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Analysis of a Three-Level Variant of Parareal

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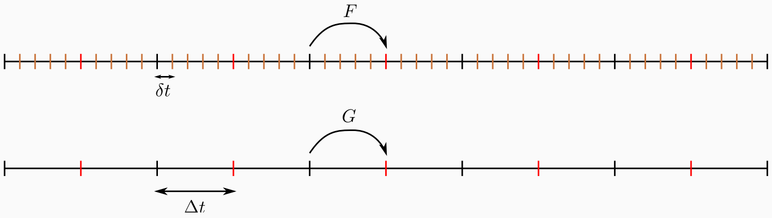
Outline

Three-level Parareal

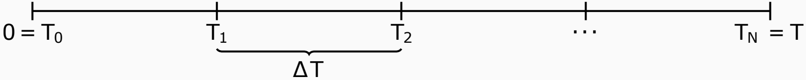
Parareal (Lions, Maday & Turinici 2001)



- Want to solve $u_t = f(t,u)$ for $t \in [0,T]$ with $u(0) = u_0$
- If the solution u is known at a set of points $t \in \{T_1, \ldots, T_N\}$, then the solution $u(t)$ on each (T_{i-1}, T_i) can be computed independently of the other intervals (and in parallel)
- Therefore, want to obtain approximations $U_n^k \approx u(t_n)$ iteratively
- Two-level method :
  - F = "exact" propagator over one interval (as an ODE, or numerically over many δt)
  - G = coarse propagator over the same interval (but with larger time steps Δt)

Parareal : algorithm

Goal : Find $U_i^k \approx u(T_i)$, $i = 1, 2, \dots$



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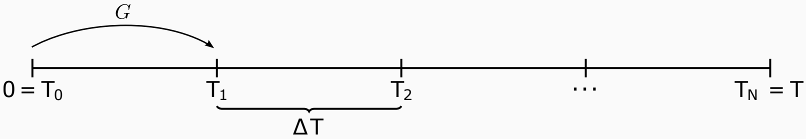
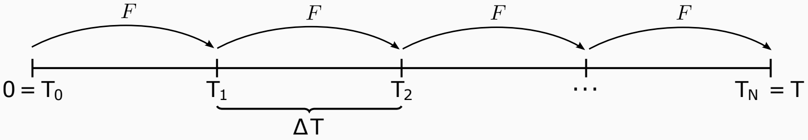


$$U_i^0 = G U_{i-1}^0$$

First, initialize U_i^0 using G.

Parareal : algorithm

Goal : Find $U_i^k \approx u(T_i)$, $i = 1, 2, \dots$



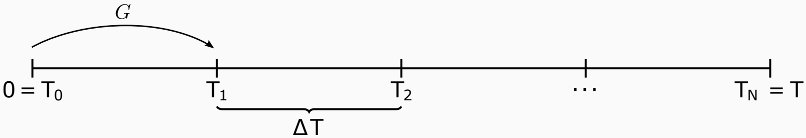
$$U_i^{k+1} = {\color{red} F U_{i-1}^k} + G U_{i-1}^{k+1} - G U_{i-1}^k$$

First, initialize U_i^0 using G. Then at step k, given U_i^k :

1. Evaluate $F U_{i-1}^k$ in **parallel** for all i (DD in time !)

Parareal : algorithm

Goal : Find $U_i^k \approx u(T_i)$, $i = 1, 2, \ldots$



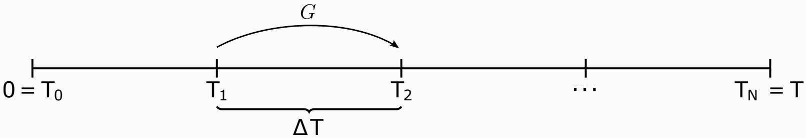
$$U_i^{k+1} = FU_{i-1}^k + GU_{i-1}^{k+1} - GU_{i-1}^k$$

First, initialize U_i^0 using G. Then at step k, given U_i^k :

1. Evaluate FU_{i-1}^k in **parallel** for all i (DD in time !)
2. Evaluate GU_{i-1}^{k+1} and update U_i^{k+1} **sequentially**.

Parareal : algorithm

Goal : Find $U_i^k \approx u(T_i)$, $i = 1, 2, \dots$



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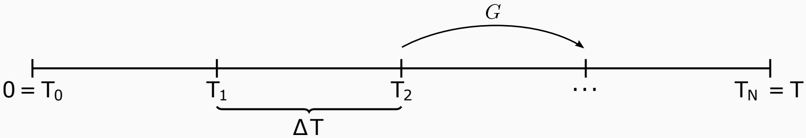

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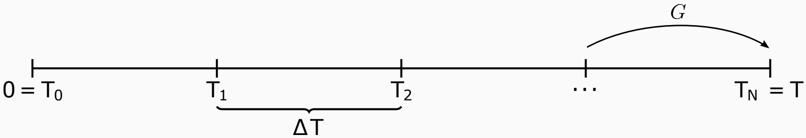

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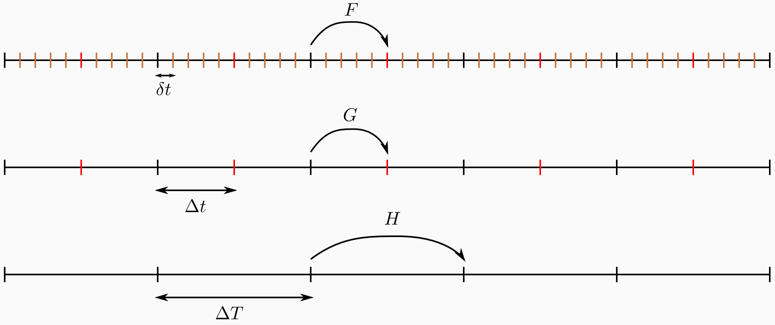
1. Evaluate FU_{i-1}^k in **parallel** for all i (DD in time !)
2. Evaluate GU_{i-1}^{k+1} and update U_i^{k+1} **sequentially**.

Repeat until convergence.

Parareal : known results

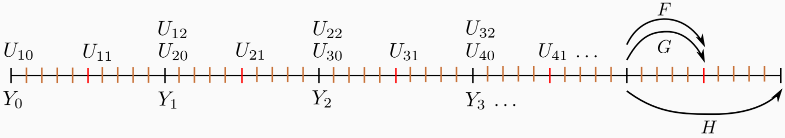
- Classical convergence results :
  - If $G =$ backward Euler, then $|U_i^k - u(T_i)| \leq C_k \Delta T^{k+1}$ (Lions, Maday & Turinici 2001)
  - If G is of order p, then $|U_i^k - u(T_i)| \leq C_k \Delta T^{p(k+1)}$ (Bal & Maday 2002, Bal 2003)
  - Superlinear convergence : $|U_i^k - u(T_i)| \leq \dfrac{C_0 (CT)^k}{k!} \Delta T^{pk}$ (Gander & Vandewalle 2007)
- Parareal can be interpreted as a multigrid-in-time method (Gander, K. & Zhang 2018)
- Parareal and MGRIT extensively analyzed for ODEs and some discretized PDEs (Gander & Hairer DD17 2008 ; Friedhoff & MacLachlan NLAA 2015 ; Dobrev et al. SISC 2017 ; Ruprecht CVS 2018 ; Southworth SIMAX 2019 ; Hessenthaler et al. SISC 2020 ; Gander & Lunet DD25 2020, Friedhoff & Southworth NLAA 2021, De Sterck et al. NLAA 2021, ...)
- Coarse solve in parareal still sequential : want to parallelize if there are many coarse intervals

