united nations educational scientific and cultural organization

international atomic energy agency

the
abdus salam
international centre for theoretical physics

SMR 1161/33

AUTUMN COLLEGE ON PLASMA PHYSICS

25 October - 19 November 1999

Computational Linear MHD: Different Approaches

Stefaan POEDTS

K.U. Leuven
Centre for Plasma Astrophysics
Belgium

Computational linear MHD: different approaches

Stefaan Poedts

Introductory remarks

Conservative form MHD equations / Different (complementary!) approaches

Steady state approach

Basic discretization techniques and applications

Spectral approach

Time evolution approach

time scale problem / time stepping schemes / applications

Concluding remarks

Conservative form MHD equations

- general form of a (scalar) conservation law: $$\frac{\partial u}{\partial t} + \nabla \cdot (f(u)) = 0$$

  u: conserved quantity (actually $\int_V u \, \mathrm{d}V$, not u)

  $f(u)$: rate of flow (or 'flux')

$\Rightarrow$ expresses that $\int_V u \, \mathrm{d}V$ can only change due to a flux $f(u)$ through the surface of volume V

$\Rightarrow$ this is the *differential form* of the conservation law

$\Rightarrow$ derived from the *integral form* (even more general):

ASSUMING u **and** $f(u)$ **are DIFFERENTIABLE!**

Derivation of differential from integral form

- e.g. scalar *integral form* in 1D:

$$\overbrace{\int_{x_1}^{x_2} \underbrace{[u(x,t_2)-u(x,t_1)]}_{\int_{t_1}^{t_2} \frac{\partial u}{\partial t}\,\mathrm{d}t}\,\mathrm{d}x}^{\text{total change of } u \text{ in } [x_1,x_2]} = \overbrace{\int_{t_1}^{t_2} \underbrace{[f(x_1,t)-f(x_2,t)]}_{-\int_{x_1}^{x_2} \frac{\partial f}{\partial x}\,\mathrm{d}x}\,\mathrm{d}t}^{\text{total flux of } u \text{ (through boundaries)}}$$

$$\Downarrow$$

(provided u and f are *differentiable*!)

$$\int_{x_1}^{x_2}\int_{t_1}^{t_2}\left[\frac{\partial u}{\partial t}+\frac{\partial f}{\partial x}\right]\mathrm{d}x\mathrm{d}t = 0$$

- must hold for all x_1, x_2, t_1, and t_2 $\Rightarrow$ $\boxed{\frac{\partial u}{\partial t}+\frac{\partial f}{\partial x}=0}$

Conservative form ideal MHD equations

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho\vec{v} \\ \frac{\rho v^2}{2} + \rho e + \frac{B^2}{2} \\ \vec{B} \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho\vec{v} \\ \rho\vec{v}\vec{v} + \left(p + \frac{B^2}{2}\right)\vec{I} - \vec{B}\vec{B} \\ \left(\frac{\rho v^2}{2} + \rho e + p\right)\vec{v} - (\vec{v}\times\vec{B})\times\vec{B} \\ \vec{v}\vec{B} - \vec{B}\vec{v} \end{bmatrix} = 0$$

⇒ *conserved quantities* (in 'closed' systems, *i.e.* with BCs: $\vec{n}\cdot\vec{v} = \vec{n}\cdot\vec{B} = 0$):

$$\underbrace{M \equiv \int_V \rho\,\mathrm{d}V}_{\textit{total mass}},\quad \underbrace{\vec{\Pi} \equiv \int_V \rho\vec{v}\,\mathrm{d}V}_{\textit{momentum}},\quad \underbrace{H \equiv \int_V \left(\frac{\rho v^2}{2} + \rho e + \frac{B^2}{2}\right)\mathrm{d}V}_{\textit{energy}},\quad \underbrace{\Phi \equiv \int_S \vec{B}\cdot\vec{n}\,\mathrm{d}\Sigma}_{\textit{magnetic flux}}$$

Conservation in ideal MHD

- e.g.

$$\frac{\partial M}{\partial t} = \int_V \frac{\partial \rho}{\partial t}\,\mathrm{d}V = -\int_V \nabla\cdot[\rho\vec{v}]\,\mathrm{d}V \stackrel{Gauss}{=} -\oint[\rho\vec{v}]\cdot\vec{n}\,\mathrm{d}\Sigma \stackrel{\vec{v}\cdot\vec{n}=0}{=} 0$$

$\Rightarrow$ M **is constant!**

- similarly for
  - total momentum, $\vec{\Pi}$
  - total energy, H
  - total magnetic flux, Φ

$\Rightarrow$ extremely powerful representation of nonlinear dynamics of plasmas

Linearized resistive MHD equations

$$\begin{aligned}
\frac{\partial \rho_1}{\partial t} &= -\nabla \cdot (\rho_0 \vec{v}_1), \\
\rho_0 \frac{\partial \vec{v}_1}{\partial t} &= -\nabla(\rho_0 T_1 + \rho_1 T_0) + (\nabla \times \vec{B}_0) \times (\nabla \times \vec{A}_1) \\
&\quad - \vec{B}_0 \times (\nabla \times (\nabla \times \vec{A}_1)), \\
\rho_0 \frac{\partial T_1}{\partial t} &= -\rho_0 \vec{v}_1 \cdot \nabla T_0 - (\gamma - 1)\rho_0 T_0 \nabla \cdot \vec{v}_1 \\
&\quad + 2\eta(\gamma - 1)(\nabla \times \vec{B}_0) \cdot (\nabla \times (\nabla \times \vec{A}_1)), \\
\frac{\partial \vec{A}_1}{\partial t} &= -\vec{B}_0 \times \vec{v}_1 - \eta \nabla \times (\nabla \times \vec{A}_1)
\end{aligned}$$

$\Rightarrow$ system of 8 PDEs for ρ_1, $\vec{v}_1$, T_1, and $\vec{A}_1$ (rem.: $\nabla \cdot \vec{B}_1 = 0$ satisfied)

of the form: $L \cdot \frac{\partial \vec{u}}{\partial t} = R \cdot \vec{u}$ with state vector $\vec{u} = (\rho_1 \;\; \vec{v}_1 \;\; T_1 \;\; \vec{A}_1)$

Three different approaches

- after spatial discretization of L and R: $$A \cdot \vec{x} = B \cdot \frac{\partial \vec{x}}{\partial t}$$

