Waveform Relaxation using Spectral Collocation in Time

Jan Van lent[1] Stefan Vandewalle

Katholieke Universteit Leuven
Department of Computer Science

Tuesday 27 July
ICCAM 2004

[1] Research Assistant of the Fund for Scientific Research - Flanders (Belgium) (F.W.O.-Vlaanderen)

Classical Iterative Methods

- system $Ax = b$
- splitting $A = A^{+} + A^{-}$
- iteration $A^{+}x^{(\nu)} + A^{-}x^{(\nu-1)} = b$
- A^{+} such that simple to solve
  - Jacobi: diagonal of A
  - Gauss-Seidel: lower triangular part of A
- iteration matrix $K = -(A^{+})^{-1}A^{-}$
- spectral radius

$$\rho(K) = \max\{|\lambda| : \lambda \in \sigma(K)\}$$

- $\rho < 1 \Rightarrow$ convergence, the smaller the better

Continuous Waveform Relaxation

- iterative method for system of ODEs

$$\dot{x} = Ax + b$$

- same splitting $A = A^+ + A^-$

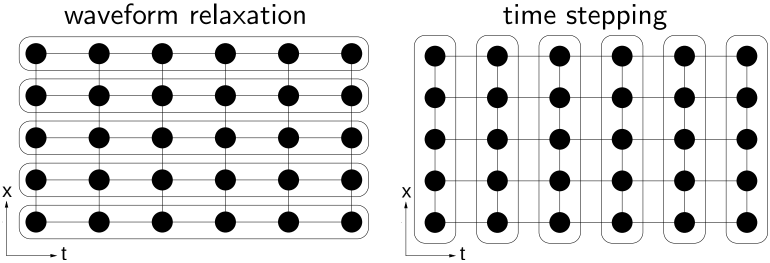
$$\dot{x}^{(\nu)} = A^+ x^{(\nu)} + A^- x^{(\nu-1)} + b$$

- e.g. Jacobi

$$\dot{x}_i^{(\nu)} + a_{ii} x_i^{(\nu)} = b_i - \sum_{j \neq i} a_{ij} x_j^{(\nu-1)}$$

Discrete Waveform Relaxation

- in practice: ODE integrator for each scalar ODE



- LMF, IRK, BVM have all been considered
- in this presentation Chebyshev Spectral Collocation

Convergence Analysis of Waveform Relaxation

- system of equations

$$(T \otimes I)x = (I \otimes A)x + b$$

- T : time derivative operator $w = Tv$
  - continuous $\quad w(t) = \frac{dv(t)}{dt}$
  - BDF1 $\quad w_i = \frac{v_i - v_{i-1}}{\Delta t}$
- $A = A^+ + A^- \longrightarrow$ iteration

$$(T \otimes I)x^{(\nu)} = (I \otimes A^+)x^{(\nu)} + (I \otimes A^-)x^{(\nu-1)} + b$$

- iteration operator

$$\mathcal{K} = (T \otimes I - I \otimes A^+)^{-1}(I \otimes A^-)$$

- spectral radius

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

- $K(z)$ iteration matrix for classical iterative method

$$K(z) = (zI - A^+)^{-1} A^-$$

- $\mathcal{K}$ non-normal operator $\rightarrow$ infinite time domains (alternatives: pseudospectrum, weighted norms)
- T operates on $v(t)$, $t \in \mathbf{R}^+$ or v_i, $i \in \mathbf{N}$
- continuous WR on $[0, \infty) \rightarrow \sigma(T) = \mathbf{C}^+$
- upper bound for A-stable methods ($\sigma(T) \subset \mathbf{C}^+$)

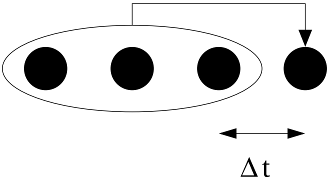
Linear Multistep Formula

$$v'(t) = f(v(t))$$

$$v_i \approx v(i\Delta t)$$

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

$$\sum_{j=-k}^{0} \alpha_{k+j} v_{i+j} = \Delta t \sum_{j=-k}^{0} \beta_{k+j} f(v_{i+j})$$



