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Parallel-in-time solutions with ParaDiag

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Outline

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Parallel-in-time motivation

The ParaDiag idea

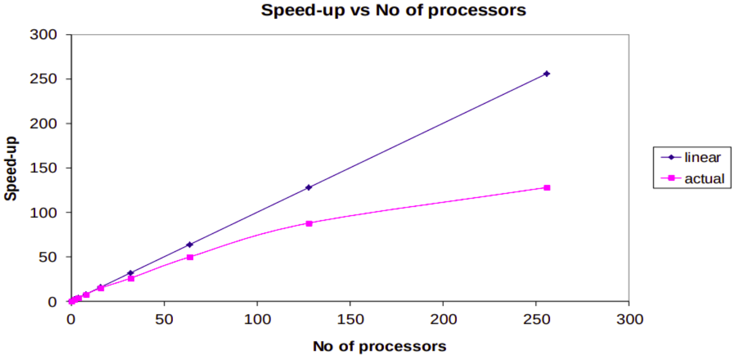
ParaDiag methods

Performance model

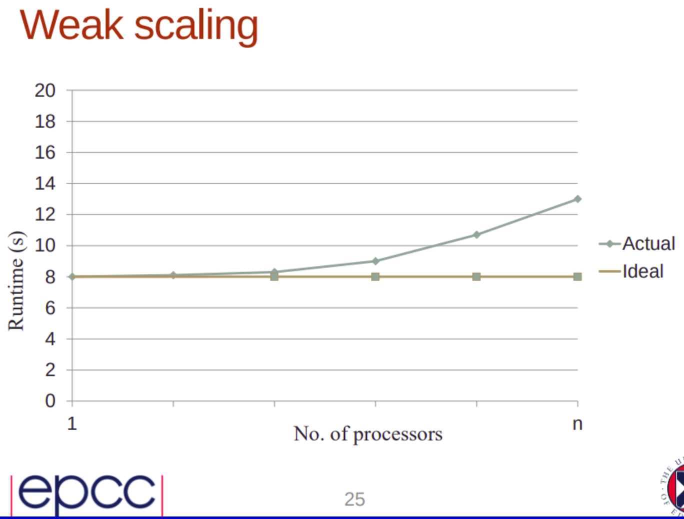
Summary

Strong scaling

Strong scaling



Weak scaling



Time-dependent O/PDEs

$$\boldsymbol{M}\partial_t u + \boldsymbol{K} u = b(t)$$

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$$\boldsymbol{M}\left(\frac{u^{n+1} - u^n}{\Delta t}\right) + \theta \boldsymbol{K}u^{n+1} + (1-\theta)\,\boldsymbol{K}u^n = b^{n+1}$$

Time-dependent O/PDEs

$$\boldsymbol{M}\partial_t u + \boldsymbol{K} u = b(t)$$

$$\boldsymbol{M}\left(\frac{u^{n+1} - u^n}{\Delta t}\right) + \theta \boldsymbol{K} u^{n+1} + (1-\theta)\,\boldsymbol{K} u^n = b^{n+1}$$

$$\left(\frac{\boldsymbol{M}}{\Delta t} + \theta \boldsymbol{K}\right) u^{n+1} = b^{n+1} - \left(\frac{-\boldsymbol{M}}{\Delta t} + (1-\theta)\,\boldsymbol{K}\right) u^n$$

Performance of serial method

$$\left(\frac{\boldsymbol{M}}{\Delta t} + \theta \boldsymbol{K}\right) u^{n+1} = \tilde{b}$$

Work: $W_s = K_s M_s N_x N_t \sim N_x N_t$

Processors: $P_s \sim N_x$

Time: $T_s = \dfrac{W_s}{P_s} = K_s M_s N_t \sim N_t$

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All-at-once system

$$\left(\frac{-\boldsymbol{M}}{\Delta t} + (1-\theta)\,\boldsymbol{K}\right) u^{n} + \left(\frac{\boldsymbol{M}}{\Delta t} + \theta \boldsymbol{K}\right) u^{n+1} = b^{n+1}$$

