Implicit time integration

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- Explicit schemes: CFL restricted time step: Courant number $C < 1$ in

$$\Delta t \leq C \min_i \left(\frac{\Delta x_i}{c_i^{\max}} \right)$$

  $\Rightarrow$ MHD: $c_i^{\max} = \mid v_i \mid + c_i^{\text{fast}}$ fast magnetosonic speed c_i^{fast}

- can be inefficient when

  $\Rightarrow$ only interested in steady state $\partial t = 0$ solution

  $\Rightarrow$ no fast waves induced (or physically unimportant): still set CFL

  $\Rightarrow$ solution: switch to implicit time integration, allowing $C > 1$!

- diffusive type source term: further limit on Δt from

$$\Delta t \leq C_{\text{diff}} \min_i \left[\frac{(\Delta x_i)^2}{\max(\eta, \nu, \kappa)} \right]$$

  $\Rightarrow$ for increasing resolution: more restrictive than CFL

  $\Rightarrow$ need to treat source term(s) implicitly

Implicit schemes

- after semi-discretization (Finite Volume spatial discretization) solve

$$\frac{d\mathbf{U}}{dt} = \mathbf{R}(\mathbf{U})$$

$\Rightarrow$ two-parameter (α, β) base scheme

$$\begin{aligned} \mathbf{U}^{n+1} \;=\; & \mathbf{U}^n + \Delta t_n \mathbf{R}(\mathbf{U}^n) + \alpha \Delta t_n \left[\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t_{n-1}} - \mathbf{R}(\mathbf{U}^n) \right] \\ & + \beta \Delta t_n \left[\mathbf{R}_{\text{impl}}(\mathbf{U}^{n+1}) - \mathbf{R}_{\text{impl}}(\mathbf{U}^n) \right] \end{aligned}$$

$\Rightarrow$ uses two time levels n and $n+1$ for $\alpha = 0$

$\Rightarrow$ three-level scheme for $\alpha \neq 0$

$\Rightarrow$ all implicitly treated terms in $\mathbf{R}_{\text{impl}}$

- Steady state simulations: fully implicit Backward Euler

  $\Rightarrow$ two-level scheme $\alpha = 0,\ \beta = 1$

  $\Rightarrow$ fully implicit: $\mathbf{R}_{\text{impl}} = \mathbf{R}$

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \Delta t_n \mathbf{R}(\mathbf{U}^{n+1})$$

- nonlinear residual $\mathbf{R}(\mathbf{U}^{n+1})$ at unknown time level $n+1$

  $\Rightarrow$ linearize $\mathbf{R}(\mathbf{U}^{n+1}) = \mathbf{R}(\mathbf{U}^n) + \frac{\partial \mathbf{R}}{\partial \mathbf{U}}\big|_n \left(\mathbf{U}^{n+1} - \mathbf{U}^n\right)$

- linearized fully implicit Backward Euler scheme: solve

$$\left[\frac{I}{\Delta t} - \frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right] [\mathbf{U}^{n+1} - \mathbf{U}^n] = \mathbf{R}(\mathbf{U}^n)$$

  $\Rightarrow$ large linear system

  $\Rightarrow$ Newton's method: $x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$ for $f(x) = 0$ for $\Delta t \to \infty$

  $\Rightarrow$ Jacobian $\partial \mathbf{R} / \partial \mathbf{U}$: numerically evaluated

- two essential ingredients: large linear systems and Jacobian evaluation
- SS: employ nearest neighbour 1st order discretization in $\partial\mathbf{R}/\partial\mathbf{U}$

  $\Rightarrow$ only interest in high order solution satisfying $\mathbf{R}(\mathbf{U}) = 0$

  $\Rightarrow$ 1D: block tri-diagonal system; 2D block penta; 3D: block hepta
- 1D block tri-diagonal systems: employ direct solver
- $>$ 1D problem: storage and accuracy problem for direct linear solvers

  $\Rightarrow$ switch to iterative linear system solvers, e.g. GMRES

Iterative methods: GMRES (Saad & Schultz 1986)

- Generalized Minimal RESidual for system $A\mathbf{x} = \mathbf{b}$
- guess $\mathbf{x}_o$ and residual $\mathbf{r}_o = \mathbf{b} - A\mathbf{x}_o$
- define Krylov subspace $K^k(A, \mathbf{x}_o) = \left\{\mathbf{r}_o, A\mathbf{r}_o, \ldots, A^{k-1}\mathbf{r}_o\right\}$
- successive approximations $\mathbf{x}_k$