Implicit Runge-Kutta Method

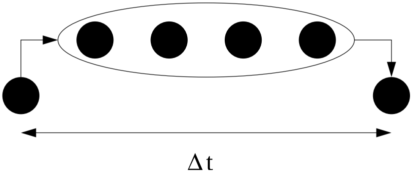
$$v'(t) = f(v(t))$$

$$v_i \approx v(i\Delta t)$$

- s stage IRK
- update approximation at point i using s "stage" values V_i

$$v_i = v_{i-1} + \Delta t b^T f(V_i)$$

$$V_i = v_{i-1} + \Delta t A f(V_i)$$

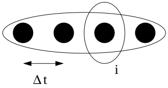


Boundary Value Method

$$v'(t) = f(v(t))$$
$$v_i \approx v(i\Delta t)$$

- k-step BVM ($k = k_1 + k_2$)
- assume boundary value problem
- use "central" LMF formula where possible

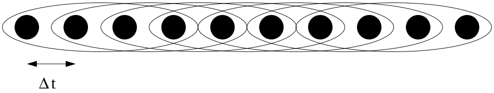
$$\sum_{j=-k_1}^{k_2} \alpha_{k_1+j} v_{i+j} = \Delta t \sum_{j=-k_1}^{k_2} \beta_{k_1+j} f(v_{i+j})$$



- additional conditions of same order near boundaries (less symmetrical)

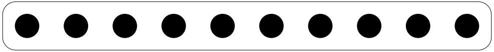
$$\tilde{\mathbf{A}}\tilde{\mathbf{y}} = \Delta t \tilde{\mathbf{B}} f(\tilde{t}, \tilde{\mathbf{y}})$$

$$\tilde{\mathbf{A}} = \begin{bmatrix}
\alpha_0^1 & \alpha_1^1 & \cdots & \alpha_k^1 & & & \\
\vdots & \vdots & \cdots & \vdots & & & \\
\alpha_0^{k_1-1} & \alpha_1^{k_1-1} & \cdots & \alpha_k^{k_1-1} & & & \\
 & \alpha_0 & & \cdots & \alpha_k & & \\
 & & \ddots & & \cdots & \ddots & \\
 & & & \alpha_0 & & \cdots & \alpha_k \\
 & & & \alpha_0^{n-k_2+1} & & \cdots & \alpha_k^{n-k_2+1} \\
 & & & \vdots & & \cdots & \vdots \\
 & & & \alpha_0^n & & \cdots & \alpha_k^n
\end{bmatrix}$$



Chebyshev Spectral Differentiation

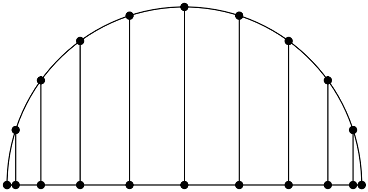
- interpolating spectral method (pseudospectral method)
- idea
  - given function $v(x)$
  - choose points x_j
  - construct interpolating polynomial $p(x_j) = v(x_j)$
  - approximate derivative $v'(x_j)$ by $w_j = p'(x_j)$



Chebyshev points

- interpolation → choice of x_j very important
- intuition: one-sidedness
  - central difference more accurate than forward or backward difference
  - points near boundary: more one-sided → higher density of points needed
- Chebyshev extreme points (Gauss-Chebyshev-Lobatto points)

$$x_j = \cos \frac{j\pi}{n}$$



Differentiation Matrix

- spectral differentiation: linear operation
  $\longrightarrow$ can be written as matrix

$$\bar{\mathbf{w}} = \bar{\mathbf{D}}\bar{\mathbf{v}}$$

- explicit formula
- on interval $[0, \Delta t]$

$$t_j = \frac{1 - x_j}{2}\Delta t$$

$$\tilde{\mathbf{D}} = -\frac{2}{\Delta t}\bar{\mathbf{D}}$$

Chebyshev Spectral Collocation for ODEs

- replace $v'(t) = f(v(t))$ by $\tilde{\mathbf{D}}\tilde{\mathbf{v}} = f(\tilde{\mathbf{v}})$
- v_j parameters of unknown function
- partition $\tilde{\mathbf{D}}$ and $\tilde{\mathbf{v}}$

$$\tilde{\mathbf{D}}\tilde{\mathbf{v}} = \left[\begin{array}{c|c} \cdot & \text{---} \\ \hline \mathbf{d_0} & \mathbf{D} \end{array}\right] \left[\begin{array}{c} v_0 \\ \hline \mathbf{v} \end{array}\right]$$

