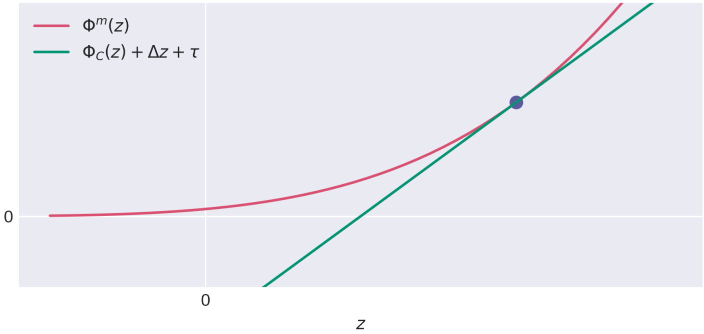


$$A_c(\mathbf{v}^{k+1}) = \mathbf{f} + \boldsymbol{\tau}$$

$$\boldsymbol{\tau} = A_*(\mathbf{v}^k) - A_c(\mathbf{v}^k)$$

Δ correction is a linear correction



$$[A_c + \Delta](\mathbf{v}^{k+1}) = \mathbf{f} + \boldsymbol{\tau}$$

$$\Delta = D_{\mathrm{u}} A_*(\mathbf{v}^k) - D_{\mathrm{u}} A_c(\mathbf{v}^k)$$

$$\boldsymbol{\tau} = A_*(\mathbf{v}^k) - A_c(\mathbf{v}^k) - \Delta \mathbf{v}^k$$

Δ correction is a generalization of Newton's method

- exact method for linear systems
- quadratic convergence for nonlinear systems

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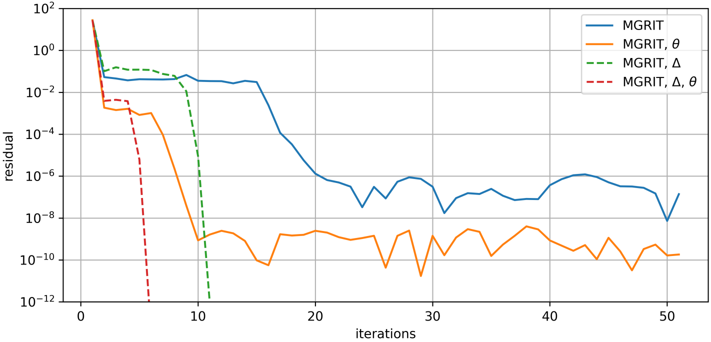
If A_c is the identity, then the coarse grid equation becomes

$$\begin{aligned}
[D_{\mathrm{u}} A_*(\mathbf{v}^k)]\mathbf{v}^{k+1} &= [D_{\mathrm{u}} A_*(\mathbf{v}^k)]\mathbf{v}^k + (\mathbf{f} - A_*(\mathbf{v}^k)) \\
\mathbf{v}^{k+1} &= \mathbf{v}^k - [D_{\mathrm{u}} A_*(\mathbf{v}^k)]^{-1}(A_*(\mathbf{v}^k) - \mathbf{f})
\end{aligned}$$

Results for Lorenz

optimal θ methods converge faster, Δ correction converges quadratically



Two-level method, Lorenz system, forward Euler fine-grid, $T_f = 8\,T_\lambda$ and $nt = 8192$

θ method improves both stability and MGRIT convergence

- Lorenz system, Forward Euler fine-grid, F-relax, $m = 2$
- T_f constant, n_t varies, iteration counts to reach residual tolerance of $1e - 10$

	T_f, n_t				
Algorithm	4, 512	4, 1024	4, 2048	4, 4096	4, 8192
MGRIT_2	*	44	22	15	12
MGRIT_2, θ	19	13	9	7	6
MGRIT_2, Δ	*	11	8	6	6
MGRIT_2, Δ, θ	8	6	5	4	4