  $\Rightarrow$ minimize $\parallel \mathbf{b} - A\mathbf{x}_k \parallel_2$ over $K^k(A, \mathbf{x}_o)$

- iterative linear system solvers for $A\mathbf{x} = \mathbf{b}$

  $\Rightarrow$ kernels: matrix-vector products and dot products

  $\Rightarrow$ condition number of A = ratio largest/smallest eigenvalue

  $\Rightarrow$ fast convergence if condition number close to unity

- for strongly non-symmetric matrix (advection dominated problems)

  $\Rightarrow$ needed: pre-conditioning!

  $\Rightarrow$ apply iterative solver to ‘pre-conditioned’ linear system

  $\Rightarrow$ pre-multiply system with approximate to inverse of A

  $\Rightarrow$ can dramatically improve convergence behavior

  $\Rightarrow$ VAC: Modified Block Incomplete LU-preconditioner

- Storage issue (as k increases): Restarted GMRES

  $\Rightarrow$ GMRESR (van der Vorst & Vuik 1994)

- Best experience with: Bi-Conjugate Gradient Stabilized

  $\Rightarrow$ Bi-CGSTAB (van der Vorst 1992)

Jacobian evaluation

- numerical evaluation: matrix-free (Newton-Krylov) (can be high order!)

  $\Rightarrow$ only need directional derivative

  $\Rightarrow$ use explicit methods to evaluate $\mathbf{R}(\mathbf{U})$ (CFL limited Δt)

$$\frac{\partial \mathbf{R}}{\partial \mathbf{U}}[\Delta \mathbf{U}] = \frac{\mathbf{R}(\mathbf{U} + \epsilon \Delta \mathbf{U}) - \mathbf{R}(\mathbf{U})}{\epsilon}$$

  $\Rightarrow$ action of Jacobian in direction $\Delta \mathbf{U}$ with numerical differentiation

  $\Rightarrow$ choice of ϵ crucial

  ◇ small enough to be physical/accurate

  ◇ avoid rounding errors (large w.r.t. machine precision)

- PROBLEM: this effectively perturbs the matrix

  $\Rightarrow$ errors at each matrix-vector product (kernel for iterative scheme)

  $\Rightarrow$ destroys orthogonality properties exploited in iterative schemes!!!

- numerical evaluation: Build the matrix

$$\frac{\partial \mathbf{R}_i^{(u)}}{\partial \mathbf{U}_j^{(w)}} = \frac{\mathbf{R}_i^{(u)}(\mathbf{U} + \epsilon_j^{(w)}) - \mathbf{R}_i^{(u)}(\mathbf{U})}{\epsilon}$$

$\Rightarrow$ still use explicit branch to evaluate $\mathbf{R}(\mathbf{U})$

$\Rightarrow$ low order $\mathbf{R} \longrightarrow$ known sparsity pattern (nearest neighbour)

$\Rightarrow$ STRUCTURED GRID: Grid masks (allows data parallelism)