1) **steady state approach**: t-dependence is *prescribed*

   $\Rightarrow$ lin. algebraic system: $(A - i\omega_d B) \cdot \vec{x} = \vec{f}$ ($\vec{f}$: from BCs (driver))

2) **eigenvalue approach**: t-dependence $\sim e^{\lambda t}$

   $\Rightarrow$ eigenvalue problem: $(A - \lambda B) \cdot \vec{x} = 0$

3) **time evolution approach**: t-dependence is *calculated*

   $\Rightarrow$ initial value problem: $A \cdot \vec{x} = B \cdot \dfrac{\partial \vec{x}}{\partial t}$ with $\vec{x}(r, t = 0)$ given

   $\Rightarrow$ driven problem: $A \cdot \vec{x} = B \cdot \dfrac{\partial \vec{x}}{\partial t} + \vec{f}$

The steady state approach

Basic discretization techniques

- recall: MHD equations = PDEs *derived from integral equations!*

  $\Rightarrow$ assuming 'smooth' solutions (derivatives exist)!

- BUT: there exist discontinuous solutions too (e.g. continuum modes, shocks, etc.)

  $\Rightarrow$ *do not satisfy the PDEs!*

$\Rightarrow$ there are two 'cures':

- impose 'Rankine-Hugoniot jump conditions'
- formulate and solve the 'weak form' of the equations

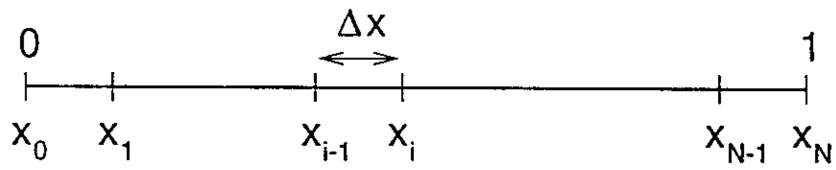
- 'model' problem: $\boxed{\dfrac{\partial^2 u}{\partial x^2} = f(x)u}$ on domain $x \in [0, 1]$

  BCs: $u(0) = 0$ and $\alpha u(1) + \beta \dfrac{\partial u}{\partial x}(1) = F$

The finite difference method (FDM)

- continuous domain $[0, 1] \Rightarrow$ finite number of *grid points*

e.g. equidistant grid: $x_i = i\Delta x = \dfrac{i}{N}$



- functions $f(x) \quad \Rightarrow \quad \{f_i \equiv f(x_i), i = 0, 1, \ldots, N\}$
- derivatives $\quad \Rightarrow \quad$ truncated Taylor series expansions, e.g.

$$u_{i\pm 1} = u_i \pm \left.\frac{\partial u}{\partial x}\right|_i \Delta x + \left.\frac{\partial^2 u}{\partial x^2}\right|_i \frac{\Delta x^2}{2!} \pm \left.\frac{\partial^3 u}{\partial x^3}\right|_i \frac{\Delta x^3}{3!} + O(\Delta x^2)$$

$$\left.\frac{\partial u}{\partial x}\right|_i = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x)$$ '1st-order forward'

$$\left.\frac{\partial u}{\partial x}\right|_i = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x)$$ '1st-order backward'

$$\Rightarrow \left.\frac{\partial u}{\partial x}\right|_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2)$$ '2nd-order Central'

- 2nd-order derivatives: substitute 2nd-order Central difference in Taylor series expansion to obtain

$$\Rightarrow \left.\frac{\partial^2 u}{\partial x^2}\right|_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(\Delta x^2) \qquad \text{(2nd-order)}$$

- higher-order derivatives: similarly

⇒ for model problem equation:

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = f(x_i)u_i \quad \Rightarrow \quad \text{tridiagonal system, BUT BCs:}$$

- $u(0) = 0 \quad \Rightarrow u_0 = 0$
- $\alpha u(1) + \beta \frac{\partial u}{\partial x}(1) = F \;\Rightarrow$ use $\frac{\partial u}{\partial x}(1) = \frac{3u_N - 4u_{N-1} + u_{N-2}}{2\Delta x}$

- FD equations easy to derive / extend / code / solve

  ⇒ FDM is very popular in MHD!

FDM: MHD examples

- 2D nonlinear time evolution driven loops (Ofman & Davila)

- 2D eigenvalue problems in coronal arcades (Oliver)

- radial direction in 3D nonlinear time evolution driven loops (Poedts, Goedbloed, Keppens)

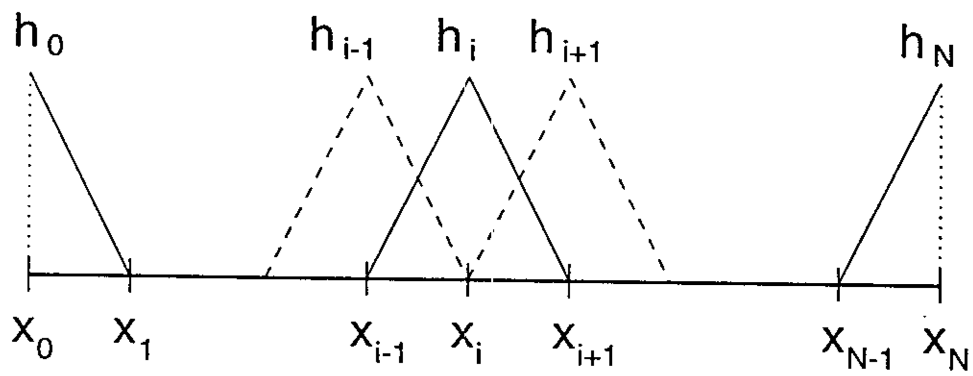
- radial direction in *many* nonlinear stability codes for tokamak plasmas (*e.g.* Kerner/Jakoby/Biskamp/Luciani/Lerbinger/etc.)