Three-level parareal



- Hierarchical decomposition :
  - Coarsest grid : $0 = T_0 < T_1 < T_2 < \cdots < T_L = T$, of size $\Delta T = T_i - T_{i-1}$
  - Intermediate grid : a subdivision of each "subdomain" $\Omega_i = [T_{i-1}, T_i]$, with time step size $\Delta t = \Delta T/M$: $T_{i-1} = t_{i0} < t_{i1} < \cdots < t_{iM} = T_i$
  - Fine grid of size $\delta t = \Delta t/N$ (not indexed)

Three-level parareal



- Unknowns :
  - $U_{ij}^k \approx u(t_{ij})$: approximate solution at t_{ij} at iteration k
  - Y_i^k : approximate solution at T_i at iteration k
- Propagators :
  - F = fine propagator over one Δt, from t_{ij} to $t_{i,j+1}$
  - G = intermediate propagator over the same Δt
  - H = coarse propagator over $\Delta T = M\Delta t$, from T_i to T_{i+1}

Algorithm

- Compute initial guess for coarsest points :

$$Y_0^0 = y_0, \qquad Y_i^0 = HY_{i-1}^0, \qquad 1 \le i \le L$$

- Compute initial guess for intermediate points (in parallel for $1 \le i \le L$) :

$$U_{i0}^0 = Y_{i-1}^0, \qquad U_{ij}^0 = GU_{i,j-1}^0, \qquad 1 \le j \le M$$

- For $k = 0, 1, 2, \ldots$:
  - Run parareal on each Ω_i : parfor $i = 1, \ldots, L$, do

$$U_{i0}^{k+1} = Y_{i-1}^k, \qquad U_{ij}^{k+1} = FU_{i,j-1}^k + GU_{i,j-1}^{k+1} - GU_{i,j-1}^k, \qquad 1 \le j \le M$$

  - Coarsely propagate values across subdomains :

$$Y_i^{k+1} = {\color{red}U_{iM}^{k+1}} + HY_{i-1}^{k+1} - HY_{i-1}^k, \qquad 1 \le i \le L$$

Relationship with MGRIT

If we write down the three-level MGRIT V-cycle with F-relaxation and nested iterations in the above notation, we get

1. Initialize Y_i^0 and U_{ij}^1 the same way as parareal
2. Initialize residuals $g_{ij}^0 = 0$, $1 \leq i \leq L$, $1 \leq j \leq M$
3. For $k = 1, 2, \ldots$
   - (Par)for $i = 1, \ldots, L$, do
     - $U_{i0}^{k+1/2} = Y_{i-1}^k$
     - $U_{ij}^{k+1/2} = g_{i,j-1}^{k-1} + GU_{i,j-1}^{k+1/2}$, $1 \leq j \leq M$
     - $g_{ij}^k = FU_{ij}^{k+1/2} - GU_{ij}^{k+1/2}$, $1 \leq j \leq M$
     - $U_{ij}^{k+1} = g_{ij}^k + GU_{i,j-1}^{k+1}$, $1 \leq j \leq M$
   - $Y_i^{k+1} = U_{iM}^{k+1} + HY_{i-1}^{k+1} - HY_{i-1}^k$, $1 \leq i \leq L$

So the three-level parareal method corresponds to three-level MGRIT with no pre-smoothing at the intermediate level.

Convergence Analysis

What do we want to know ?

- Two-level parareal is known to work well for dissipative problems (e.g. heat equation), but less well for wave or advection-dominated problems
- To predict the behaviour for a given problem, need a convergence analysis that takes into account properties of the spatial operator (e.g. eigenvalues, Lipschitz constants, etc.)
- We present three different error estimates :
  - Nonlinear analysis (uses Lipschitz constants)
  - Linear analysis (analyzes one eigenmode at a time for linear operators)
  - Simplified linear estimates (to get compact formulas useful for further analysis)

Nonlinear analysis

- In the style of Gander & Hairer (DD17 Proceedings, 2008)
- We define the errors at intermediate and coarse points :

$$E_{ij}^k = U_{ij}^k - u(t_{ij}), \qquad D_i^k = Y_i^k - u(T_i).$$

- Assume the Lipschitz constants

$$\|(F-G)y-(F-G)z\| \leq \tau\|y-z\|, \quad \|Fy-Fz\| \leq \beta_F\|y-z\|, \quad \|Gy-Gz\| \leq \beta_G\|y-z\|.$$

- Parareal on the fine level :

$$\begin{aligned} U_{ij}^{k+1} &= FU_{i,j-1}^k + GU_{i,j-1}^{k+1} - GU_{i,j-1}^k \\ U_{ij}^{k+1} - u(t_{ij}) &= (F-G)U_{i,j-1}^k - (F-G)u(t_{i,j-1}) + GU_{i,j-1}^{k+1} - Gu(t_{i,j-1}) \\ \|E_{ij}^{k+1}\| &\leq \tau\|E_{i,j-1}^k\| + \beta_G\|E_{i,j-1}^{k+1}\| \end{aligned}$$

- Parareal on the coarse level :

$$\begin{aligned} Y_i^{k+1} &= U_{iM}^{k+1} + HY_{i-1}^{k+1} - HY_{i-1}^{k} \\ Y_i^{k+1} - u(T_i) &= U_{iM}^{k+1} - F^M u(T_{i-1}) + HY_{i-1}^{k+1} - HY_{i-1}^{k} \\ &= U_{iM}^{k+1} - F^M Y_{i-1}^{k} + HY_{i-1}^{k+1} - Hu(T_{i-1}) \\ &\quad + (F^M - H)Y_{i-1}^{k} - (F^M - H)u(T_{i-1}) \\ \|D_i^{k+1}\| &\leq \|U_{iM}^{k+1} - F^M Y_{i-1}^{k}\| + \beta_H^M \|D_{i-1}^{k+1}\| + \rho\|D_{i-1}^{k}\|, \end{aligned}$$

where

$$\|(F^M - H)y - (F^M - H)z\| \leq \rho\|y - z\|, \qquad \|Hy - Hz\| \leq \beta_H^M \|y - z\|.$$

- Need a recurrence on the **sub-interval truncation error** $\mathcal{E}_{ij}^{k+1} = U_{ij}^{k+1} - F^j Y_{i-1}^{k}$:

$$\begin{aligned} \mathcal{E}_{ij}^{k+1} &= (F - G)E_{i,j-1}^{k} - (F - G)E_{i,j-1}^{k+1} + FU_{i,j-1}^{k+1} - F^j Y_{i-1}^{k} \\ \|\mathcal{E}_{ij}^{k+1}\| &\leq \tau\|E_{i,j-1}^{k}\| + \tau\|E_{i,j-1}^{k+1}\| + \beta_F\|\mathcal{E}_{i,j-1}^{k+1}\| \end{aligned}$$