1	2	3

1D

1	2	3	4	5
3	4	5	1	2
5	1	2	3	4
2	3	4	5	1
4	5	1	2	3

2D

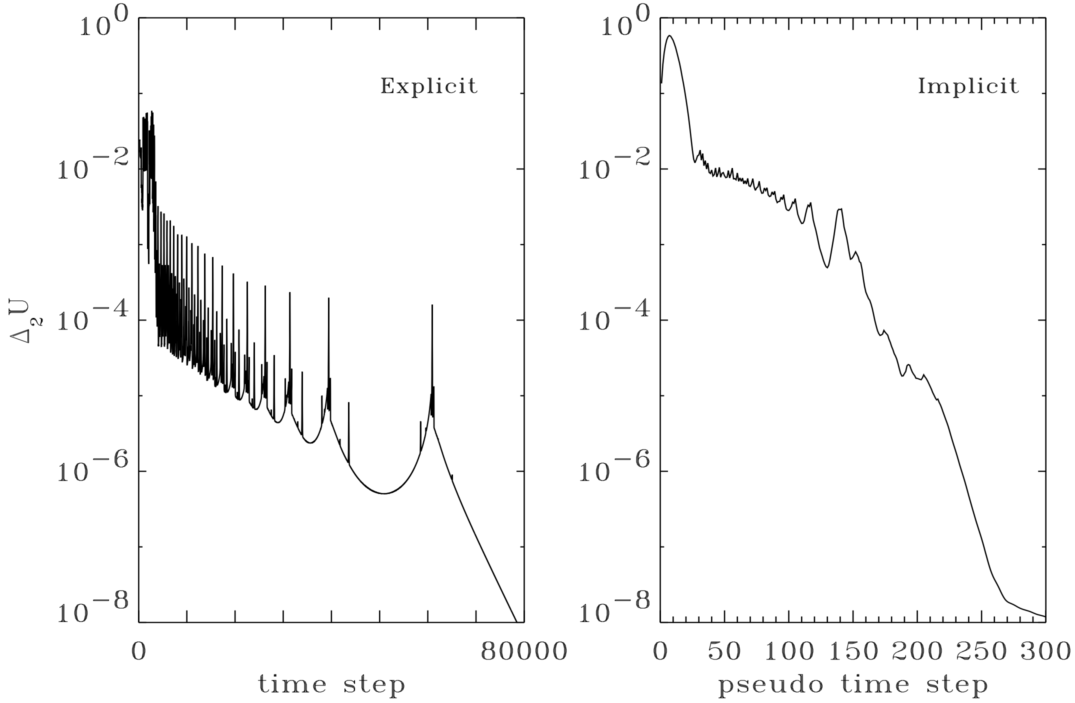
x $\rightarrow$	1	2	3	4	5	6	7
y $\rightarrow$	1	3	5	7	2	4	6
z $\rightarrow$	1	4	7	3	6	2	5

3D

$\Rightarrow$ divide grid into 3, 5^2, 7^3 blocks, tiled using method stencil

Accretion onto black hole

- 1D HD problem: Steady State transonic accretion onto black hole
- Convergence behaviour Superior to explicit scheme.
- speedup by factor of 40: compare residual behavior explicit/implicit

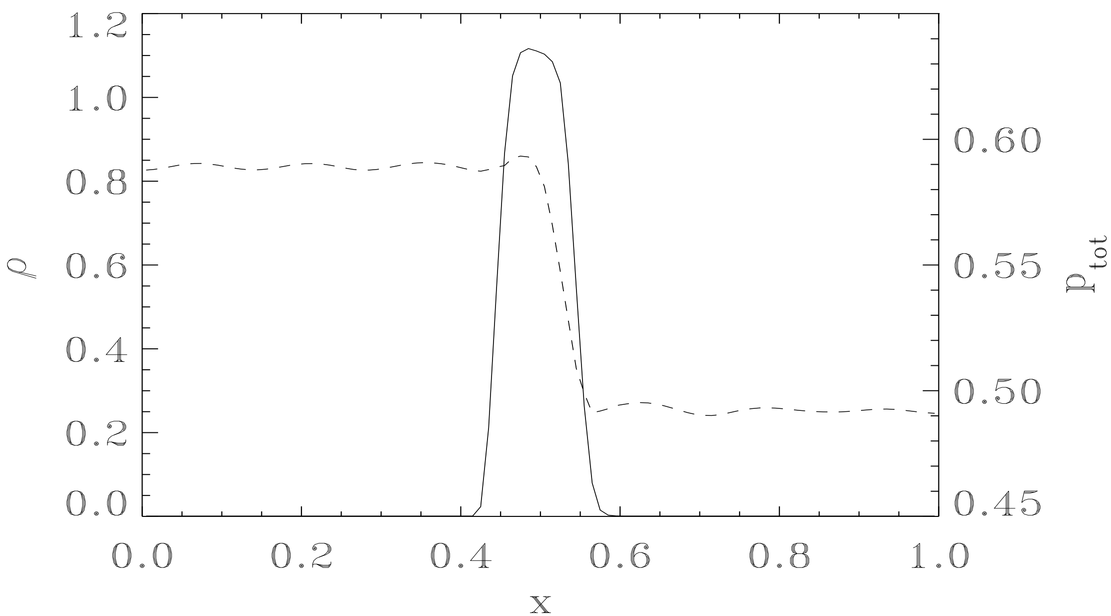


Oscillating plasma sheet

- 1D MHD problem: fully implicit ($\mathbf{R}_{\mathrm{impl}} = \mathbf{R}$) Time Accurate calculation
  - ⇒ Models: Oscillating plasma sheet in magnetized Vacuum
  - ⇒ Challenge for explicit scheme due to ‘infinite’ sound speed!
- use three-level BDF2 (Backward Differentiation Formula) scheme