All-at-once system

$$\boldsymbol{A}_0 u^n + \boldsymbol{A}_1 u^{n+1} = b^{n+1}$$

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$$\boldsymbol{A}_0 u^n + \boldsymbol{A}_1 u^{n+1} = b^{n+1}$$

$$\boldsymbol{A}_0 u^0 + \quad \boldsymbol{A}_1 u^1 \qquad = b^1$$

All-at-once system

$$A_0 u^n + A_1 u^{n+1} = b^{n+1}$$

$$\begin{aligned}
A_0 u^0 + \quad A_1 u^1 \quad & & = b^1 \\
A_0 u^1 + \quad A_1 u^2 & & = b^2
\end{aligned}$$

All-at-once system

$$\boldsymbol{A}_0 u^n + \boldsymbol{A}_1 u^{n+1} = b^{n+1}$$

$$\begin{array}{lllll} \boldsymbol{A}_0 u^0 + & \boldsymbol{A}_1 u^1 & & & = b^1 \\ & \boldsymbol{A}_0 u^1 + & \boldsymbol{A}_1 u^2 & & = b^2 \\ & & \boldsymbol{A}_0 u^2 + & \boldsymbol{A}_1 u^3 & = b^3 \end{array}$$

All-at-once system

$$\boldsymbol{A}_0 u^n + \boldsymbol{A}_1 u^{n+1} = b^{n+1}$$

$$\begin{array}{ccccccc}
\boldsymbol{A}_0 u^0 + & \boldsymbol{A}_1 u^1 & & & & = & b^1 \\
& \boldsymbol{A}_0 u^1 + & \boldsymbol{A}_1 u^2 & & & = & b^2 \\
& & \boldsymbol{A}_0 u^2 + & \boldsymbol{A}_1 u^3 & & = & b^3 \\
& & & \boldsymbol{A}_0 u^3 + & \boldsymbol{A}_1 u^4 & = & b^4
\end{array}$$

All-at-once system

$$\boldsymbol{A}_0 u^n + \boldsymbol{A}_1 u^{n+1} = b^{n+1}$$

$$\begin{pmatrix} \boldsymbol{A}_1 & & & \\ \boldsymbol{A}_0 & \boldsymbol{A}_1 & & \\ & \boldsymbol{A}_0 & \boldsymbol{A}_1 & \\ & & \boldsymbol{A}_0 & \boldsymbol{A}_1 \end{pmatrix} \begin{pmatrix} u^1 \\ u^2 \\ u^3 \\ u^4 \end{pmatrix} = \begin{pmatrix} b^1 - \boldsymbol{A}_0 u^0 \\ b^2 \\ b^3 \\ b^4 \end{pmatrix}$$

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{b}$$

Diagonalising the all-at-once system

$$\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^{-1}$$

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{b} \implies \boldsymbol{\Lambda}\left(\boldsymbol{V}^{-1}\boldsymbol{u}\right) = \left(\boldsymbol{V}^{-1}\boldsymbol{b}\right) \implies \boldsymbol{\Lambda}\tilde{\boldsymbol{u}} = \tilde{\boldsymbol{b}},$$

$$\boldsymbol{u} = \boldsymbol{V}\tilde{\boldsymbol{u}}, \quad \tilde{\boldsymbol{b}} = \boldsymbol{V}^{-1}\boldsymbol{b}$$

$$\begin{pmatrix} \boldsymbol{\Lambda}_1 & & & \\ & \boldsymbol{\Lambda}_2 & & \\ & & \boldsymbol{\Lambda}_3 & \\ & & & \boldsymbol{\Lambda}_4 \end{pmatrix} \begin{pmatrix} \tilde{u}^1 \\ \tilde{u}^2 \\ \tilde{u}^3 \\ \tilde{u}^4 \end{pmatrix} = \begin{pmatrix} \tilde{b}^1 \\ \tilde{b}^2 \\ \tilde{b}^3 \\ \tilde{b}^4 \end{pmatrix}$$