Linear analysis

- The "wrong" sign leads to pessimistic bounds when E_{ij}^{k+1} is not much smaller than E_{ij}^{k}, i.e., when the speed of convergence is modest.
- Linear analysis : assume
    - F, G and H are linear in the initial conditions (e.g. for linear DEs)
    - Assume F, G and H simultaneously diagonalizable (e.g. same spatial differential operator)
    - Analyze method for scalar ODE, keeping sign information in the error equations
- Example : for $y_t = -\lambda y$, Backward Euler gives

$$F = \frac{1}{(1 + \lambda \Delta t / N)^N}, \qquad G = \frac{1}{1 + \lambda \Delta t}, \qquad H = \frac{1}{1 + \lambda M \Delta t}.$$

Recurrences for linear analysis

- Intermediate level :

$$
\begin{aligned}
E_{ij}^{k+1} &= \tau E_{i,j-1}^{k} + G E_{i,j-1}^{k+1}, && 1 \le j \le M,\ k \ge 0 \\
E_{ij}^{0} &= G E_{i,j-1}^{0} - \tau u(t_{i,j-1}), && 1 \le j \le M \\
E_{i0}^{k+1} &= D_{i-1}^{k}, && k \ge 0
\end{aligned}
$$

- Coarse level :

$$
\begin{aligned}
D_{i}^{k+1} &= \mathcal{E}_{iM}^{k+1} + \rho D_{i-1}^{k} + H D_{i-1}^{k+1}, && k \ge 0 \\
D_{i}^{0} &= H D_{i-1}^{0} - \rho u(T_{i-1}) \\
D_{0}^{k} &= 0, && k \ge 0
\end{aligned}
$$

- Sub-interval truncation error :

$$
\begin{aligned}
\mathcal{E}_{ij}^{k} &= \tau E_{i,j-1}^{k-1} - \tau E_{i,j-1}^{k} + F \mathcal{E}_{i,j-1}^{k}, && 1 \le j \le M,\ k \ge 1 \\
\mathcal{E}_{i0}^{k} &= 0, && k \ge 1.
\end{aligned}
$$

- To solve these recurrences, use generating functions :

$$E(\xi, \eta, z) = \sum_{i\geq 1}\sum_{j\geq 0}\sum_{k\geq 0} E_{ij}^k \eta^i \xi^j z^k, \qquad D(\eta, z) = \sum_{i\geq 1}\sum_{k\geq 0} D_i^k \eta^i z^k$$

- After a lot of algebra, we get $D_l(z) = \sum_{k\geq 0} D_l^k z^k$, where

$$\begin{aligned} D_l(z) &= \sum_{p=0}^{l-1} \left[(G+\tau z)^M z + H(1-z)\right]^p (d_{l-p} + \cdots) \\ &= \sum_{p=0}^{l-1} \left[((G+\tau z)^M - G^M)z + (G^M - H)z + H\right]^p (d_{l-p} + \cdots) \\ &= \sum_{p=0}^{l-1} \left[\sum_{n=2}^{M+1} \binom{M}{n-1} G^{M-n+1}(F-G)^{n-1} z^n + (G^M - H)z + H\right]^p (d_{l-p} + \cdots) \end{aligned}$$

- To find D_l^k, compute the coefficient of z^k in the series expansion of $D_l(z)$

Finite termination property

Theorem : For $l = 1, 2, 3, \ldots$, the kth iterate of three-level parareal satisfies

$$Y_l^k = u(T_l)$$

whenever $k \geq Ml + l$.

Proof : For a linear scalar problem, the generating function

$$D_l(z) = \sum_{p=0}^{l-1} \left[(G + \tau z)^M z + H(1-z)\right]^p$$
$$\times \left[d_{l-p} + \left((G+\tau z)^M - G^M\right) \sum_{i=0}^{l-p-1} H^i d_{l-p-i-1} + \sum_{j=1}^{M-1} \left((G+\tau z)^{M-j} - G^{M-j}\right) e_{l-p,j}\right]$$

is a polynomial of degree $(l-1)(M+1) + M = lM + l - 1$ in z, so the coefficient of z^k is zero for $k \geq lM + l$. A similar argument holds for the nonlinear problem.

Simplified error bounds

$$D_l(z) = \sum_{p=0}^{l-1} \left[(G+\tau z)^M z + H(1-z)\right]^p$$
$$\times \left[d_{l-p} + \left((G+\tau z)^M - G^M\right) \sum_{i=0}^{l-p-1} H^i d_{l-p-i-1} + \sum_{j=1}^{M-1} \left((G+\tau z)^{M-j} - G^{M-j}\right) e_{l-p,j} \right]$$

- For a fixed time $t = T_l$, the error at all iterations k can be written in terms of block vectors and matrices :

$$\mathbf{D}_l = \begin{bmatrix} D_l^0 \\ D_l^1 \\ \vdots \end{bmatrix} = \sum_{p=0}^{l-1} \mathcal{Q}^p \mathbf{f}_p, \qquad \text{where} \qquad \mathcal{Q} = \begin{bmatrix} L & & & \\ R & L & & \\ & R & L & \\ & & \ddots & \ddots \end{bmatrix}, \qquad \mathbf{f}_p = \begin{bmatrix} f_{p0} \\ f_{p1} \\ \vdots \end{bmatrix},$$

- Use the relationship between Toeplitz matrices and generating functions to bound powers of $\mathcal{Q}$ applied to $\mathbf{f}_p$
- Must choose norm carefully to get useful estimates **within** the same block !

Convergence of three-level Parareal

Theorem (K. 2022) : Let $|G|, |H| < 1$. Let $D_k^l = Y_l - u(T_l)$ be the error of three-level parareal after $k = (M+1)q + r$ iterations, where $q \geq 0$ and $0 \leq r \leq M$. Then

$$D_l^k \leq \binom{l}{q+1} b_r \|R\|_*^q \cdot (D+E) \|u\|_{L^\infty(0,T_l)},$$

where $(b_i)_{i=0}^\infty$ is the coefficient of z^i in the Taylor expansion of

$$B(z) = \frac{1-H}{1-H-z((G+|\tau|z)^M - G^M + |\gamma|)}$$

and

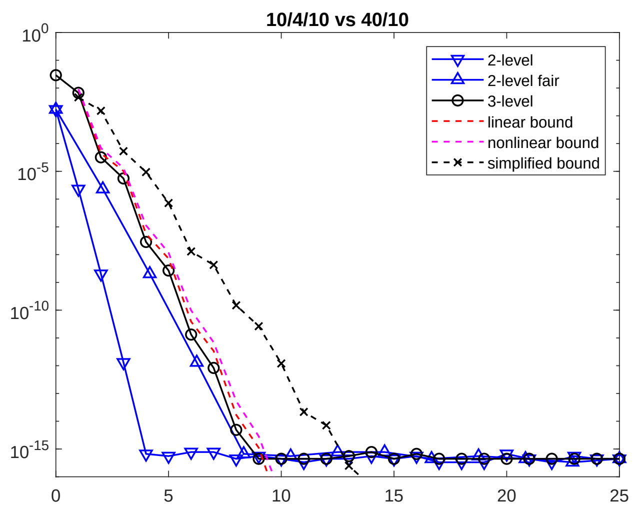
$$\|R\|_* = \max_{0 \leq i \leq M} \frac{b_{i+M+1}}{b_i}, \quad D = \frac{|\rho|}{1-H}\left(1 - |\gamma|(1-H) + \frac{\|R\|_*}{b_M}\right), \quad E = \max_{1 \leq s \leq M} \frac{|\tau|^{s+1}}{b_s G (1-G)^{s+1}}.$$