- initial value condition $v(0) = v_0$
  $\rightarrow$ ignore first row of $\tilde{\mathbf{D}}$
- system of equation to solve

$$\mathbf{Dv} = -\mathbf{d_0} v_0 + f(\mathbf{v})$$

Features

- simple explicit formula for **D**
- if smooth $\rightarrow$ use high order $\rightarrow$ small number of unknowns
- spectral convergence
- all time steps simultaneously (like BVM)
- dense matrix
- expensive when applied mindlessly to large system of ODEs
- **but** in Jacobi and GS WR only scalar ODEs
- A-stable for any order $\rightarrow$ good WR convergence

Similarities to IRK and BVM

- k-step BVM is collocation with spline of order k
  $k = n \rightarrow$ polynomial
- block BVM = apply BVM on subintervals
- block CSC = apply CSC on subintervals
  = spectral elements
  $\approx$ IRK/block BVM
- polynomial collocation using same collocation points
  $\rightarrow$ essentially the same method

CSC as BVM

- CSC

$$\mathbf{d_0} v_0 + \mathbf{D} v = f(\mathbf{v})$$

- BVM on general grids $\mathbf{H} = \mathrm{diag}(\Delta t_i)$

$$\mathbf{a_0} v_0 + \mathbf{A} v = \mathbf{H}\mathbf{b_0} f(v_0) + \mathbf{H}\mathbf{B} f(\mathbf{v})$$

- high order A-stable BVMs $\rightarrow$ more points near boundaries
- n-step GBDF ($\mathbf{b_0} = 0$, $\mathbf{B} = \mathbf{I}$)
  on Gauss-Chebyshev-Lobatto points
  $\mathbf{d_0} = \mathbf{H}^{-1}\mathbf{a_0}$, $\mathbf{D} = \mathbf{H}^{-1}\mathbf{A}$
- methods to calculate coefficients of BVMs and spectral methods on general grids are very similar

CSC as IRK

- CSC $\quad \mathbf{d_0} v_0 + \mathbf{D} v = f(\mathbf{v})$

  $\times \mathbf{D}^{-1} \rightarrow \quad \mathbf{v} = -\mathbf{D}^{-1}\mathbf{d_0} v_0 + \mathbf{D}^{-1} f(\mathbf{v})$
- IRK $\quad \mathbf{v} = v_0 + \Delta t \mathbf{A} f(\mathbf{v})$

IRK as BVM

- IRK methods derived using order conditions
  but shown to be polynomial collocation methods
- e.g. Gauss, Radau, Lobatto
  based on Gauss-Legendre, Gauss-Legendre-Radau, Gauss-Legendre-Lobatto points
- n-step GBDF on Gauss-Radau points = RadauIIA

Waveform Relaxation

- Classical Iterative Methods
- Continuous and Discrete Waveform Relaxation
- Convergence Analysis

Time Discretisation

- LMF, IRK, BVM
- Chebyshev Spectral Collocation
- Similarities to IRK and BVM

Results

- Model Problem
- Convergence Analysis Results
- Numerical Results

Model Problem

- linear parabolic equation on unit square $(x, y) \in [0, 1]^2$

$$u_t = (au_x)_x + (bu_y)_y + cu + f$$

- finite difference in space (method of lines)
- stiff system of ODEs

$$\dot{u} = Lu + f$$

- L large sparse structured matrix
- adapt multigrid method for elliptic equation $(u_t = \dot{u} = 0)$