Requirements on the diagonalisation

$$\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^{-1},$$

1. Exists (not as trivial as it sounds)
2. $\boldsymbol{V}$ and $\boldsymbol{V}^{-1}$ are:
   - relatively cheap to compute
   - easily parallelisable
3. The cost to solve $\boldsymbol{\Lambda}_i$ is comparable to the serial problem

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Kronecker products

$$\boldsymbol{A} \in \mathbb{R}^{n\times n}, \quad \boldsymbol{B} \in \mathbb{R}^{m\times m}, \quad \boldsymbol{A}\otimes\boldsymbol{B} \in \mathbb{R}^{nm\times nm}$$

$$\boldsymbol{A}\otimes\boldsymbol{B} = \begin{pmatrix} a_{00}\boldsymbol{B} & a_{01}\boldsymbol{B} & a_{02}\boldsymbol{B} \\ a_{10}\boldsymbol{B} & a_{11}\boldsymbol{B} & a_{12}\boldsymbol{B} \\ a_{20}\boldsymbol{B} & a_{21}\boldsymbol{B} & a_{22}\boldsymbol{B} \end{pmatrix}$$

$$(\boldsymbol{AC})\otimes(\boldsymbol{BD}) = (\boldsymbol{A}\otimes\boldsymbol{B})(\boldsymbol{C}\otimes\boldsymbol{D})$$

$$\boldsymbol{A}\otimes\boldsymbol{B} = (\boldsymbol{A}\otimes\boldsymbol{I})(\boldsymbol{I}\otimes\boldsymbol{B}) = (\boldsymbol{I}\otimes\boldsymbol{B})(\boldsymbol{A}\otimes\boldsymbol{I})$$

ParaDiag-I: A diagonalisable integrator

$$\begin{pmatrix} \frac{1}{\Delta t_1} & & & \\ \frac{-1}{\Delta t_1} & \frac{1}{\Delta t_2} & & \\ & \frac{-1}{\Delta t_2} & \frac{1}{\Delta t_3} & \\ & & \frac{-1}{\Delta t_3} & \frac{1}{\Delta t_4} \end{pmatrix} \otimes \boldsymbol{M} + \begin{pmatrix} \theta & & & \\ (1-\theta) & \theta & & \\ & (1-\theta) & \theta & \\ & & (1-\theta) & \theta \end{pmatrix} \otimes \boldsymbol{K}$$

$$\boldsymbol{A} = \boldsymbol{B}_1 \otimes \boldsymbol{M} + \boldsymbol{B}_2 \otimes \boldsymbol{K}$$

ParaDiag-I: A diagonalisable integrator

$$\begin{pmatrix} \frac{1}{\Delta t_1} & & & \\ \frac{-1}{\Delta t_1} & \frac{1}{\Delta t_2} & & \\ & \frac{-1}{\Delta t_2} & \frac{1}{\Delta t_3} & \\ & & \frac{-1}{\Delta t_3} & \frac{1}{\Delta t_4} \end{pmatrix} \otimes \boldsymbol{M} + \begin{pmatrix} \theta & & & \\ (1-\theta) & \theta & & \\ & (1-\theta) & \theta & \\ & & (1-\theta) & \theta \end{pmatrix} \otimes \boldsymbol{K}$$

$$\begin{aligned} \boldsymbol{A} &= \boldsymbol{B}_1 \otimes \boldsymbol{M} + \boldsymbol{B}_2 \otimes \boldsymbol{K} \\ \hat{\boldsymbol{A}} &= \left(\boldsymbol{B}_2^{-1}\boldsymbol{B}_1\right) \otimes \boldsymbol{M} + \boldsymbol{I} \otimes \boldsymbol{K} \\ &= (\boldsymbol{V} \otimes \boldsymbol{I}_x)\,(\boldsymbol{D} \otimes \boldsymbol{M} + \boldsymbol{I} \otimes \boldsymbol{K})\left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right) \end{aligned}$$