Scalar test problems : $y_t = -\lambda y$

- Total number of time steps $= 100M$, $M = 4, 8, 16, 32, 64, 128$
  - 3-level : $10 \times M \times 10$ steps
  - 2-level : either $10 \times 10M$ steps or $10M \times 10$ steps
- We compare :
  - "Linear/nonlinear bound" : calculate polynomials in Matlab
  - "Simplified bound" : use expression from theorem
- For a cost-adjusted comparison of 2- and 3-level parareal, let C_F, C_G and C_H be the cost of doing a single step of the fine, intermediate and coarse integration. Then ignoring communication cost, we have

Type	#Coarse $\times$ Fine steps	Cost/iter.	Iter. for exact conv.
2-level	$LM \times N$	$N \cdot C_F + LM \cdot C_G$	LM
2-level	$L \times MN$	$NM \cdot C_F + L \cdot C_G$	L
3-level	$L \times M \times N$	$N \cdot C_F + M \cdot C_G + L \cdot C_H$	$LM + L$

Backward Euler, $y_t = -0.1y$



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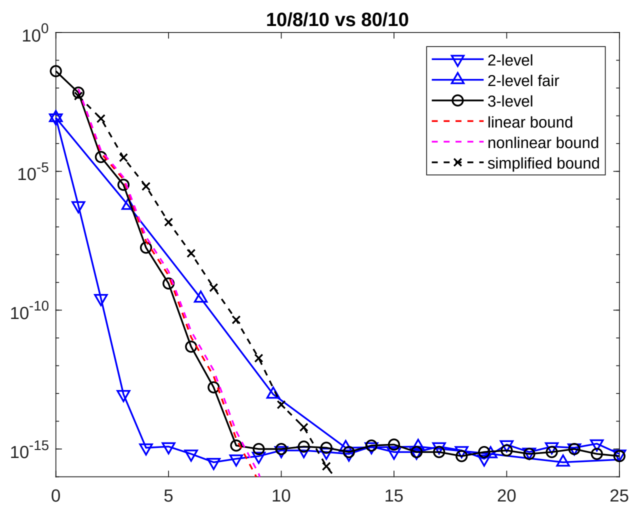

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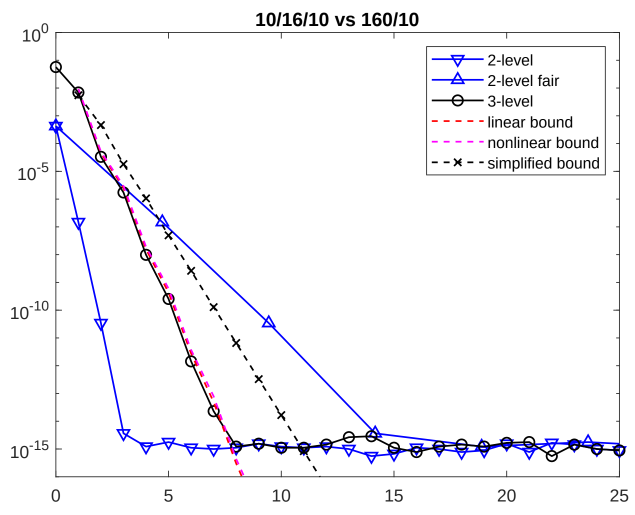

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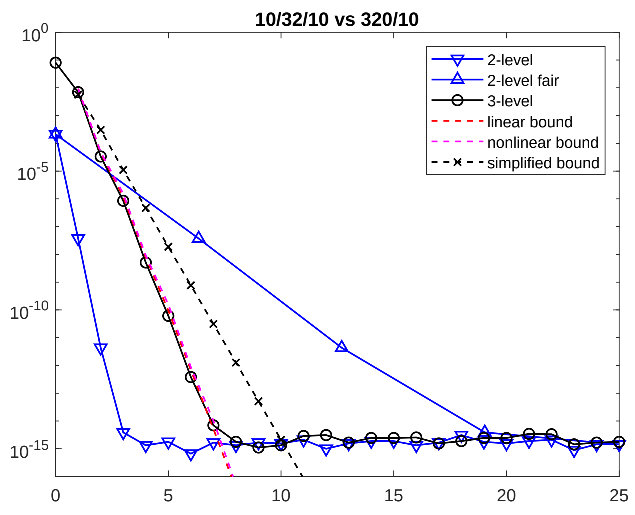

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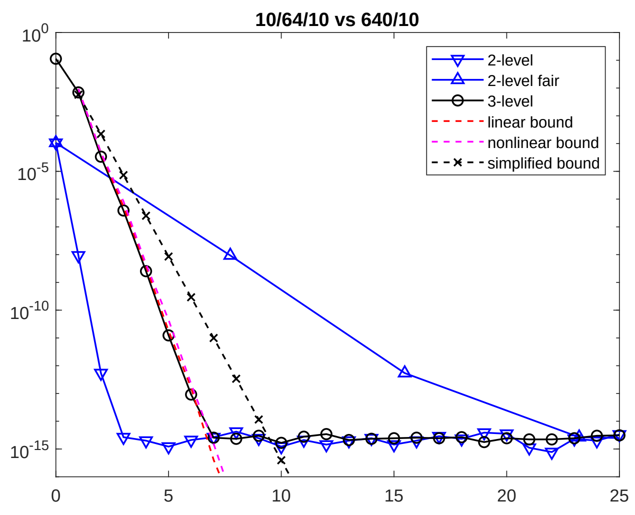

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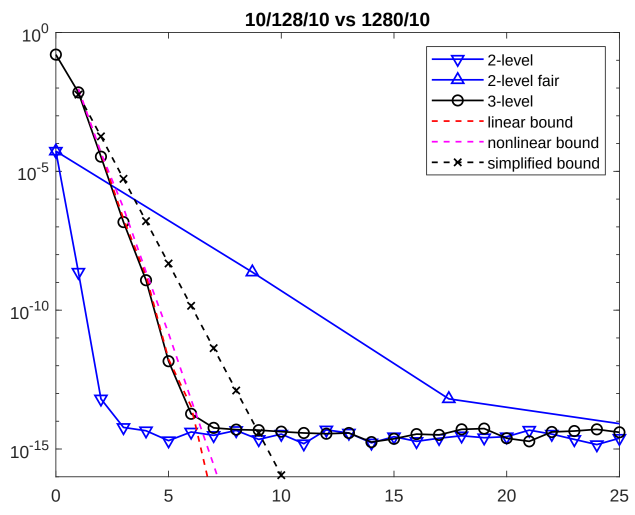
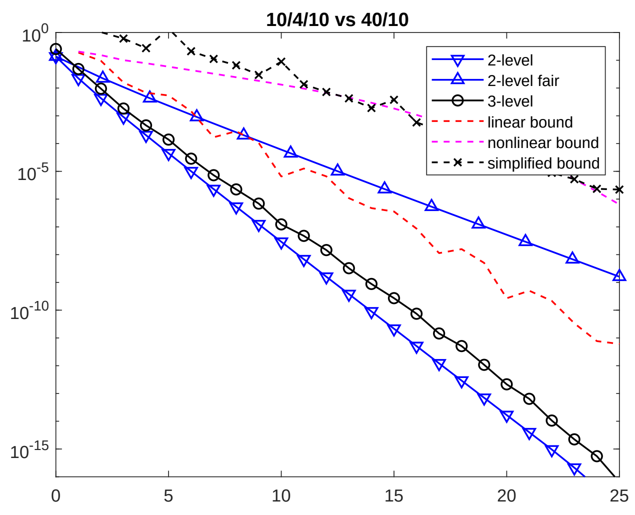