The finite element method (FEM)

- domain discretized as in FDM
- dependent variables: approximated by finite set of local piecewise polynomials $h_i(x)$

$$\Rightarrow \quad u(x) \approx \hat{u}(x) = \sum_{i=0}^{N} u_i h_i(x)$$

e.g. linear elements:



Weighted residual formulation

- require: $$\int_0^1 w_l \underbrace{\left[\frac{\partial^2 \hat{u}}{\partial x^2} - f(x)\hat{u}\right]}_{residual} \mathrm{d}x = 0, \quad l = 0, 1, \ldots, N$$

$\Rightarrow$ linear algebraic system for $\{u_i\}$

Galerkin method

- take the 'shape' functions $h_i(x)$ as weight functions:

$$\Rightarrow \int_0^1 h_l \left[\frac{\partial^2 \hat{u}}{\partial x^2} - f(x)\hat{u} \right] \mathrm{d}x = 0 \quad l = 0, 1, \ldots, N$$

$\Rightarrow$ linear algebraic system for $\{u_i\}$ $\quad \left(\hat{u}(x) = \sum_{i=0}^{N} u_i h_i(x) \right)$

Weak form

- integrating by parts on highest-order derivatives:

$$\Rightarrow \left[h_l \frac{\partial \hat{u}}{\partial x} \right]_0^1 - \int_0^1 \frac{\partial h_l}{\partial x} \frac{\partial \hat{u}}{\partial x} \mathrm{d}x - \int_0^1 h_l f(x) \hat{u} \, \mathrm{d}x = 0 \quad l = 0, 1, \ldots, N$$

$\Rightarrow$ allows less 'smooth' solutions (continuously differentiable to a lower order)

$\Rightarrow$ *closer to integral form of the equation!*

The (pseudo-)spectral method (SPM)

- similar to FEM but finite set of global shape functions

$$e.g.\ \boxed{u(x) \approx \hat{u}(x) = \sum_{k=-N}^{N} u_k e^{ik2\pi x}} \quad \text{for } x \in [0,1]$$

- weighted residual formulation / weak form / Galerkin method

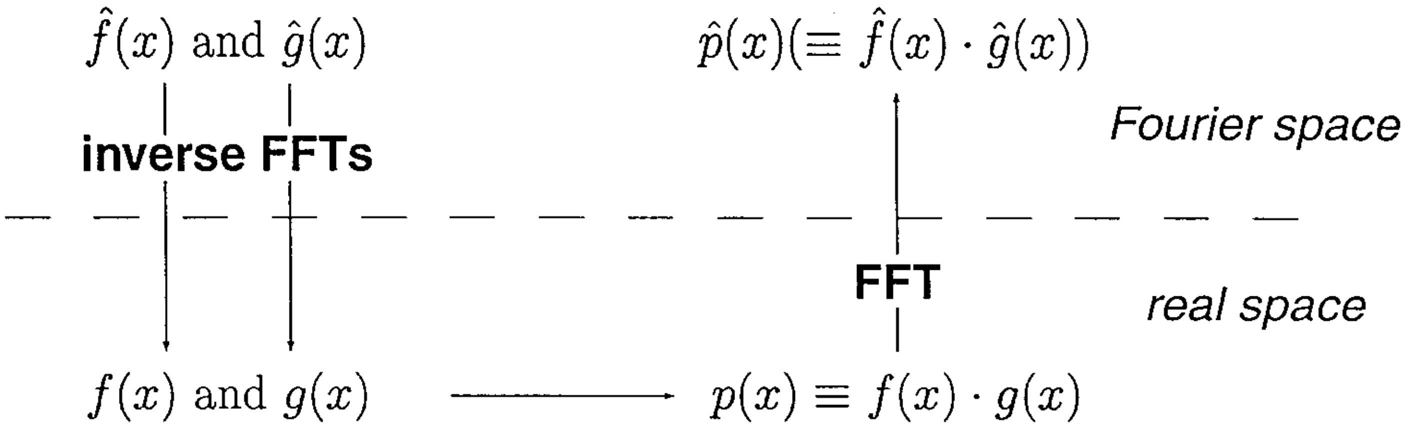
  $\Rightarrow$ 2D complication: coefficient functions also approximated $\Rightarrow$ full matrices!

- disadvantages:

  - periodicity $\Rightarrow$ poor approximation near non-periodic boundaries
  - nonlinear terms: CPU time consuming convolutions ($\sim N^2$ calculations)

$$e.g.\ f(x)g(x) \approx \hat{f}(x)\hat{g}(x) = \sum_{k=-N}^{N} \left[\sum_{l=-N+k}^{N} f_l g_{k-l} \right] e^{ik2\pi x}$$

- determination quadratic terms in *pseudo-spectral method*:



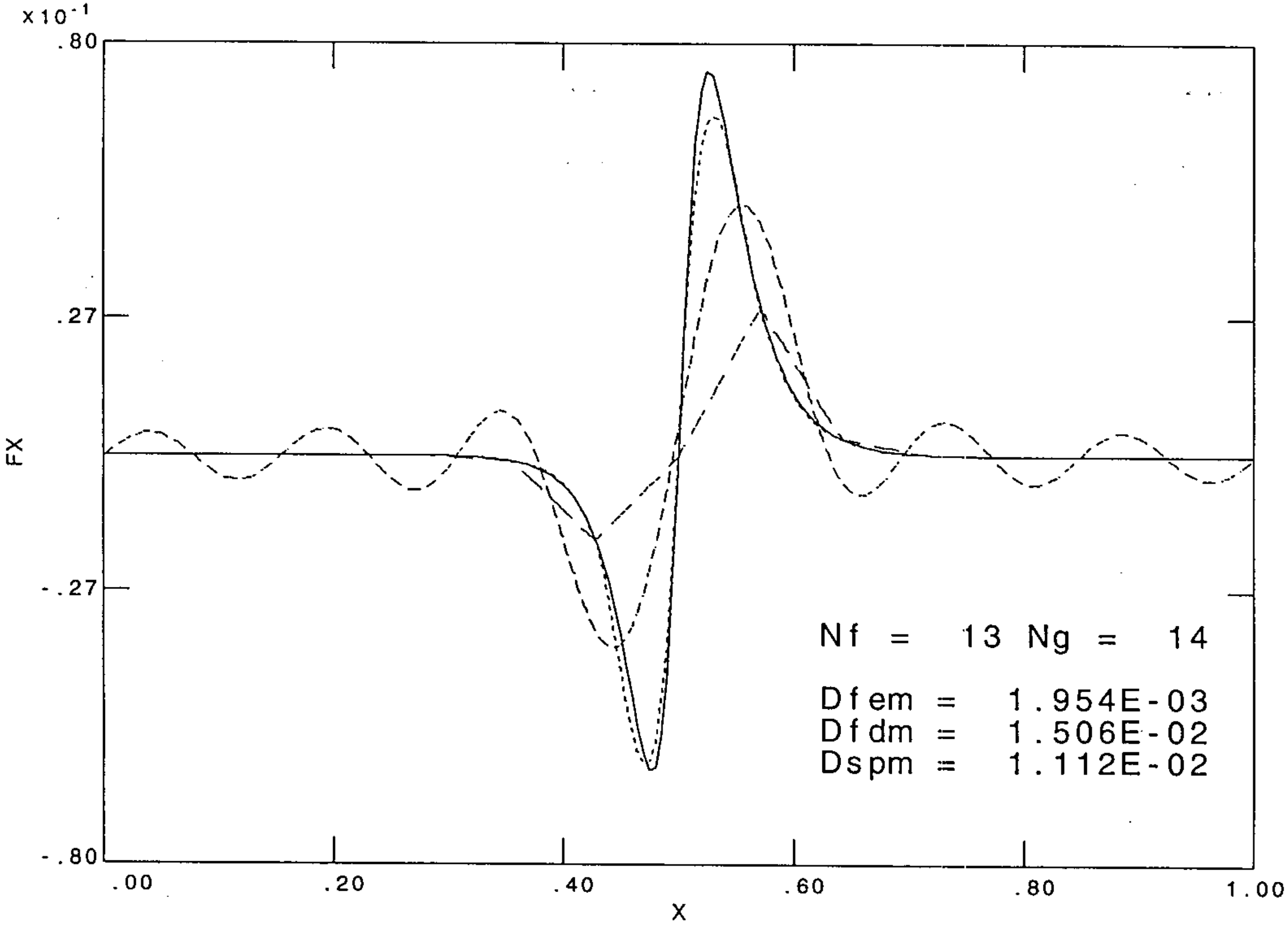
$\Rightarrow$ FFTs require $\sim N\log N$ calculations