- $\boldsymbol{B}_2^{-1}\boldsymbol{B}_1 = \boldsymbol{V}\boldsymbol{D}\boldsymbol{V}^{-1}$ is diagonalisable if Δt_i are all different

ParaDiag-II: Circulant all-at-once system

$$\begin{pmatrix} \frac{1}{\Delta t} & & & \frac{-1}{\Delta t} \\ \frac{-1}{\Delta t} & \frac{1}{\Delta t} & & \\ & \frac{-1}{\Delta t} & \frac{1}{\Delta t} & \\ & & \frac{-1}{\Delta t} & \frac{1}{\Delta t} \end{pmatrix} \otimes \boldsymbol{M} + \begin{pmatrix} \theta & & & (1-\theta) \\ (1-\theta) & \theta & & \\ & (1-\theta) & \theta & \\ & & (1-\theta) & \theta \end{pmatrix} \otimes \boldsymbol{K}$$

$$\boldsymbol{P} = \boldsymbol{C}_1 \otimes \boldsymbol{M} + \boldsymbol{C}_2 \otimes \boldsymbol{K} \approx \boldsymbol{A}$$

$$\boldsymbol{P} = (\boldsymbol{V} \otimes \boldsymbol{I}_x)(\boldsymbol{D}_1 \otimes \boldsymbol{M} + \boldsymbol{D}_2 \otimes \boldsymbol{K})\left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)$$

- $\boldsymbol{C}_{1,2} = \boldsymbol{V}\boldsymbol{D}_{1,2}\boldsymbol{V}^{-1}$ are *simultaneously* diagonalisable

ParaDiag-II: Circulant all-at-once system

$$\begin{pmatrix} \frac{1}{\Delta t} & & & \frac{-\alpha}{\Delta t} \\ \frac{-1}{\Delta t} & \frac{1}{\Delta t} & & \\ & \frac{-1}{\Delta t} & \frac{1}{\Delta t} & \\ & & \frac{-1}{\Delta t} & \frac{1}{\Delta t} \end{pmatrix} \otimes \boldsymbol{M} + \begin{pmatrix} \theta & & & \alpha(1-\theta) \\ (1-\theta) & \theta & & \\ & (1-\theta) & \theta & \\ & & (1-\theta) & \theta \end{pmatrix} \otimes \boldsymbol{K}$$

$$\boldsymbol{P}^{(\alpha)} = \boldsymbol{C}_1^{(\alpha)} \otimes \boldsymbol{M} + \boldsymbol{C}_2^{(\alpha)} \otimes \boldsymbol{K} \approx \boldsymbol{A}$$

$$\boldsymbol{P}^{(\alpha)} = (\boldsymbol{V} \otimes \boldsymbol{I}_x)(\boldsymbol{D}_1 \otimes \boldsymbol{M} + \boldsymbol{D}_2 \otimes \boldsymbol{K})\left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)$$

- $\boldsymbol{C}_{1,2}^{(\alpha)} = \boldsymbol{V}\boldsymbol{D}_{1,2}\boldsymbol{V}^{-1}$ are *simultaneously* diagonalisable
- $\alpha \in (0, 1]$, and in practice can be very small ($\approx 10^{-4}$)

Circulant diagonalisation

$$\boldsymbol{P} = \boldsymbol{C}_1 \otimes \boldsymbol{M} + \boldsymbol{C}_2 \otimes \boldsymbol{K}, \qquad \boldsymbol{C}_j = \boldsymbol{V}\boldsymbol{D}_j\boldsymbol{V}^{-1},$$

$$\boldsymbol{P} = \left(\boldsymbol{V} \otimes \boldsymbol{I}_x\right)\left(\boldsymbol{D}_1 \otimes \boldsymbol{M} + \boldsymbol{D}_2 \otimes \boldsymbol{K}\right)\left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)$$

Circulant diagonalisation

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$$\boldsymbol{\Lambda}_k = \left(\lambda_{1,k}\boldsymbol{M} + \lambda_{2,k}\boldsymbol{K}\right) \quad \forall k \in [1, N_t]$$