Backward Euler, $y_t = -10y$



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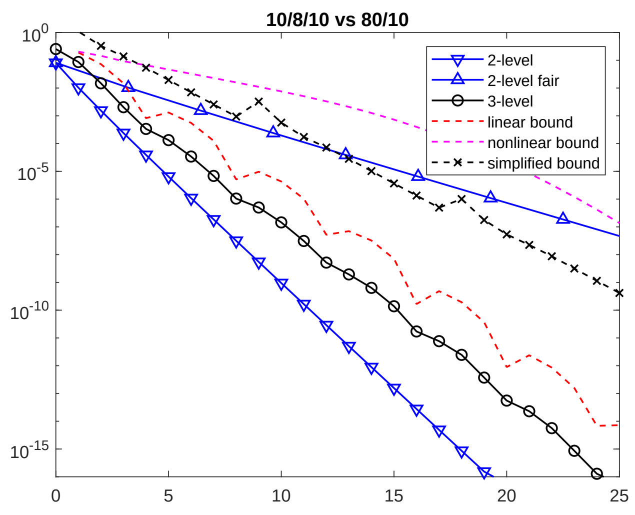

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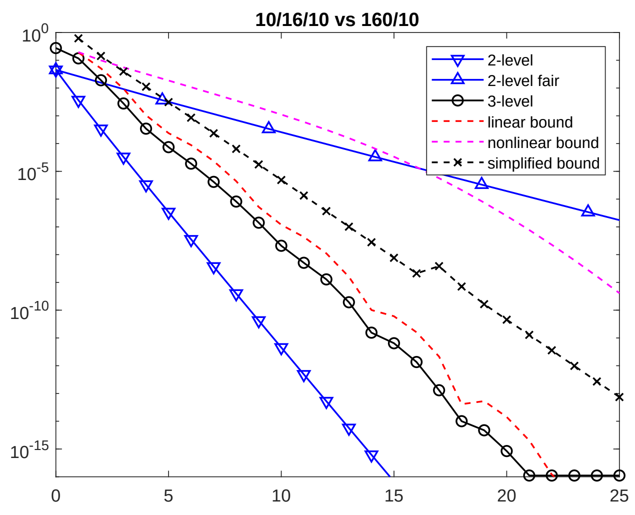

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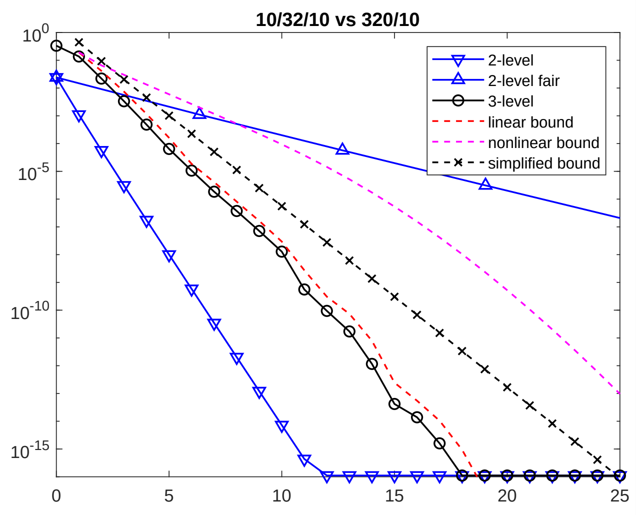

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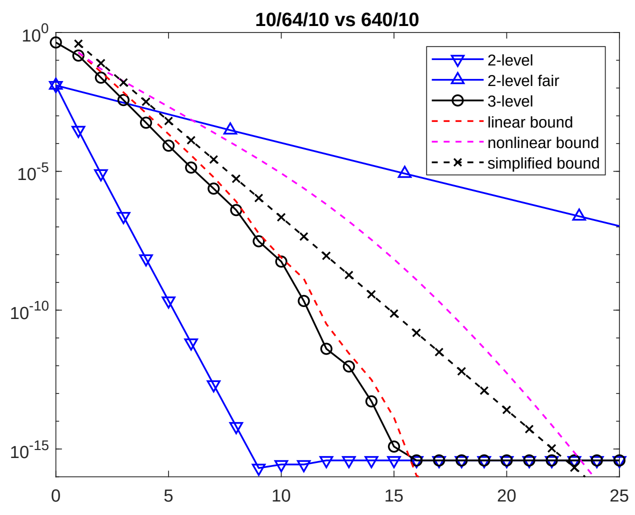

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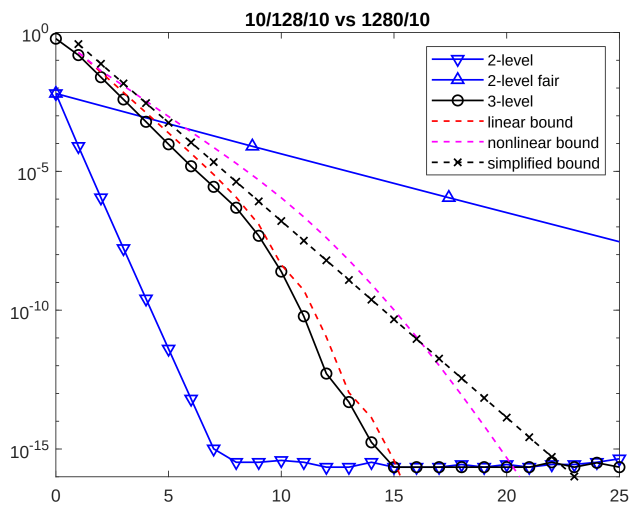


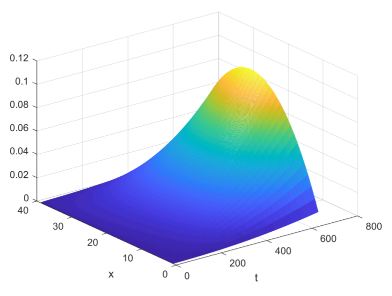
PDE examples

Heat equation

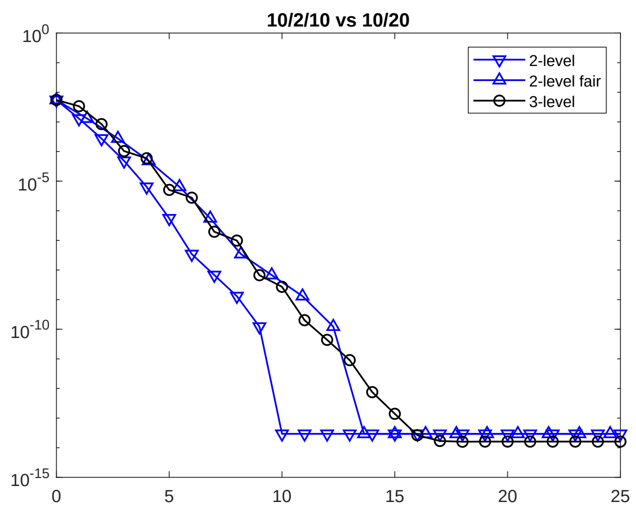
- Solve

$$u_t - u_{xx} = x^4(1-x) + t^2, \qquad (x,t) \in (0,1) \times (0,1)$$

- Initial condition : $u(x,0) = 0$
- Homogeneous Dirichlet boundary condition in space
- Centred 2nd order FD in space ($h = 1/40$)
- Backward Euler on all levels



