Multigrid for Time-Dependent PDEs

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Typical Problem

- parabolic PDE

$$u_t = \mathcal{L}u + f$$

- example : 1D Poisson

$$u_t = u_{xx} + f$$

- discretise
  - time : implicit Euler
  - space : finite differences

$$\Delta t^{-1}(u_{i,j} - u_{i-1,j}) = \Delta x^{-2}(u_{i,j-1} - 2u_{i,j} + u_{i,j+1} + f_{i,j})$$

- matrix notation

$$(T \otimes I)u = (I \otimes L)u + f$$

System of Equations

$$(T \otimes I)u = (I \otimes L)u + f, \qquad L : m \times m$$

	1D	2D	3D
$m \approx$	n_x	$n_x n_y$	$n_x n_y n_z$

- implicit Euler : T triangular

$$m \times m$$

- s-stage IRK : T has dense $s \times s$ blocks

$$sm \times sm$$

- k-step BVM, n time steps : T $n \times n$, bandwith k
- Can we use high order time discretisation schemes?

Two Worlds

- parabolic PDE

$$u_t = \mathcal{L}u + f$$

- aspects of
  - ODE

$$\frac{du}{dt} = f(u)$$

  - elliptic PDE

$$\mathcal{L}u + f = 0$$

- PDE approach : (reduce to) simple time discretisation
- ODE approach :
  - simple preconditioners for large system
  - preconditioner for time discretisation
  - special time discretisation schemes
- Best of both worlds?

ODEs

- typical equation

$$\frac{du}{dt} = f(u)$$

- implicit Euler

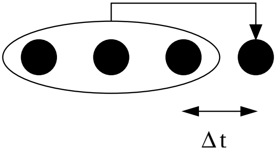
$$\frac{u_i - u_{i-1}}{\Delta t} = f(u_i)$$

- stability : A-stable
  - test equation $\frac{du}{dt} = \lambda u$
  - continuous solution bounded
  - $\Rightarrow$ discrete solution bounded
- order 1 : error $\sim \Delta t^{-1}$

Linear Multistep Method

$$\frac{du}{dt}(t) = f(u(t))$$

$$u_i \approx u(i\Delta t)$$



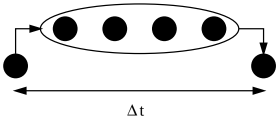
- k-step LMF
- update approximation at point i
  using k previous points $i-1, \ldots, i-k$

$$\alpha_k u_i + a^T U_i = \Delta t \beta_k f(u_i) + \Delta t b^T f(U_i)$$

- only A-stable up to order 2

Implicit Runge-Kutta Method

$$\frac{du}{dt}(t) = f(u(t))$$
$$u_i \approx u(i\Delta t)$$



- s stage IRK
- update approximation at point i using s stage values U_i

$$U_i = u_{i-1} + \Delta t A f(U_i)$$
$$u_i = u_{i-1} + \Delta t b^T f(U_i)$$

- A-stable methods for all orders

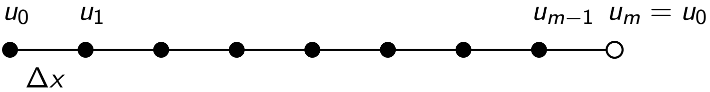
Elliptic PDE

- typical equation : 1D Poisson

$$u_{xx} + f = 0$$

- discretisation : e.g., finite differences

$$u_{i-1} - 2u_i + u_{i+1} = \Delta x^{-2} f_i$$



- system of equations

$$Lu = f$$

- 2D, 3D → large systems → iterative methods

Simple Iterations

- system

$$Lu = f$$

- splitting $L = L^+ + L^-$

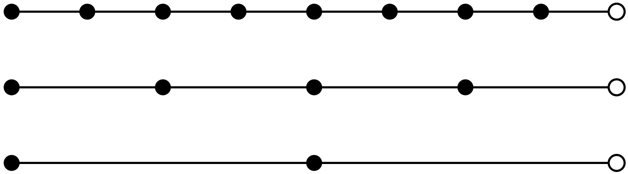
$$L^+ u^{(\nu)} + L^- u^{(\nu-1)} = f$$

- e.g., Jacobi, **Gauss-Seidel**

$$u_i^{(\nu)} = \frac{1}{2}(u_{i-1}^{(\nu)} + u_{i+1}^{(\nu-1)} - \Delta x^{-2} f_i)$$