Circulant diagonalisation

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$$\boldsymbol{\Lambda}_k = \left(\lambda_{1,k}\boldsymbol{M} + \lambda_{2,k}\boldsymbol{K}\right) \quad \forall k \in [1, N_t]$$

$$\boldsymbol{V} = \boldsymbol{\Gamma}_\alpha^{-1}\boldsymbol{\mathcal{F}}^{-1}, \quad \boldsymbol{D}_j = \mathtt{diag}\left(\mathcal{F}\boldsymbol{\Gamma}_\alpha\boldsymbol{c}_j\right), \quad \boldsymbol{\Gamma}_\alpha = \mathtt{diag}\left(\alpha^{\frac{k-1}{N_t}}\right)\forall k \in [1, N_t]$$

Circulant linear solves

$$\boldsymbol{P} = (\boldsymbol{V} \otimes \boldsymbol{I}_x)(\boldsymbol{D}_1 \otimes \boldsymbol{M} + \boldsymbol{D}_2 \otimes \boldsymbol{K})\left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)$$

$$\boldsymbol{P}\boldsymbol{x} = \boldsymbol{b}$$

Circulant linear solves

$$\boldsymbol{P} = \left(\boldsymbol{V} \otimes \boldsymbol{I}_x\right)\left(\boldsymbol{D}_1 \otimes \boldsymbol{M} + \boldsymbol{D}_2 \otimes \boldsymbol{K}\right)\left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)$$

$$\boldsymbol{P}\boldsymbol{x} = \boldsymbol{b}$$

- Step-(a) $\boldsymbol{y}_1 = \left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)\boldsymbol{b}$

Circulant linear solves

$$\boldsymbol{P} = \left(\boldsymbol{V} \otimes \boldsymbol{I}_x\right) \left(\boldsymbol{D}_1 \otimes \boldsymbol{M} + \boldsymbol{D}_2 \otimes \boldsymbol{K}\right) \left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)$$

$$\boldsymbol{P}\boldsymbol{x} = \boldsymbol{b}$$

- Step-(a) $\boldsymbol{y}_1 = \left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right) \boldsymbol{b}$
- Step-(b) $\left(\lambda_{1,j}\boldsymbol{M} + \lambda_{2,j}\boldsymbol{K}\right) \boldsymbol{y}_{2,n} = \boldsymbol{y}_{1,n} \quad \forall j \in [1, N_t]$

Circulant linear solves

$$\boldsymbol{P} = (\boldsymbol{V} \otimes \boldsymbol{I}_x)(\boldsymbol{D}_1 \otimes \boldsymbol{M} + \boldsymbol{D}_2 \otimes \boldsymbol{K})\left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)$$

$$\boldsymbol{P}\boldsymbol{x} = \boldsymbol{b}$$

- Step-(a) $\boldsymbol{y}_1 = \left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)\boldsymbol{b}$
- Step-(b) $\left(\lambda_{1,j}\boldsymbol{M} + \lambda_{2,j}\boldsymbol{K}\right)\boldsymbol{y}_{2,n} = \boldsymbol{y}_{1,n} \quad \forall j \in [1, N_t]$
- Step-(c) $\boldsymbol{x} = (\boldsymbol{V} \otimes \boldsymbol{I}_x)\,\boldsymbol{y}_2$

Circulant linear solves

$$\boldsymbol{P} = (\boldsymbol{V} \otimes \boldsymbol{I}_x)(\boldsymbol{D}_1 \otimes \boldsymbol{M} + \boldsymbol{D}_2 \otimes \boldsymbol{K})\left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)$$

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- Step-(a) $\boldsymbol{y}_1 = \left(\boldsymbol{V}^{-1} \otimes \boldsymbol{I}_x\right)\boldsymbol{b}$
- Step-(b) $\left(\lambda_{1,j}\boldsymbol{M} + \lambda_{2,j}\boldsymbol{K}\right)\boldsymbol{y}_{2,n} = \boldsymbol{y}_{1,n} \quad \forall j \in [1, N_t]$
- Step-(c) $\boldsymbol{x} = (\boldsymbol{V} \otimes \boldsymbol{I}_x)\,\boldsymbol{y}_2$