Δ correction extends the length of the time-domain

- Lorenz system, Forward Euler fine-grid, $m = 2$
- T_f, n_t vary, iteration counts to reach residual tolerance of $1e-10$

	T_f, n_t			
Algorithm	2, 4096	4, 8192	8, 16384	12, 24576
MGRIT_2	10	13	64	-
MGRIT_2, θ	4	5	7	-
MGRIT_2, Δ	5	6	8	94
MGRIT_2, Δ, θ	3	4	5	48

RK4-θ method allows us to reach very coarse grids for Lorenz

- 4-level method, RK4 fine-grid, 4th order θ method coarse grid, $m = 4$
- T_f, n_t vary, iteration counts to reach residual tolerance of $1e - 10$

	T_f, n_t			
Algorithm	2, 2048	4, 4096	8, 8192	12, 12288
MGRIT_4	*	*	*	*
MGRIT_4, θ	15	29	-	-
MGRIT_4, Δ	*	*	*	*
MGRIT_4, Δ, θ	6	9	18	51

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- 4-level method, RK4 fine-grid, 4th order θ method coarse grid, $m = 4$
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Algorithm	2, 2048	4, 4096	8, 8192	12, 12288
MGRIT_4	$*$	$*$	$*$	$*$
MGRIT_4, θ	15	29	-	-
MGRIT_4, Δ	$*$	$*$	$*$	$*$
MGRIT_4, Δ, θ	6	9	18	51

coarsest grids have 32 and 64 time-points, respectively!

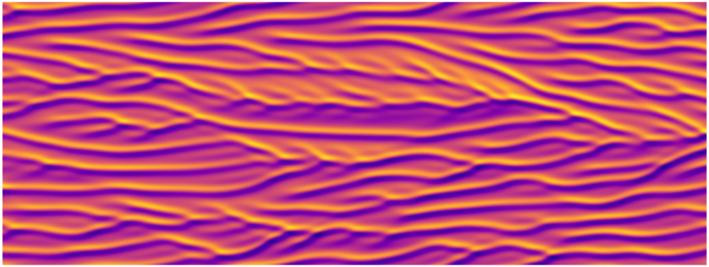
Low rank Δ correction for chaotic PDEs

Δ correction is too expensive for PDEs

- For Lorenz, the Δ_i are 3×3 matrices
- For a 1D PDE, they are $n_x \times n_x$
- For a 2D PDE...
- Jacobians might not be available

The Kuramoto-Sivashinsky (KS) equation

$$\mathbf{u}_t = -\mathbf{u}_{xx} - \mathbf{u}_{xxxx} - \mathbf{u}\mathbf{u}_x$$
$$\mathbf{u}(t, 0) = \mathbf{u}(t, L)$$



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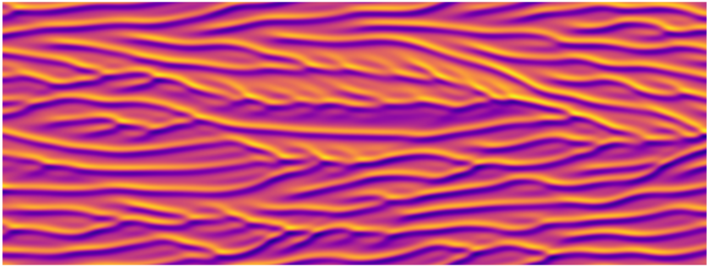

- Infinitely many Lyapunov exponents, λ
- Finitely many $\lambda > 0$
- Why correct for modes which already converge well?