$\Rightarrow$ for $N \gg 1$: $\quad N^2 \gg N\log N$

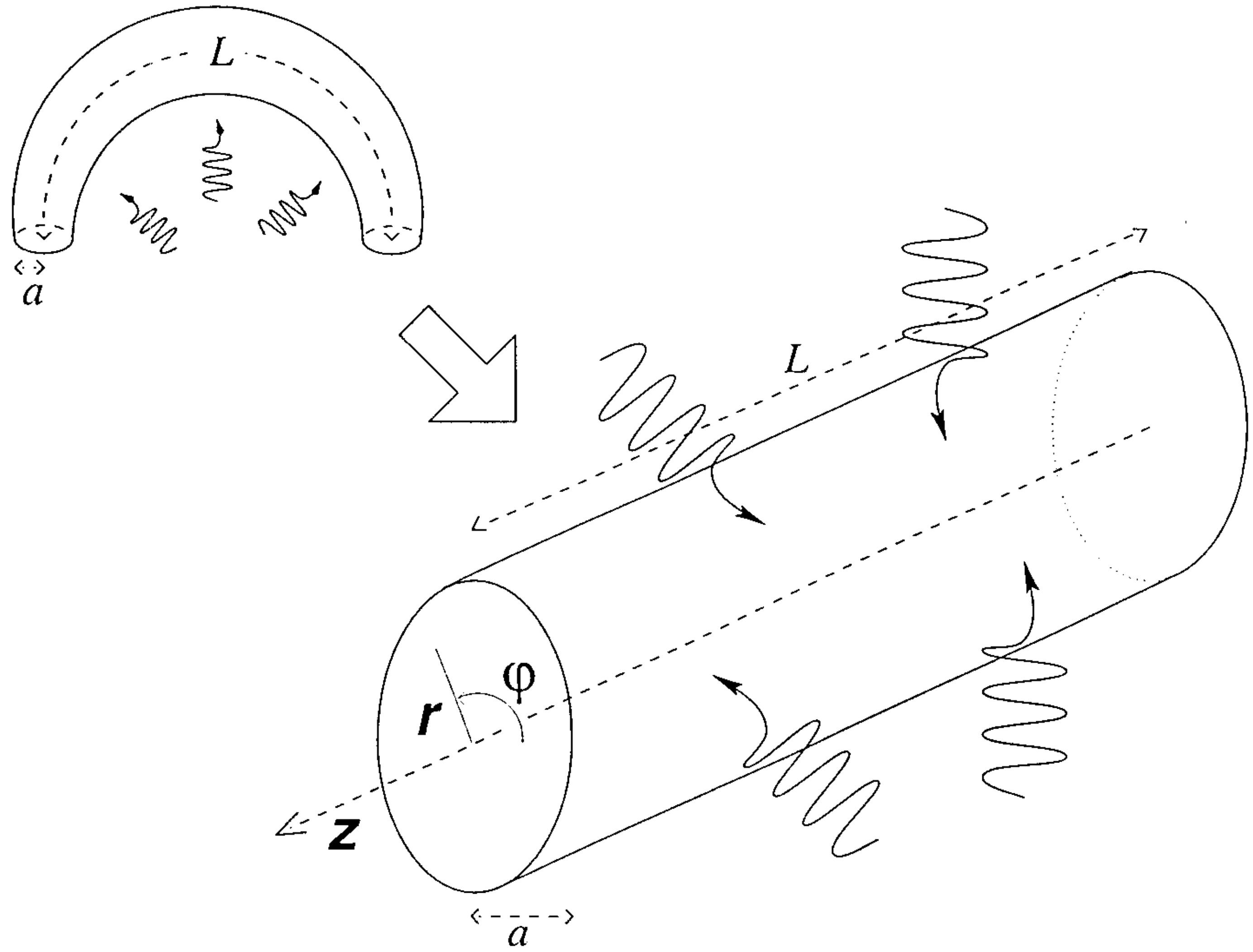
- problem: 'aliasing' $\quad\Rightarrow\quad$ de-aliasing techniques

  - drop 50% of modes OR do 2 FFTs (one on shifted grid)