All-at-once solution strategies

- Preconditioned Krylov method: $\boldsymbol{P}^{-1}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{P}^{-1}\boldsymbol{b}$
  $\boldsymbol{P}^{-1}\boldsymbol{A}$ has N_x non-unit eigenvalues
- Richardson iteration: $\boldsymbol{P}\boldsymbol{x}^{k+1} = (\boldsymbol{P} - \boldsymbol{A})\,\boldsymbol{x}^{k} + \boldsymbol{b}$
  Convergence rate bounded by $\alpha/(1-\alpha)$
- Roundoff error: $\mathcal{O}(\epsilon N_t \alpha^{-2})$ if ϵ is machine precision

Outline

Performance model vs time-serial method

$$\left(\beta_1 \boldsymbol{M} + \beta_2 \boldsymbol{K}\right) x = \tilde{b}$$

Serial: $(\beta_1 = 1/\Delta t,\ \beta_2 = \theta)$

$$W_s = K_s\, M_s\, (N_x\, N_t)$$

$$P_s \sim N_x$$

$$T_s \sim \frac{W_s}{P_s} = K_s\, M_s\, N_t$$

Parallel: $(\beta_1 = \lambda_1,\ \beta_2 = \lambda_2)$

$$W_p = 2\, K_p\, M_p\, (N_x\, N_t)$$

$$P_p \sim 2 N_x\, N_t$$

$$T_p \sim \frac{W_p}{P_p} = K_p\, M_p + T_c$$

Ideal speedup bound

Speedup: $S = \dfrac{T_s}{T_p} = \left(\dfrac{N_t}{\gamma\omega}\right)\dfrac{1}{1 + T_c/T_b}$

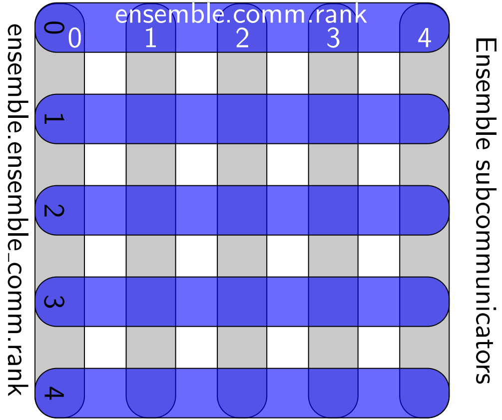
"Difficulty" measures: $\gamma = \dfrac{K_p}{K_s}, \quad \omega = \dfrac{M_p}{M_s}$

Block solve time: T_b

Communication time: T_c

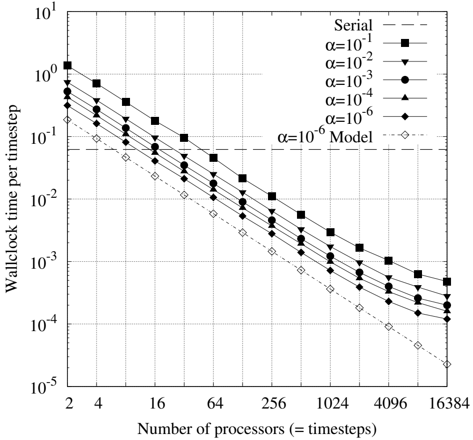
Efficiency: $E = \dfrac{S}{P_p/P_s} = \dfrac{1}{2\gamma\omega}\dfrac{1}{1 + T_c/T_b}$