Multigrid Principle

- convergence of Jacobi and Gauss-Seidel very slow
- for elliptic PDEs: multigrid
- idea: use calculations on a coarse grid (cheaper) to accelerate iteration on fine grid



Convergence

- iteration

$$u^{(\nu)} = Mu^{(\nu-1)} + g$$

- convergence factor

$$\rho^{(\nu)} = \frac{\|u^{(\nu)} - u\|}{\|u^{(\nu-1)} - u\|}$$

- spectral radius

$$\lim_{\nu\to\infty} \rho^{(\nu)} = \rho = \max|\sigma(M)|$$

- typical MG convergence

$$\rho \approx 0.1$$

independent of mesh size

Time and Space

- discretise space
- discretise time
- large system
- iterative methods
- elliptic PDE

$$-Lu = \cdots$$

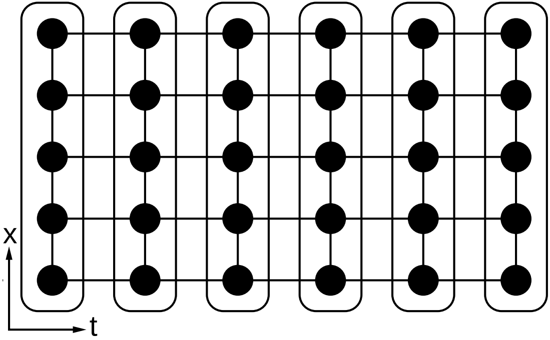
  MG
- implicit Euler/LMM

$$\alpha I - \Delta t \beta L = \cdots$$

  still MG
- IRK, BVM?

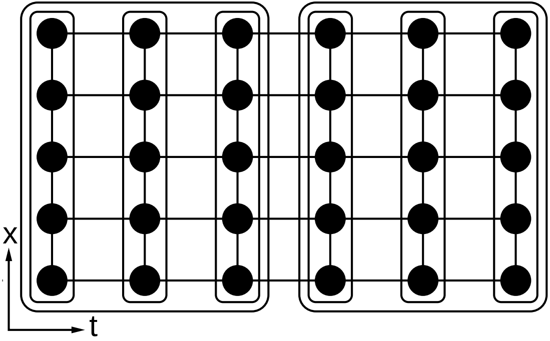
LMM Time Stepping

loop over time steps
  loop over grid points (MG)



IRK Time Stepping

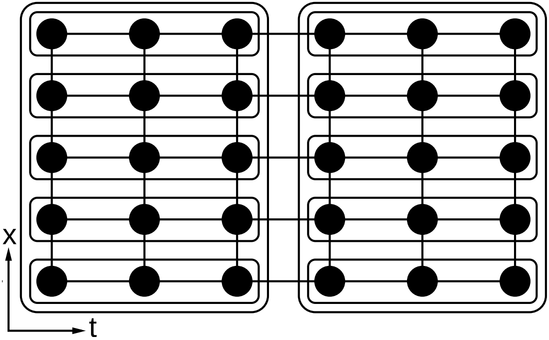
loop over time steps
  loop over stages
    loop over grid points (MG)



- slow because of strong coupling

Reorder Loops : Block Time Stepping

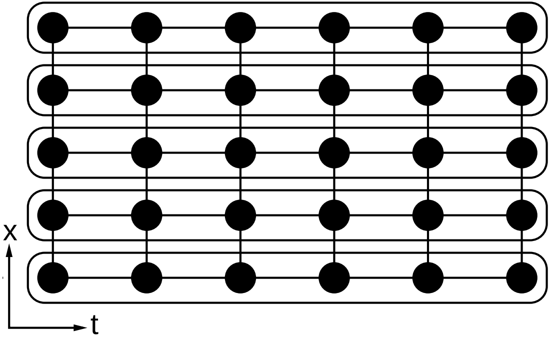
loop over time steps
  loop over grid points (MG)
    solve stages



- strong coupling handled by small dense solve

Waveform Relaxation

- carry idea through : all time steps together



- useful for BVP, periodic, delay
- for theory : solve ODE in each grid point
- interesting ideas, but do they work?