$$\alpha = \frac{\Delta t_n}{2\Delta t_n + \Delta t_n - 1} = 1 - \beta$$

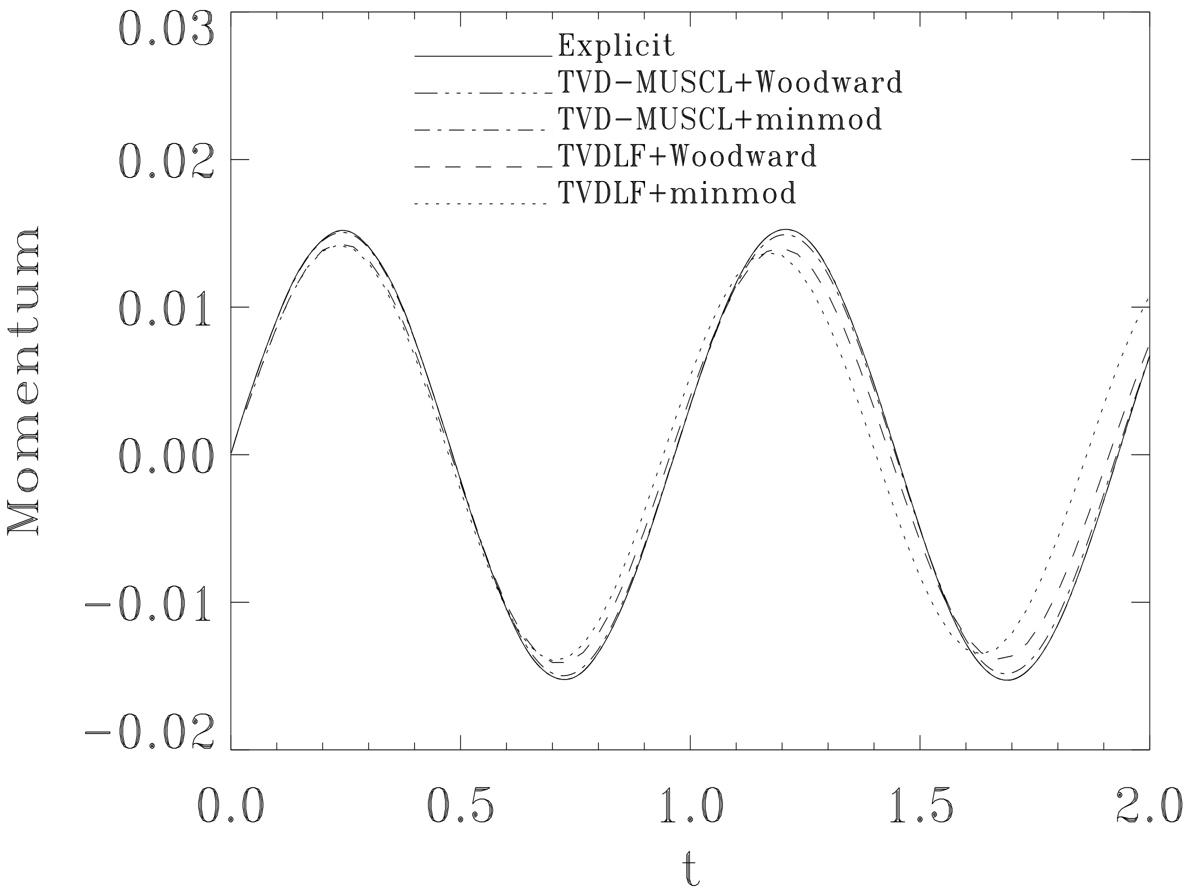
  - ⇒ first time step: Backward Euler (1st order: $\alpha = 0, \beta = 1$)
  - ⇒ first step at second order: trapezoidal method $\alpha = 0$, $\beta = 1/2$



- Trade-off efficiency-diffusion: more diffusive solution: faster

  $\Rightarrow$ speedup can be up to 30!

  $\Rightarrow$ total x-momentum evolution (known amplitude and frequency)



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