Space-time parallelism



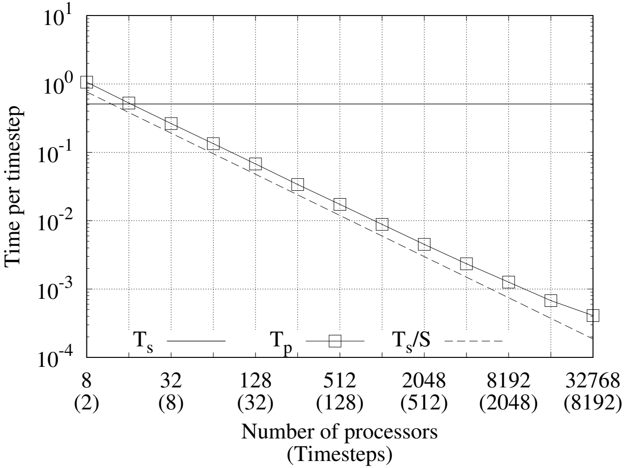
Spatial subcommunicators

Scalar advection scaling



$$S = \frac{N_t/(\gamma\omega)}{1 + T_b/T_c}$$

Linear shallow water equations scaling



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Summary

Summary:

- Solve for entire all-at-once system in one swoop
- Find suitable diagonalisation in time to expose parallelism
- Circulant preconditioner is diagonalisable with FFT
- Very good convergence $\mathcal{O}(\alpha)$ for linear systems

Nonlinear all-at-once system

$$\boldsymbol{M}\partial_t \boldsymbol{u} + \boldsymbol{f}(\boldsymbol{u}) = 0$$

$$\begin{pmatrix} \frac{1}{\Delta t} & & & \\ \frac{-1}{\Delta t} & \frac{1}{\Delta t} & & \\ & \frac{-1}{\Delta t} & \frac{1}{\Delta t} & \\ & & \frac{-1}{\Delta t} & \frac{1}{\Delta t} \end{pmatrix} \otimes \boldsymbol{M} + \left(\begin{pmatrix} \theta & & & \\ (1-\theta) & \theta & & \\ & (1-\theta) & \theta & \\ & & (1-\theta) & \theta \end{pmatrix} \otimes \boldsymbol{I}_x \right) \begin{pmatrix} \boldsymbol{f}(\boldsymbol{u}^1) \\ \boldsymbol{f}(\boldsymbol{u}^2) \\ \boldsymbol{f}(\boldsymbol{u}^3) \\ \boldsymbol{f}(\boldsymbol{u}^4) \end{pmatrix}$$

Nonlinear all-at-once Jacobian

$$\boldsymbol{M}\partial_t \boldsymbol{u} + \boldsymbol{f}(\boldsymbol{u}) = 0$$

$$\begin{pmatrix} \theta\nabla\boldsymbol{f}(\boldsymbol{u}^1) & & & \\ (1-\theta)\nabla\boldsymbol{f}(\boldsymbol{u}^1) & \theta\nabla\boldsymbol{f}(\boldsymbol{u}^2) & & \\ & (1-\theta)\nabla\boldsymbol{f}(\boldsymbol{u}^2) & \theta\nabla\boldsymbol{f}(\boldsymbol{u}^3) & \\ & & (1-\theta)\nabla\boldsymbol{f}(\boldsymbol{u}^3) & \theta\nabla\boldsymbol{f}(\boldsymbol{u}^4) \end{pmatrix} \otimes \boldsymbol{I}_x$$

Nonlinear all-at-once Jacobian

$$\boldsymbol{M}\partial_t \boldsymbol{u} + \boldsymbol{f}(\boldsymbol{u}) = 0$$

$$\begin{pmatrix} \theta\nabla\overline{\boldsymbol{f}(\boldsymbol{u})} & & & \\ (1-\theta)\,\overline{\nabla\boldsymbol{f}(\boldsymbol{u})} & \theta\nabla\overline{\boldsymbol{f}(\boldsymbol{u})} & & \\ & (1-\theta)\,\overline{\nabla\boldsymbol{f}(\boldsymbol{u})} & \theta\nabla\overline{\boldsymbol{f}(\boldsymbol{u})} & \\ & & (1-\theta)\,\overline{\nabla\boldsymbol{f}(\boldsymbol{u})} & \theta\overline{\nabla\boldsymbol{f}(\boldsymbol{u})} \end{pmatrix} \otimes \boldsymbol{I}_x$$