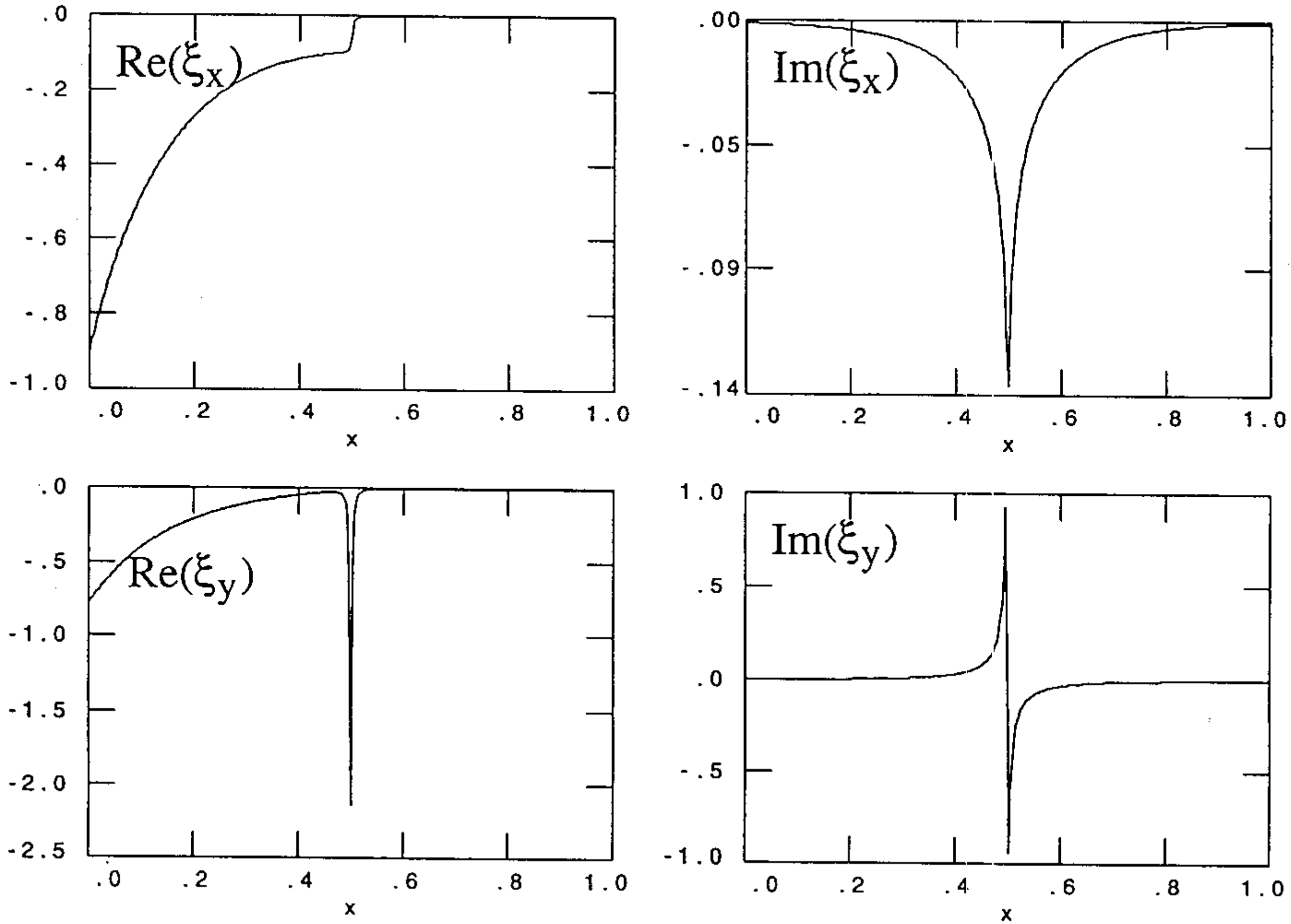
  $\Rightarrow$ some overhead still but much more acceptable for $N \gg 1$



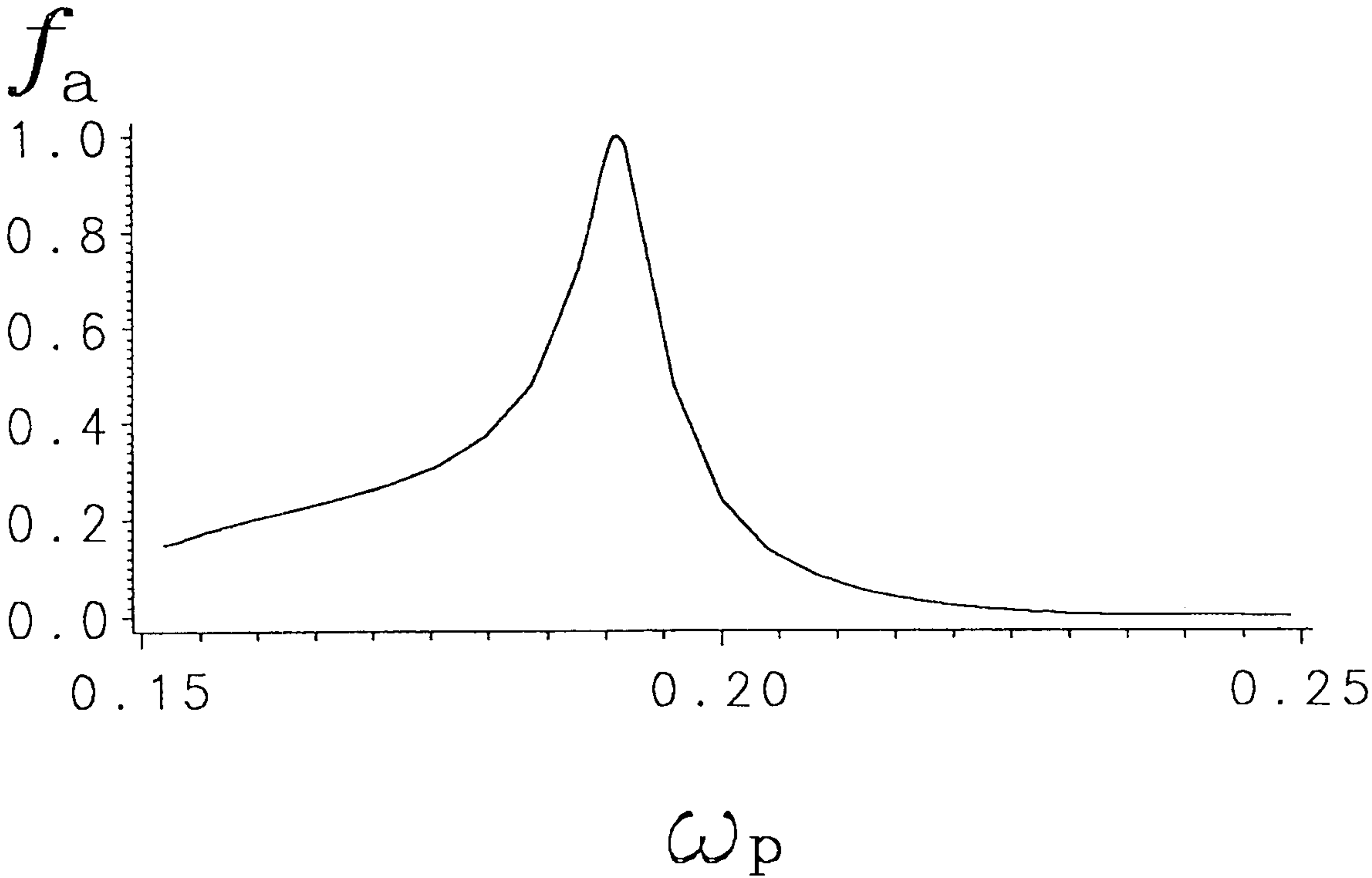
Comparison of FDM, FEM, and SPM discretizations for a localized function