Low-rank Δ correction

Given a rank k orthogonal basis for the unstable manifold: Ψ_i

$$\hat{\Delta}_i = (\Delta_i \Psi_i) \Psi_i^T$$

Low-rank Δ correction

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$$\hat{\Delta}_i = (\Delta_i \Psi_i)\Psi_i^T$$

- Only have to store the factors Ψ_i and $\Delta_i \Psi_i$
- The columns of $\Delta_i \Psi_i$ are directional derivatives (matrix free)

Backward Lyapunov Vectors

Given a trajectory $\{\mathbf{u}_i\}$ satisfying

$$\begin{aligned} \mathbf{u}_0 &= \mathbf{f}_0 \\ \mathbf{u}_{i+1} &= \Phi(\mathbf{u}_i) + \mathbf{f}_{i+1} \qquad\qquad i = 0, 1, 2, \ldots, n, \end{aligned}$$

the backward Lyapunov Vectors are an orthonormal set satisfying the tangent equation

$$\Psi_{i+1} R_{i+1} = [D_u \Phi(\mathbf{u}_i)] \Psi_i$$

Low-rank Δ correction solves state and tangent equations simultaneously

- Given a trajectory $\mathbf{u}$ we can find the Lyapunov Vectors Ψ
- Given the Lyapunov Vectors Ψ, we can accelerate the solution of $\mathbf{u}$

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- Given a trajectory $\mathbf{u}$ we can find the Lyapunov Vectors Ψ
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- So low-rank Δ correction uses the same MGRIT cycle to solve for both iteratively

Results for the KS equation

Discretization

- 4th order finite-differencing in space
- 2nd order Lobatto IIIC method in time (Stiffly accurate 2nd order Runge Kutta method)

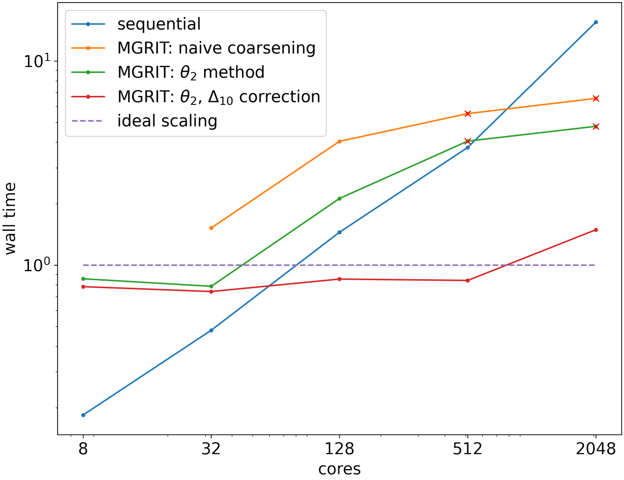
$$\begin{array}{c|cc} 0 & \frac{1}{2} & -\frac{1}{2} \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

- second order θ method constructed from combination of second order Lobatto methods, along with stiff constraint

$$\lim_{z \to -\infty} \phi(z) = 0$$

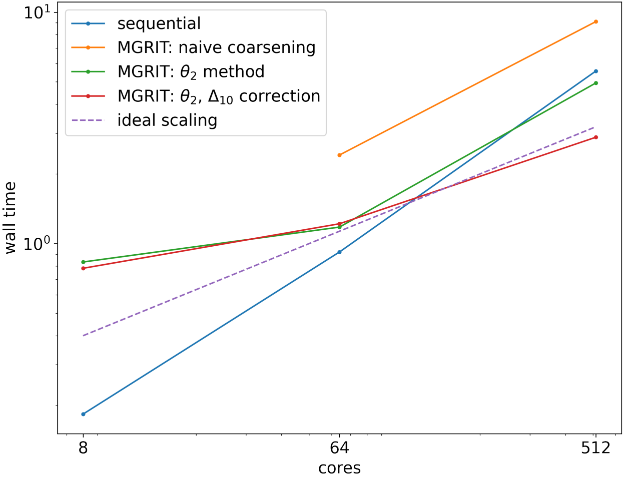
Weak scaling

Figure 1: $T_f = 4T_\lambda$, $n_x = 128$, $n_t = 128$, refinement in time only



Weak scaling

$T_f = 4T_\lambda$, $n_x = 128$, $n_t = 128$, refinement in both time and space (parallel in time only)



Future work

- space-time parallel for KS equation
- extend θ methods to wide range of applications
- convergence on arbitrary time-domains