Fixed coarse grid + refinement of second-level grid



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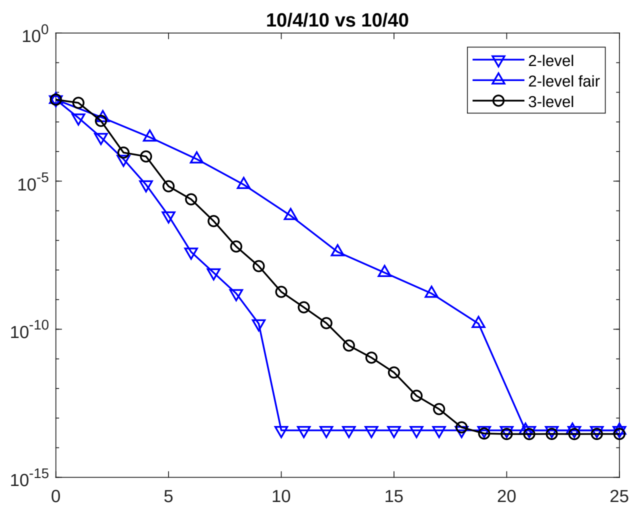

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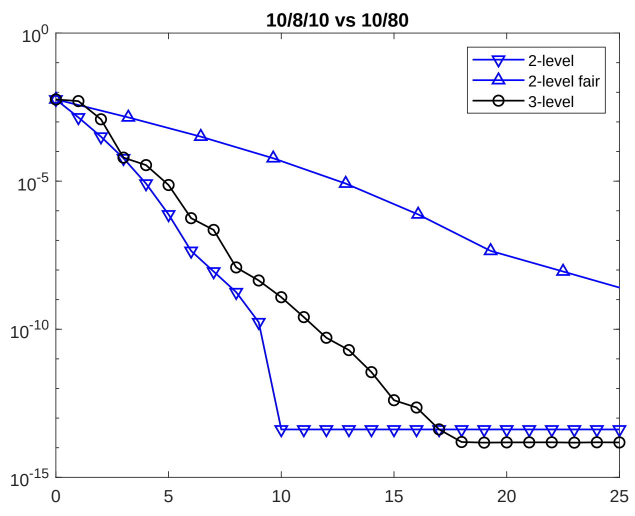

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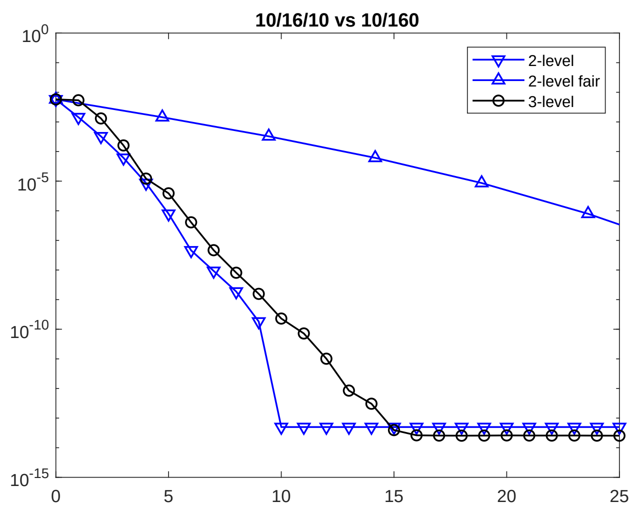

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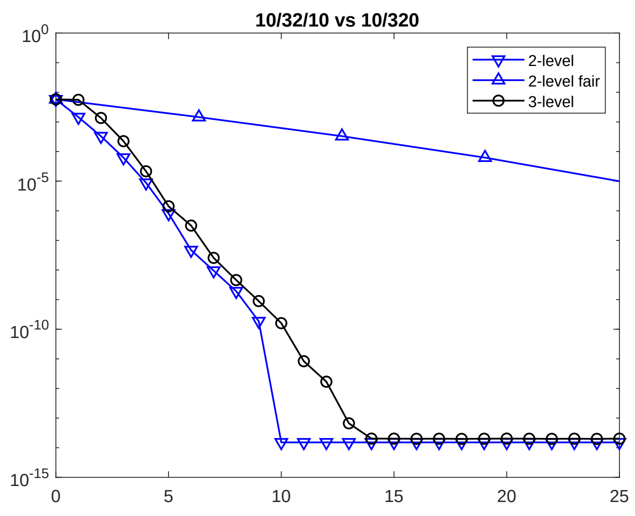

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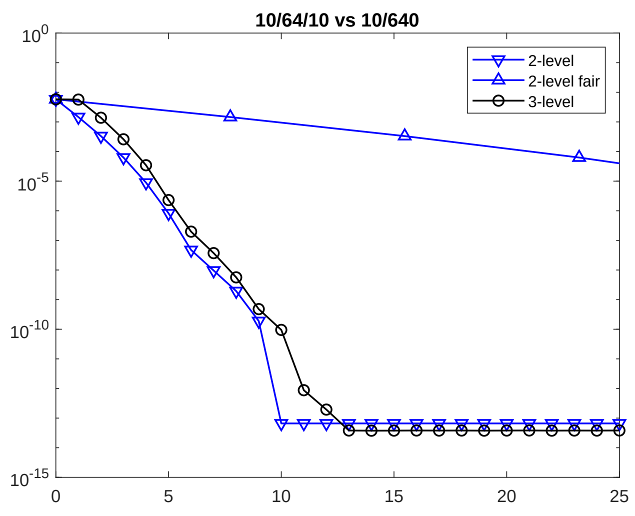
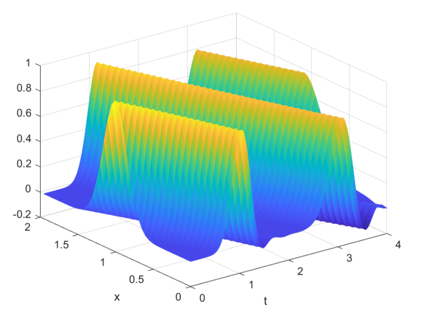


Advection diffusion equation

- Solve

$$u_t = u_x + \nu u_{xx}, \qquad (x,t) \in (0,2) \times (0,4)$$

- Initial condition : $u(x,0) = e^{-20(x-1)^2}$
- Periodic boundary conditions
- Backward Euler on all levels



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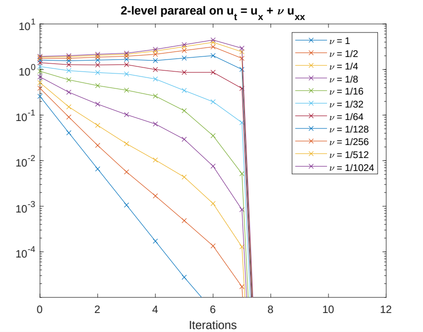
- Same behaviour for 3-level parareal ?