Overview

- system

$$(T \otimes I)u = (I \otimes L)u + f$$

- reduce to simple scheme

$$(T^+ \otimes I)u^{(\nu)} + (T^- \otimes I)u^{(\nu-1)} = (I \otimes L)u^{(\nu)} + f$$

- then MG on $\theta I - L$
- MG with block smoother

$$(T \otimes I)u^{(\nu)} = (I \otimes L^+)u^{(\nu)} + (I \otimes L^-)u^{(\nu-1)} + f$$

- then dense solve on $T - \lambda I$

1. Methods

2. Convergence Analysis
   - Functional Calculus Framework
   - ODEs
   - DDEs

Simplifications

- linear systems
- constant coefficients
- fixed regular grid
- periodic or infinite grid
- two levels
- fixed time step

Convergence Analyses

- system

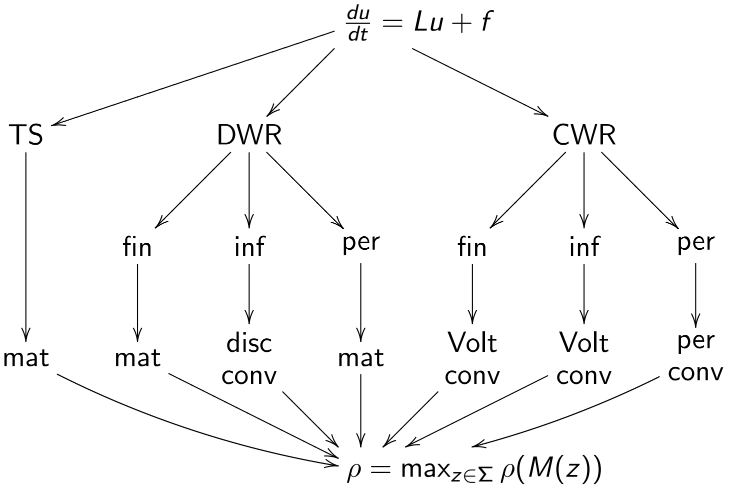
$$(T \otimes I)u = (I \otimes L)u + f$$

- MG smoother

$$(T \otimes I)u^{(\nu)} = (I \otimes L^{+})u^{(\nu)} + (I \otimes L^{-})u^{(\nu-1)} + f$$

- traditionally separate analysis for each T
- convergence analyses similar
- different theories and tools

Traditional Convergence Analysis Approach



Functional Calculus Framework

- analyses can be unified using functional calculus
- matrix $T \in \mathbb{C}^{n \times n}$
- function of a matrix
- well known examples : T^2, $\exp(T)$, $\cos(T)$, etc.
- function $f : \mathbb{C} \to \mathbb{C}$

$$f(z) = \sum_i c_i z^i$$

- analytic in $\Omega \supset \sigma(T)$
- matrix $f(T) \in \mathbb{C}^{n \times n}$

$$f(T) = \sum_i c_i T^i$$

Calculation Rules

- linearity

$$\alpha f(T) + \beta g(T) = (\alpha f + \beta g)(T)$$

- multiplication

$$f(T) \cdot g(T) = (f \cdot g)(T)$$

- function composition

$$g(f(T)) = (g \circ f)(T)$$

- spectral mapping theorem

$$\sigma(f(T)) = \{f(z) : z \in \sigma(T)\} =: f(\sigma(T))$$

Functional Calculus for Matrix-Valued Functions

- matrix $T \in C^{n \times n}$
- matrix-valued function $F : \mathbb{C} \to \mathbb{C}^{m \times p}$

$$F(z) = \sum_i C_i z^i$$

- analytic in $\Omega \supset \sigma(T)$
- definition $F(T) \in \mathbb{C}^{mn \times pn}$

$$F(T) = \sum_i C_i \otimes T^i$$

Calculation Rules

- linearity

$$\alpha F(T) + \beta G(T) = (\alpha F + \beta G)(T)$$

- multiplication

$$F(T) \cdot G(T) = (F \cdot G)(T)$$

- function composition

$$G(F(T)) = (G \circ F)(T)$$

- spectral mapping theorem

$$\sigma(F(T)) = \bigcup_{z \in \sigma(T)} \sigma(F(z)) =: \sigma(F(\sigma(T)))$$