External driving of a plasma by incident waves



Resonant dissipation: small length scales due to resonances



Fractional absorption versus driving frequency.

Eigenvalue problems

- MHD spectrum $\Rightarrow$ insight in dynamics ('MHD spectroscopy')
- linear MHD waves determine stepsize (Δt) of explicit and (semi-) implicit schemes for wave related problems
- definition: $\vec{x}$ is a (right) *eigenvector* of $n \times n$ matrix A

  with corresponding *eigenvalue* λ if $\boxed{A \cdot \vec{x} = \lambda \, \vec{x}}$
- consequences:
  - $|A - \lambda \, 1| = 0$: characteristic equation (n roots)

    $\Rightarrow$ there are always n eigenvalues (may be *degenerate*)
  - eigenvalues can be shifted (*same eigenvectors*):

    $$(A + \tau 1) \cdot \vec{x} = (\lambda + \tau) \, \vec{x}$$

    $\Rightarrow$ zero eigenvalue has no particular meaning

- idem 'left' eigenvector if $\boxed{\vec{x} \cdot A = \lambda \vec{x}}$

  $\Rightarrow$ *'left' eigenvalues = 'right' eigenvalues*

  (since $\vec{a}^T \cdot \vec{x}^T = \lambda \vec{x}^T$ and $|A| = |A^T|$)

- X_R = matrix with right eigenvectors in columns

  X_L = matrix with left eigenvectors in rows

  $\Rightarrow X_R^{-1} \cdot A \cdot X_R = \text{diag}(\lambda_1, \ldots, \lambda_n)$

  = special *'similarity transform'* $(A \to Z^{-1} \cdot A \cdot Z)$

  $\Rightarrow$ *eigenvalues not affected* since

  $$\left|Z^{-1} \cdot A \cdot Z - \lambda 1\right| = \left|Z^{-1} \cdot (A - \lambda 1) \cdot Z\right| = \left|Z^{-1}\right| \, |A - \lambda 1| \, |Z| = |A - \lambda 1|$$

$\Rightarrow$ *strategy of modern eigenvalue solvers*:

- reduce A to simpler form by similarity transforms

$$A \to P_1^{-1} \cdot A \cdot P_1 \to P_2^{-1} \cdot P_1^{-1} \cdot A \cdot P_1 \cdot P_2 \to \ldots$$

- start an iterative procedure

Ideal MHD stability codes

- ERATO: 2D ideal MHD / $\sim e^{in\varphi}$
  - straight field line coordinates: (ψ, θ, φ)
  - finite hybrid element approach
  - $\Rightarrow A \cdot \vec{x} = \omega^2 \, B \cdot \vec{x}$ with A and B symmetric, block structured
  - $\Rightarrow$ shift: $(A - \omega_0^2 B) \cdot \vec{x} = (\omega^2 - \omega_0^2) \, B \cdot \vec{x}$
- PEST: 2D ideal MHD / same coordinates: (ψ, θ, φ)
  - ψ-direction: combination of linear and constant elements
  - θ-direction: spectral method $\left(\sum_m e^{im\theta}\right)$
  - φ-direction: spectral method $(e^{in\varphi})$
- NOVA-W:
  - cubic B-spline elements in ψ-direction (4th-order accurate)

Resistive MHD spectral codes

- LEDA: 1D resistive cylinder / slab
  - r-direction: cubic Hermite and quadratic elements
  - θ- and z-direction: $e^{im\theta+inkz}$

- CASTOR / POLLUX: 2D resistive torus / loop
  - ψ-direction: cubic Hermite and quadratic elements
  - θ-direction: spectral method $(\sum_m e^{im\theta})$
  - φ-direction: spectral method $(e^{in\varphi})$

$\Rightarrow$ use different eigenvalue solvers: QR-solver, inverse vector iteration, Krylov subspace techniques

- MHD example: resistive MHD spectrum of a cylindrical plasma column (from Poedts et al. '89)

  (only Alfvén and slow magnetosonic sub-spectrum are shown)