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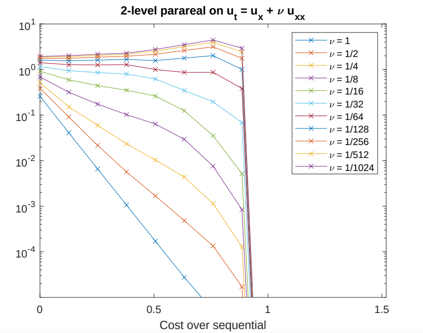
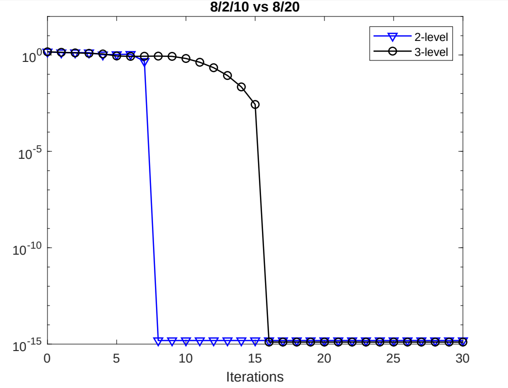
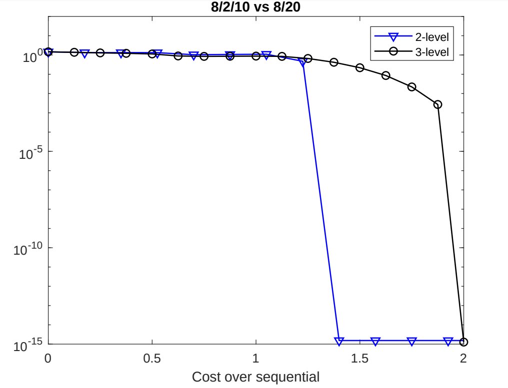
- Same behaviour for 3-level parareal ?
- Instead of counting iterations, normalize by cost of sequential solve



Advection-Diffusion Equation

- $\nu = 1/1024$
- 8 coarse intervals
- Refine second-level grid from 2 to 64 intervals





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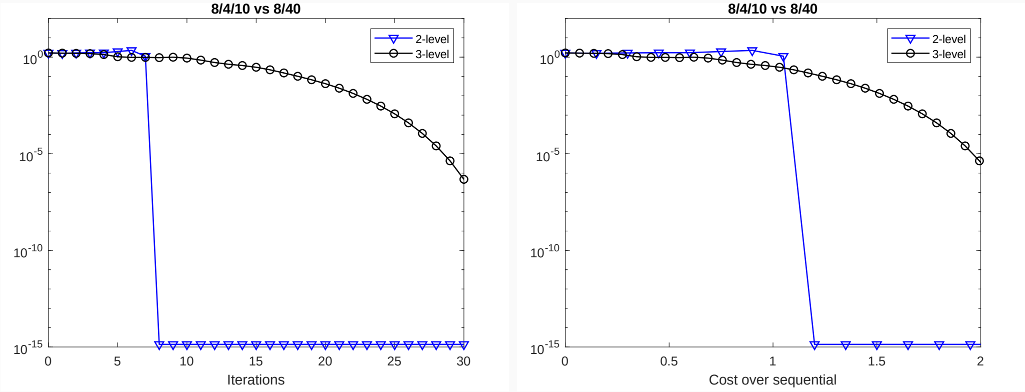

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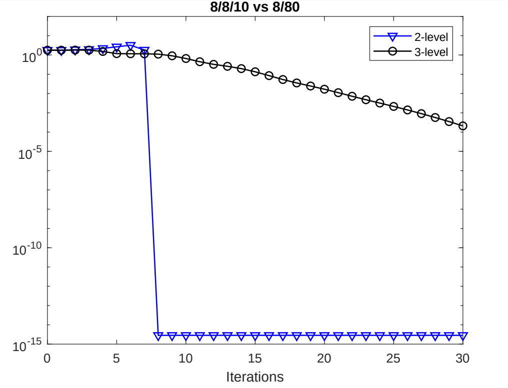

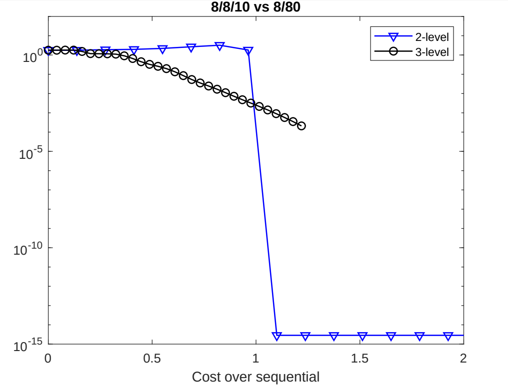

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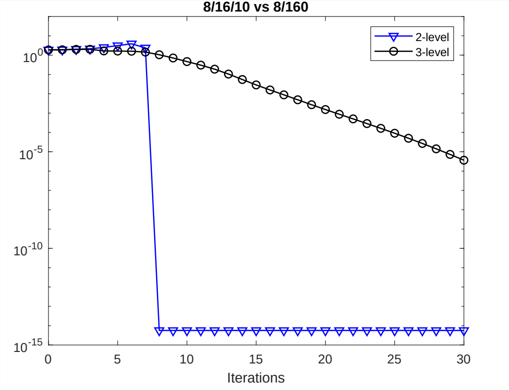

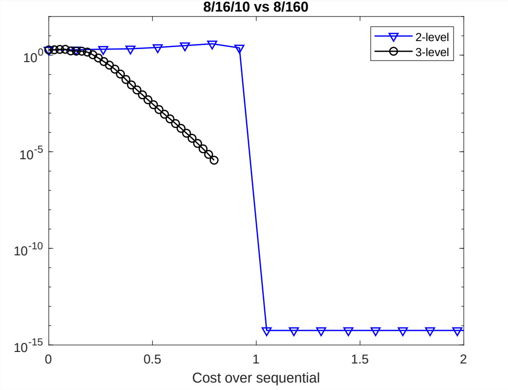

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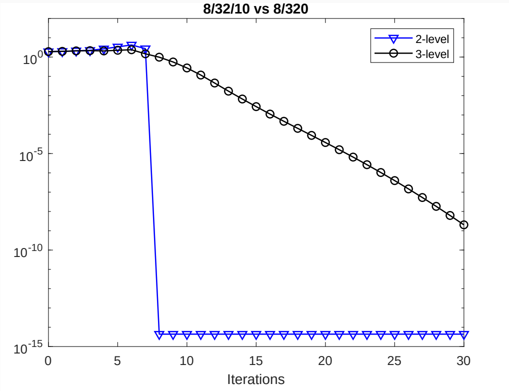

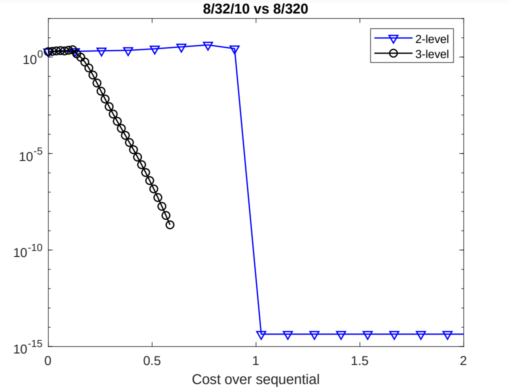

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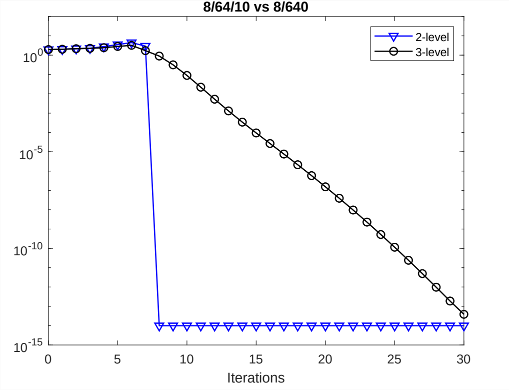