Nonlinear all-at-once Jacobian

$$\boldsymbol{M}\partial_t \boldsymbol{u} + \boldsymbol{f}(\boldsymbol{u}) = 0$$

$$\begin{pmatrix} \frac{1}{\Delta t} & & & \\ \frac{-1}{\Delta t} & \frac{1}{\Delta t} & & \\ & \frac{-1}{\Delta t} & \frac{1}{\Delta t} & \\ & & \frac{-1}{\Delta t} & \frac{1}{\Delta t} \end{pmatrix} \otimes \boldsymbol{M} + \begin{pmatrix} \theta & & & \\ (1-\theta) & \theta & & \\ & (1-\theta) & \theta & \\ & & (1-\theta) & \theta \end{pmatrix} \otimes \overline{\nabla \boldsymbol{f}(\boldsymbol{u})}$$

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$$\begin{pmatrix} \frac{1}{\Delta t} & & & \\ \frac{-1}{\Delta t} & \frac{1}{\Delta t} & & \\ & \frac{-1}{\Delta t} & \frac{1}{\Delta t} & \\ & & \frac{-1}{\Delta t} & \frac{1}{\Delta t} \end{pmatrix} \otimes \boldsymbol{M} + \begin{pmatrix} \theta & & & \\ (1-\theta) & \theta & & \\ & (1-\theta) & \theta & \\ & & (1-\theta) & \theta \end{pmatrix} \otimes \overline{\nabla \boldsymbol{f}(\boldsymbol{u})}$$

$$\overline{\nabla \boldsymbol{f}(\boldsymbol{u})} = \sum_n^{N_t} \frac{\nabla \boldsymbol{f}(\boldsymbol{u}^n)}{N_t} \quad \text{or} \quad \overline{\nabla \boldsymbol{f}(\boldsymbol{u})} = \nabla \boldsymbol{f}\left(\sum_n^{N_t} \frac{\boldsymbol{u}^n}{N_t}\right)$$

Nonlinear all-at-once Jacobian

$$\boldsymbol{M}\partial_t \boldsymbol{u} + \boldsymbol{f}(\boldsymbol{u}) = 0$$

$$\begin{pmatrix} \frac{1}{\Delta t} & & & \frac{-1}{\Delta t} \\ \frac{-1}{\Delta t} & \frac{1}{\Delta t} & & \\ & \frac{-1}{\Delta t} & \frac{1}{\Delta t} & \\ & & \frac{-1}{\Delta t} & \frac{1}{\Delta t} \end{pmatrix} \otimes \boldsymbol{M} + \begin{pmatrix} \theta & & & (1-\theta) \\ (1-\theta) & \theta & & \\ & (1-\theta) & \theta & \\ & & (1-\theta) & \theta \end{pmatrix} \otimes \overline{\nabla \boldsymbol{f}(\boldsymbol{u})}$$

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Nonlinear problems

Nonlinear system: $\boldsymbol{M}\partial_t u + \boldsymbol{f}(u)$

All-at-once system: $(\boldsymbol{B}_1 \otimes \boldsymbol{M})\,\boldsymbol{u} + (\boldsymbol{B}_2 \otimes \boldsymbol{I}_x)\,\boldsymbol{F}(\boldsymbol{u})$

All-at-once Jacobian: $(\boldsymbol{B}_1 \otimes \boldsymbol{M}) + (\boldsymbol{B}_2 \otimes \boldsymbol{I}_x)\,\nabla \boldsymbol{F}(\boldsymbol{u})$

ParaDiag Jacobian: $(\boldsymbol{C}_1 \otimes \boldsymbol{M}) + (\boldsymbol{C}_2 \otimes \nabla \boldsymbol{f}(\overline{\boldsymbol{u}}))$

Time average: $\overline{\boldsymbol{u}} = \sum_n^{N_t} \boldsymbol{u}^n / N_t$