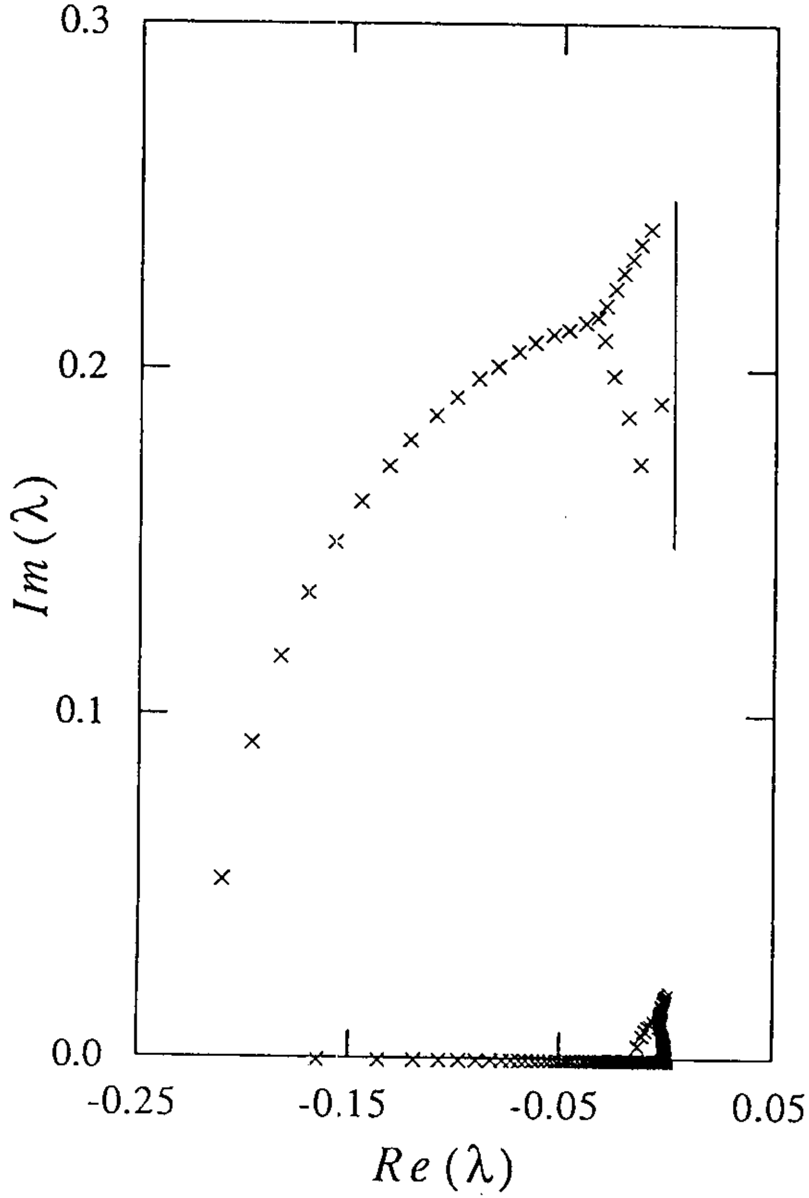
⇒ resistive modes lie on fixed curves in complex frequency plane (independent of resistivity!)

⇒ ideal continuous spectrum only approximated at end points

⇒ ideal quasi-mode clearly visible!

- collective mode
- weakly damped

⇒ easily excited!



Time evolution schemes

Time scale problem

- linear MHD spectrum $\Rightarrow$ widely separated time scales in resistive MHD!
- for hot, elongated, low-β plasmas (tokamaks, coronal loops):
  - $\tau_{\text{fast}} \equiv \dfrac{a}{v_f} \approx \dfrac{a}{v_A}$, since $\beta \equiv 2p/B^2 \ll 1 \Rightarrow v_f \approx v_A$
  - $\tau_{\text{Alfv}} \equiv \dfrac{L}{v_A}$ ($L = 2\pi R_0$ in tokamaks), with $L \gg a$)
  - $\tau_{\text{diff}} \equiv \dfrac{\mu_0 a^2}{\eta}$: where $\eta \ll 1$ (hot plasmas)

  $\Rightarrow$ $\boxed{\tau_{\text{fast}} \ll \tau_{\text{Alfv}} \ll \tau_{\text{diff}}}$

$\Rightarrow$ wave problems in loops and tokamaks lead to *stiff equations!*

Semi-discretization

- nonlinear schemes (lect. 3) are 'fully' discrete (discretized in space and time)
- <u>*semi-discrete methods*</u>: first discretize only in space

$\Rightarrow$ PDEs $\Rightarrow$ ODEs in time $\Rightarrow$ solvable by any ODE solver ($e.g.$ Runge-Kutta)

$e.g.$ after spatial discretization: $\boxed{\dfrac{\mathrm{d}\vec{u}}{\mathrm{d}t} = \vec{f}(\vec{u})}$

$$\Rightarrow \vec{u}^{n+1} = \vec{u}^{n} + \Delta t \left[\theta \vec{f}(\vec{u}^{n+1}) + (1-\theta)\vec{f}(\vec{u}^{n})\right]$$

$\theta = \frac{1}{2}$: trapezoidal rule

$\theta = 0$: backward Euler scheme

$\Rightarrow$ *useful approach* when higher-order accuracy (> 2) is needed or when extending to two or more spatial dimensions

$\Rightarrow$ *powerful*: any spatial discretization method to any accuracy can be coupled to any ODE solver for the time discretization!

Linear MHD application

- semi-discretization $\Rightarrow$ $\boxed{A \cdot \vec{a}(t) = B \cdot \frac{\mathrm{d}\vec{a}}{\mathrm{d}t} + \vec{f}(t)}$ = ODE in t