Example 1: Problem

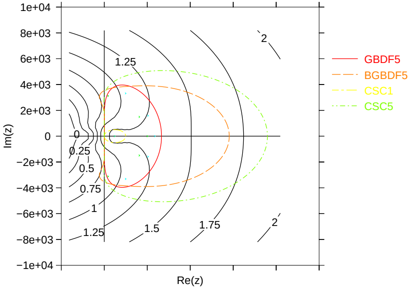
- diffusion equation ($a = b = 1$, $c = 0$)

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

- multigrid waveform relaxation
- convergence analysis
  - $\rho(\mathbf{M}(z))$ calculated using standard multigrid analysis
  - continuous WR on infinite intervals $z \in i\mathbf{R}$
  - CSC $z \in \sigma(\mathbf{D})$
  - block CSC on infinite sequences
    $z \in \sigma(w\mathbf{d_0}\mathbf{e_n}^T + \mathbf{D}), \quad |w| \leq 1$

Example 1: Convergence Analysis

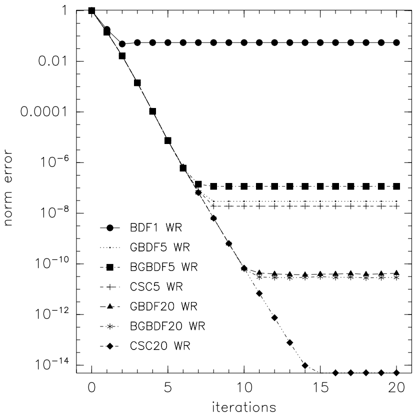
- $R(z) = -log_{10}\rho(\mathbf{M}(z))$
- $R = \min_{z \in \sigma(T)} R(z)$ digits per iteration (asymptotic)
- spectral picture



GBDF5	BGBDF5	CSC1	CSC5
0.80	0.74	1.13	0.79

Example 1: Numerical Results

- discretisation error
  - $u(x,y,t) = sin(\frac{2\pi t}{10})$
  - $\Delta x = \Delta y = \frac{1}{8}$
  - time interval and #unknowns fixed
- convergence
  - $u(x,y,t) = 0$
  - $\Delta x = \Delta y = \frac{1}{32}$
  - $\rho^{(\nu)} = \frac{\|u^{(\nu)}\|}{\|u^{(\nu-1)}\|}$
  - $R^{(\nu)} = -\log_{10}\rho^{(\nu)}$



BDF1	GBDF5	BGBDF5	CSC5	GBDF20	BGBDF20	CSC20
0.97	0.87	0.87	0.87	0.11	0.10	0.88

Example 2

$$u_t = (au_x)_x + (bu_y)_y + cu + f$$

- $a(x,y,t) = e^{10(x-y)}$, $b(x,y,t) = e^{-10(x-y)}$, $c(x,y,t) = 0$, $u(x,y,t) = 0$
- anisotropic (coefficients depend on x and y)
- standard MG does not work
  (same for corresponding elliptic equation)
- adapt special MG methods to the parabolic case
- e.g. "multigrid as smoother", a multiple semicoarsening method
- convergence factor $\approx 6 \cdot 10^{-2}$

Concluding Remarks

- WR inspired by classical iterative methods
- WR converges depends on stability of time discretisation
- if continuous WR converges on $[0, \infty)$
  $\rightarrow$ any A-stable ODE integrator will too
- for WR it is worth considering time discretisation schemes that would be too expensive in other cases
- CSC well suited for WR,
  if high order needed and possible (smooth problem)
- many time discretisation schemes are closely related
- more extensive comparisons are needed

Further Reading

- WR convergence (Miekkala and Nevanlinna '87)
- IRK (Hairer and Wanner; Butcher)
- BVM (Brugnano and Trigiante)
- CSC (Trefethen; Boyd)
- ODE/PDE/WR (Burrage)
- MG (Briggs, Henson and McCormick; Trottenberg, Oosterlee and Schüller)
- MG WR (Lubich and Ostermann '89; Vandewalle)
- MGS (Washio and Oosterlee '95, '98)