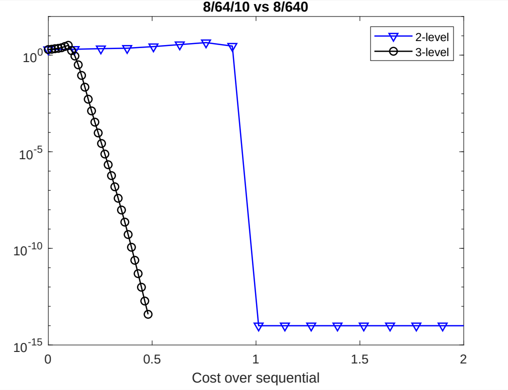

Summary

- 3-level variant of parareal + interpretation as an MGRIT method
- Finite termination property
- Linear (and nonlinear) analysis by generating functions
- Some speedup possible for advection-diffusion for small ν
- Ongoing work :
  - Adapt estimates to $y_t = \lambda y$ for complex λ
  - Optimize distribution of coarse/intermediate/fine levels
  - Nonlinear problems
  - Adapt framework to study more general Parareal/MGRIT methods

THANK YOU !

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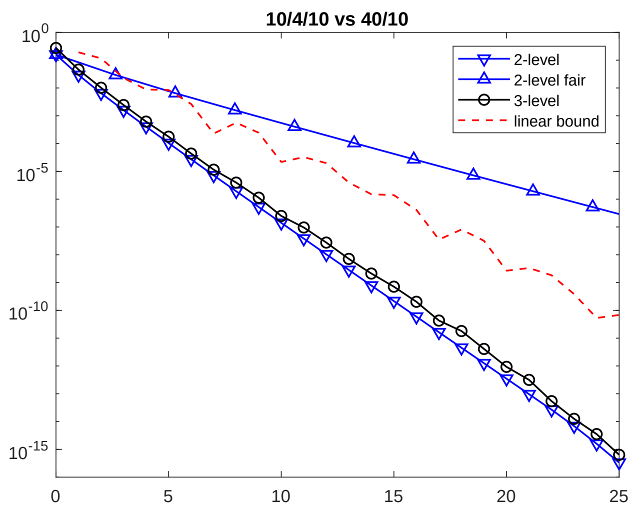
SDIRK23 + Backward Euler, $y_t = -10y$



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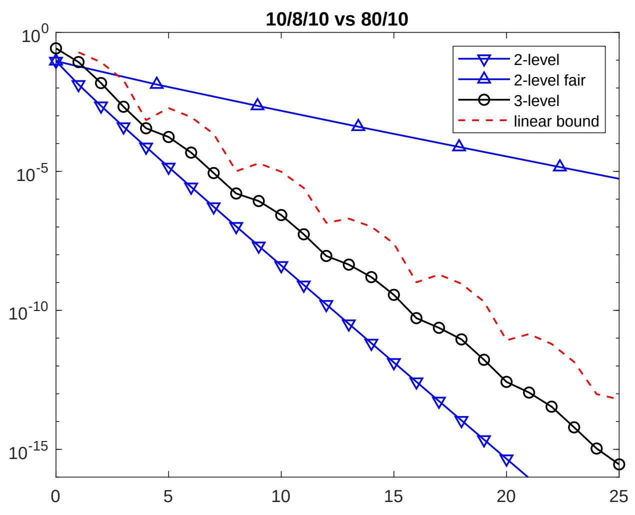

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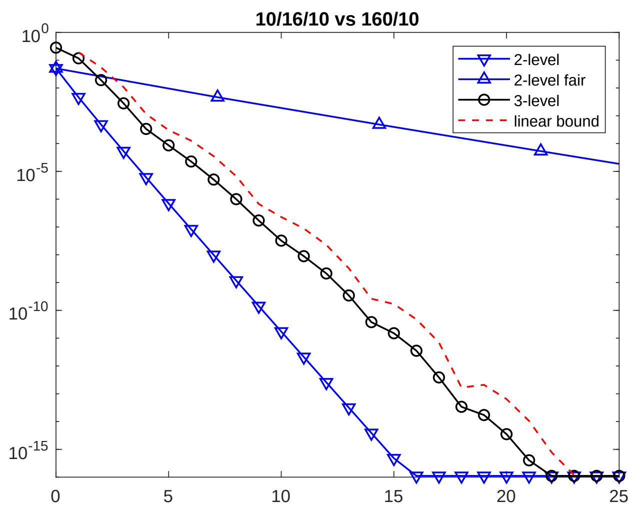

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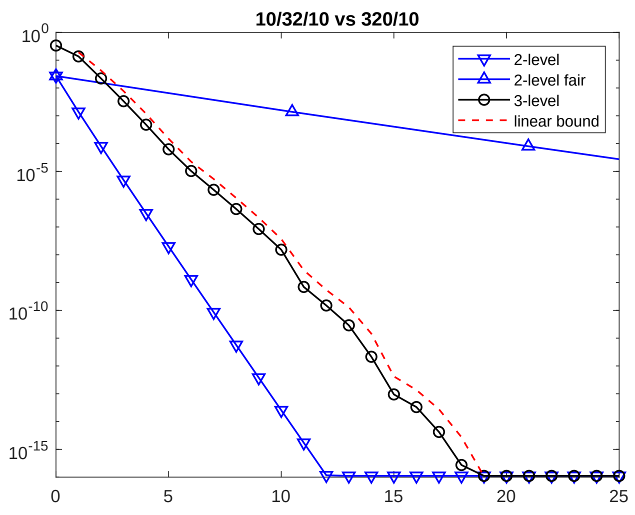

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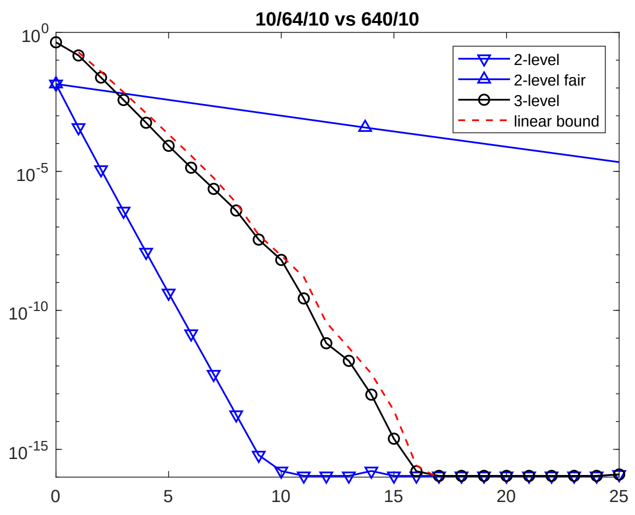

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