- corollary

$$\rho(F(T)) = \max_{z \in \sigma(T)} \rho(F(z))$$

Extensions

- F values in Banach algebra
- T element of Banach algebra
  - bounded operators on a Banach space

$$(Su)_i = u_{i-1}$$

$$(Tu)_i = \frac{u_i - u_{i-1}}{\Delta t} = \Delta t^{-1}(I - S)$$

  - Banach space : $l^p(n),\ l^p(\infty)$
- T closed unbounded operator

$$Tu = u_t$$

  - Banach space : $L^p(0, t_F),\ L^p(0, \infty)$

Result

- spectrum of MG for

$$(T \otimes I)u = (I \otimes L)u + f$$

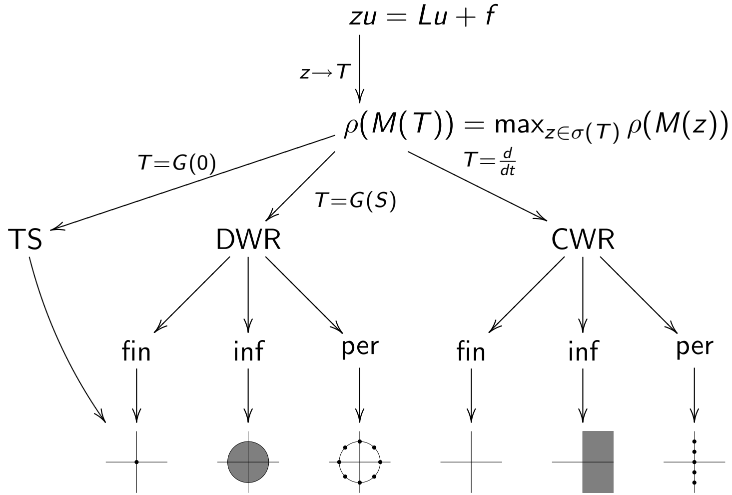
- spectrum of MG for

$$zu = Lu + f$$

- for $z \in \sigma(T)$
- spectral radius

$$\rho = \max_{z \in \sigma(T)} \rho(M(z))$$

Convergence Analysis using Functional Calculus

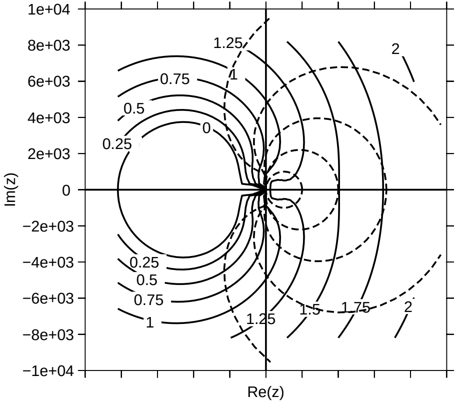


Example

- heat equation

$$u_t = u_{xx} + u_{yy} + f$$

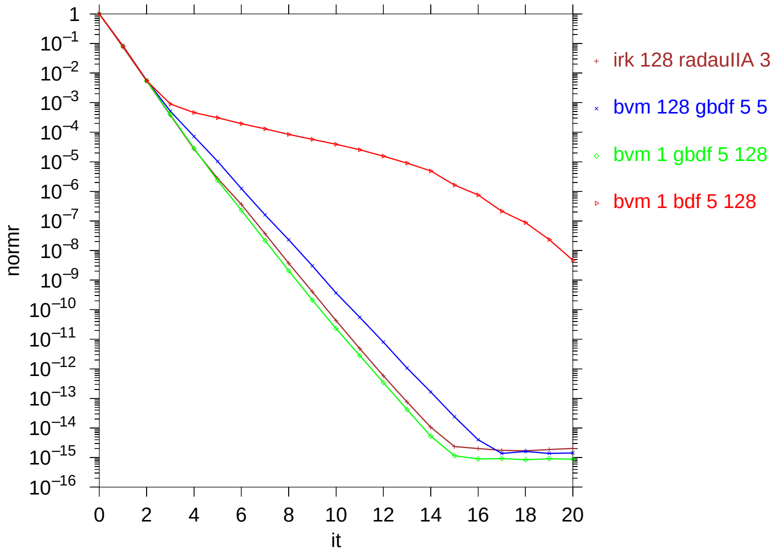
- finite differences
  $\Delta x = \Delta y = \frac{1}{32}$, $\Delta t = 10^{-3}$
- MG WR
- $\rho(\mathbf{M}(z))$ using two-grid analysis
- contour lines of
  $R(z) = -\log_{10} \rho(M(z))$
- $\sigma(T)$ for BDF1–5