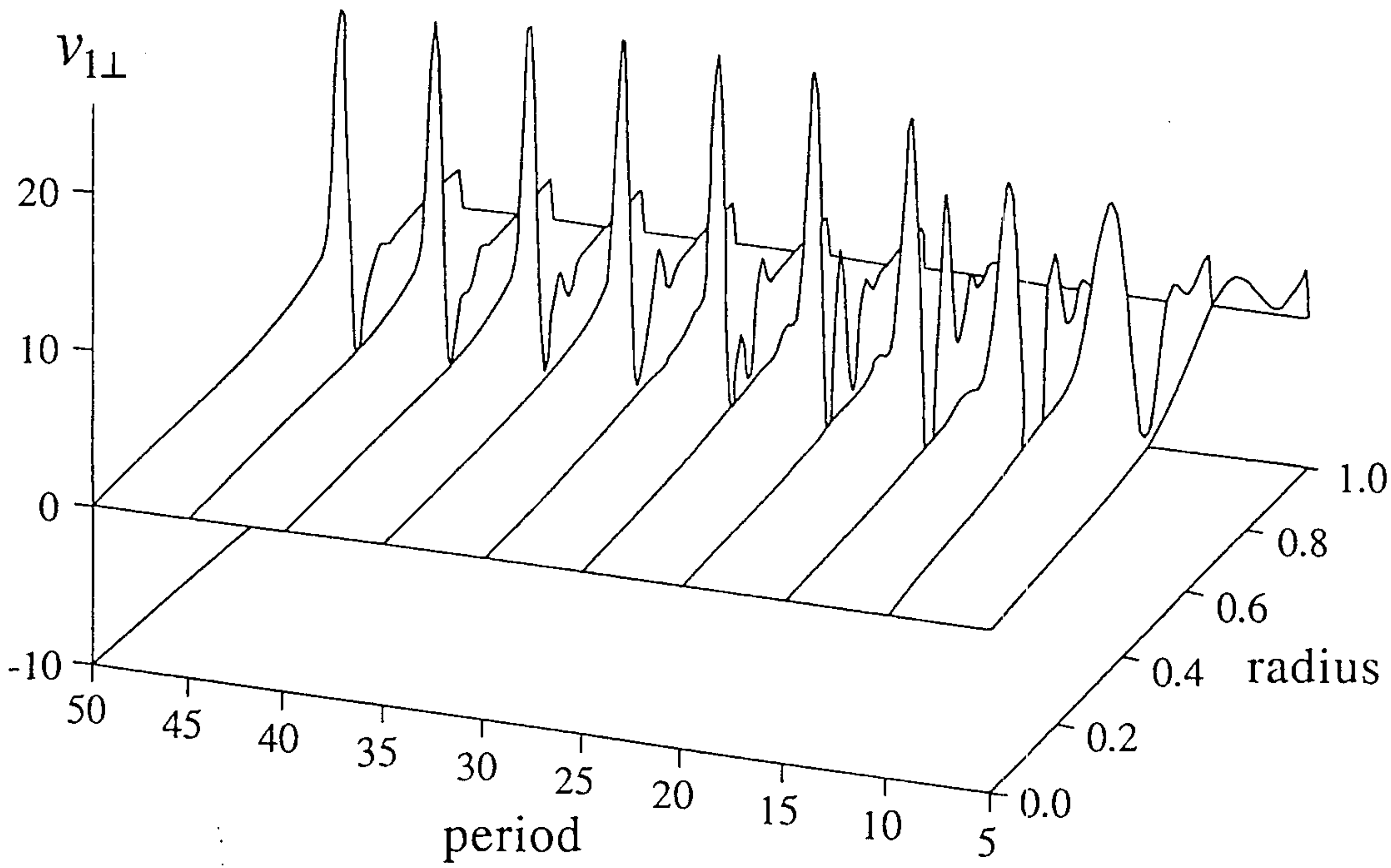
- trapezoidal method: $\vec{a}^{n+1} = \vec{a}^n + \Delta t\,(1-\alpha)\,\dot{\vec{a}}^n + \Delta t\,\alpha\,\dot{\vec{a}}^{n+1}$

$$\Rightarrow \underbrace{(-B + \Delta t\,\alpha\,A)}_{\equiv \hat{A}} \cdot \vec{a}^{n+1} = \underbrace{-[B + \Delta t\,(1-\alpha)\,A)}_{\equiv \hat{B}} \cdot \vec{a}^n$$

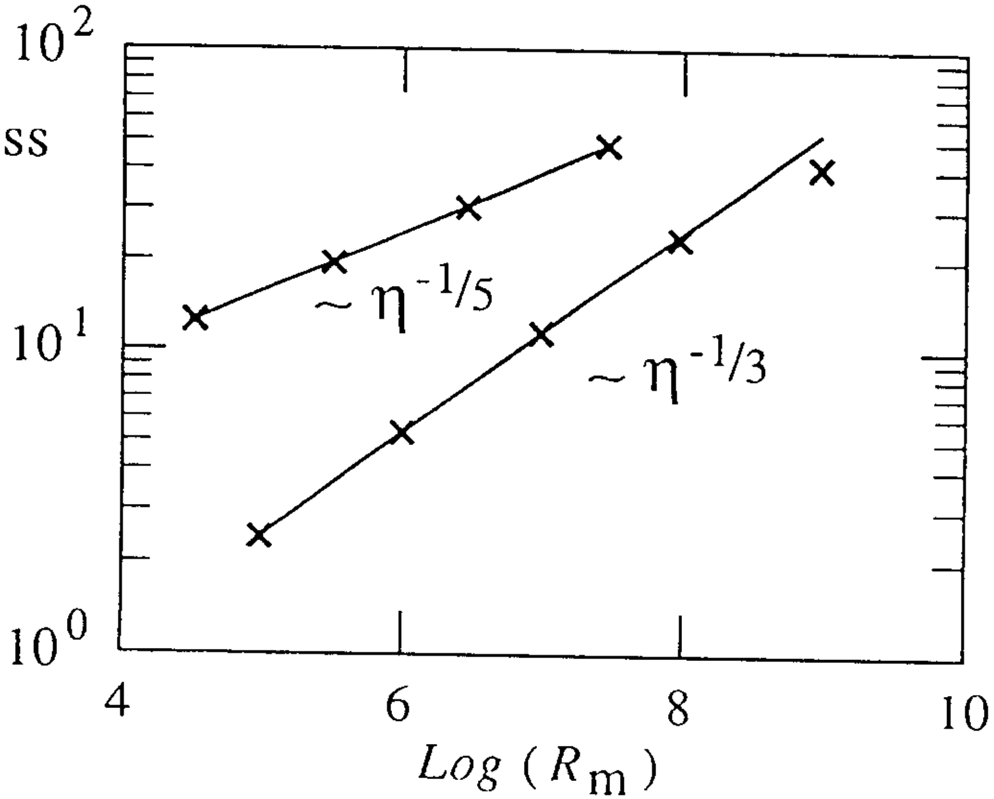
$$+ \underbrace{\Delta t\,[(1-\alpha)\,\vec{f}^n + \alpha\,\vec{f}^{n+1}]}_{\equiv \hat{\vec{f}}}$$

$$\Rightarrow \boxed{\hat{A} \cdot \vec{a}^{n+1} = \hat{B} \cdot \vec{a}^n + \hat{\vec{f}}(t)}$$

- LU factorization of $\hat{A}$ (only once!, with LAPACK's SGBFA)
- solution (typical 10^4 times, with LAPACK routine SGBSL)



Snapshots of the $v_1 \perp$ every 5 driving periods.



Time scales to reach the steady state of resonance dissipation.

Selection criteria for numerical methods

- consistency: approximation should *converge* to real solution in the limit $\Delta t, \Delta x \to 0$

- numerical stability: round-off errors should not grow

- accuracy: approximation should be of higher order in Δx and Δt or, better, in the dimensionless parameters $\delta = \left| \frac{\Delta x}{u} \frac{\partial u}{\partial x} \right|$ and $C = v \frac{\Delta t}{\Delta x}$

- monotonicity: (locally) monotone solution at t should remain monotonous at $t + \Delta t$, $i.e.$ at later times

- efficiency: CPU time and memory should be optimized (for a given accuracy)