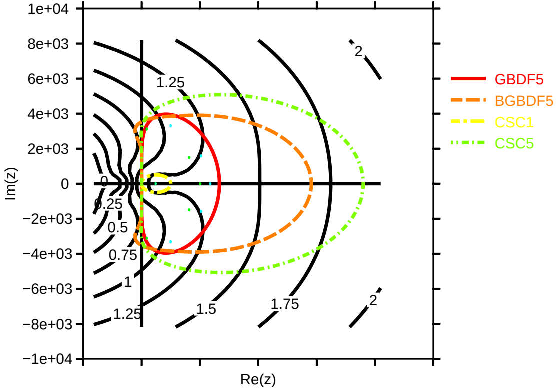
Stability and Convergence

- test equation $\frac{dy}{dt} = \lambda y$
- $y(t) \rightarrow 0$ if $\lambda \in \mathbb{C}^-$
- open stability domain S : λ for which $y_i \rightarrow 0$
- for DWR on infinity sequences : $\sigma(T) = \mathbb{C} \setminus S$
- importance of stability : stiff ODEs, step size restriction
- here also for convergence
- A-stable method : $S \subset \mathbb{C}^-$
- useful upper bound : $\max_{z \in i\mathbb{R}} \rho(M(z))$

Stability and Convergence : Example



High Order Schemes



GBDF5	BGBDF5	CSC1	CSC5
0.80	0.74	1.13	0.79

Problems with Delay

- DDE

$$\frac{du}{dt} = Lu - u(t-\tau)$$

- Picard iteration

$$\frac{du^{(\nu)}}{dt} = L^{+}u^{(\nu)} + L^{-}u^{(\nu-1)} - u^{(\nu-1)}(t-\tau)$$

- non-Picard iteration

$$\frac{du^{(\nu)}}{dt} = L^{+}u^{(\nu)} + L^{-}u^{(\nu-1)} - u^{(\nu)}(t-\tau)$$

- derivative operator : $(T_1 u)(t) = \frac{du}{dt}(t)$
- delay operator : $(T_2 u)(t) = u(t-\tau)$
- system

$$(T_1 \otimes I)u = (I \otimes L)u - (T_2 \otimes I)u$$

Convergence Analysis

- functional calculus for commuting operators
- T_1 and T_2 commute
- $F : \mathbb{C} \times \mathbb{C} \to \mathbb{C}^{m \times m}$
- $\sigma(F(T_1, T_2)) = \sigma(F(\sigma(T_1, T_2)))$
- joint spectrum $\sigma(T_1, T_2) \in \mathbb{C} \times \mathbb{C}$
- in this case

$$\sigma(T_1, T_2) = \{(z, e^{-\tau z}) : z \in \bar{\mathbb{C}}^{+}\}$$

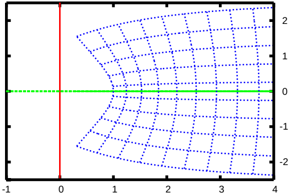
Example : non-Picard MG

- smoother

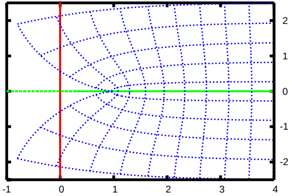
$$F(z_1, z_2) = ((z_1 + e^{-\tau z_1})I - L^+)^{-1} L^-$$

- reuse MG analysis for $zu = Lu + f$

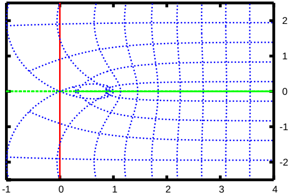
$\tau = \frac{1}{2}$



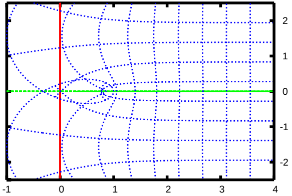
$\tau = 1$



$\tau = \frac{\pi}{2}$

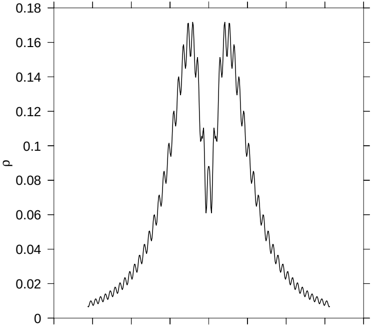


$\tau = 2$



Example (cont.)

$$u_t(t) = a\big(u_{xx}(t) + u_{yy}(t)\big) + bu(t-\tau)$$



- delay manifests itself as a wiggle on top of the curve for the equation without delay ($b = 0$)
- amplitude and frequency depend on the choice of parameters

Summary

- MG for time-dependent PDEs : block smoothers
- convergence analysis based on functional calculus
- stability of time discretisation important for convergence
- high order methods no problem (if stable)
- MG for delay PDEs