The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2292-5

School and Conference on Analytical and Computational Astrophysics

14 - 25 November - 2011

Dynamics of the Solar Wind

William H. Matthaeus
University of Delaware, Bartol Research Institute, Newark
USA

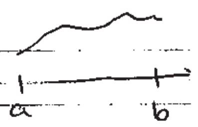
CONTENTS [Bill's Spectral Mthds Notes, Dartmouth?]

I Basic Properties of Spectral Methods

A. Approximations to a function by Least Squares

① Representation of a function in Hilbert Space.

$f(x) \quad a \le x \le b$ "suitably well behaved"



$\{\phi_n\} \quad n = 0, 1, \dots \infty$ defined on $[a, b]$

orthonormal basis $(\phi_n, \phi_m) = \delta_{nm}$

and "complete"

seek expansion $f(x) = \sum_{n=0}^{\infty} A_n \phi_n(x)$

$$A_n = (\phi_n, f)$$

② Best approximation using a finite set $\{\phi_n\}$

$\| f \| =$ Euclidean (L_2) norm. $\sqrt{(f, f)} = \left(\int_a^b f^* f \, dx \right)^{1/2}$

$\| f \| =$ weighted L_2 norm $\sqrt{(f, f)} = \left(\int_a^b f^* f \, w(x) \, dx \right)^{1/2}$

seek approximation to f

$$f(x) \simeq \sum_{n=0}^{N-1} \phi_n A_n = f_N$$

that minimizes the norm of the residual

$$\| f - f_N \| = \| f - \sum_{n=0}^{N-1} \phi_n A_n \|$$

Minimize this with respect to A_ℓ, all ℓ.

same as minimizing $\| f - f_N \|^2$ since norm is positive

$\therefore$ it is a least squares fit

$$\frac{\partial}{\partial A_e}(f-f_N, f-f_N) = 0 \quad \left[\text{and } \frac{\partial}{\partial A_e^*}(f-f_N, f-f_N) = 0\right]$$

$$\frac{\partial}{\partial A_e}\left\{\int_a^b f^* f\,dx + \sum_n \int_a^b A_n^* A_n |\phi_n|^2 dx - \sum_n \int_a^b f^* A_n \phi_n\,dx - \sum_n \int_a^b A_n^* \phi_n^* f\,dx\right\} = 0$$

$$\Rightarrow \quad A_e^*(\phi_e, \phi_e) - \underbrace{\int_a^b f^* \phi_e\,dx}_{(f,\phi_e)} = 0$$

$$A_e^* = (f, \phi_e)$$

$$\frac{\partial}{\partial A_e^*}(f-f_N, f-f_N) = 0 \Rightarrow A_e = (\phi_e, f)$$

Note

- the approximate (least-squares) expression for A_e is the same as the exact one.
- The approximate A_e is independent of N

(3) Approximation with a non-orthonormal, but linearly independent set $\{\psi_n\}$ $n = 0, \cdots N-1$

look for an approximation $f(x) \simeq \sum_{n=0}^{N-1} B_n \psi_n \equiv f_N$

(for convenience assume everything is real)

Also, to get a little more general result assume the norm may be a discrete "seminorm", or continuous

in discrete case $\{x_i\}$ $\quad \|g\|_d = \sqrt{\sum_i |g(x_i)|^2}$

$$(g, f)_{\text{discrete}} = \sum_i g(x_i) f(x_i)$$

Seek the least squares approximation that minimizes

$$\| f - \sum_{n=0}^{N-1} B_n \psi_n \|^2 = \| f - f_N \|^2$$

Use a different approach here because we have linear independence to use, but not orthogonality.

A CONDITION on the SOLUTION:

Consider an arbitrary series, distinct from f_N, $\sum C_n \psi_n$

trivially, $\sum C_n \psi_n - f = \sum (C_n - B_n) \psi_n + f_N - f$

and

$$\| \sum C_n \psi_n - f \|^2 = \| \sum (C_n - B_n) \psi_n \|^2 + \| f_N - f \|^2$$

$$+ 2 (\sum (C_n - B_n) \psi_n , f_N - f)$$

Suppose the residual $f_N - f$ is orthogonal to every ψ_n. Then it is also orthogonal to $\sum (C_n - B_n) \psi_n$. The remainder is sum of two positive terms, thus

$$\| \sum C_n \psi_n - f \|^2 \geq \| f_N - f \|^2$$

<u>therefore</u> f_N is the best (least square) solution provided that $(f_N - f, \psi_n) = 0 \quad \forall n$.

But this is simply the statement that

$$(\sum_n B_n \psi_n - f , \psi_e) = \sum_n B_n (\psi_n , \psi_e) - (f, \psi_e) = 0$$

These are the <u>NORMAL EQUATIONS</u>, a matrix problem.

$$\begin{pmatrix} (\psi_i, \psi_j) & \cdots \\ \vdots & \psi_{ij} \end{pmatrix} \begin{pmatrix} B_0 \\ \vdots \\ B_{N-1} \end{pmatrix} = \begin{pmatrix} (f, \psi_0) \\ \vdots \\ (f, \psi_{N-1}) \end{pmatrix}$$

if $(\psi_n , \psi_e) = \delta_{ne}$ it reduces to the previous result the solution to the Normal equations exists and is unique:

$$\sum_n (\psi_m, \psi_e) B_n = (f, \psi_e) \qquad l = 0, 1 \dots N-1$$

the matrix problem has a solution unless the homogeneous problem has a solution, the homogeneous problem is

$$\sum_{n=0}^{N-1} (\psi_m, \psi_e) B_n = 0 \qquad l = 0, 1 \dots N-1$$

if it has a solution with at least one $B_n \neq 0$ then

$$\|\sum B_n \psi_n\|^2 = \left(\sum B_n \psi_m, \sum B_e \psi_e \right)$$

$$= \sum_n \underbrace{\sum_e (\psi_m, \psi_e) B_n}_{=0} B_e$$

$$= \sum_n 0 \cdot B_e = 0$$

but then $\{\psi_m\}$ are not linearly independent

$\therefore$ if $\{\psi_n\}$ are linearly independent the least squares approximation is non trivial and unique.

(4) Completeness and complete orthonormal sets for use in Approximations:

$\Rightarrow$ A few facts from finite dimensional vector space theory (u, v, w are vectors in vector space V)

- inner product $\rightarrow$ $(u, v) = (v, u)^*$
  - $\rightarrow$ $(\alpha u + \beta v, w) = \alpha^*(u, w) + \beta^*(v, w)$
  - $\rightarrow$ $(u, u) \geq 0 \ \forall x$, $= 0$ iff $x = 0$

- Bessels inequality: suppose $\{u_i\}$ $i = 1, 2 \dots n$ are linearly independent, then for all V

$$\|V\|^2 = (V, V) \geq \sum_i (u_i, V)$$

- the linearly independent set $\{u_i\} = U$ can always be made orthonormal by Gram-Schmidt procedure.

Completeness of the set $\{u_i\} = \mathcal{U}$ $(i = 1, \dots n)$ Amounts to any one of the following, each of which follows from any of the others:

- $\mathcal{U}$ is complete (in $\mathcal{V}$)
- if $(w, u_i) = 0$ for $i = 1, 2, \dots n$ then $w = 0$
- $\mathcal{U}$ spans $\mathcal{V}$
- if w is in $\mathcal{V}$ then $w = \sum_i (u_i, w) u_i$
- if v, w are in $\mathcal{V}$ then $(w, v) = \sum_i (w, u_i)(u_i, v)$
- if v is in $\mathcal{V}$ then $\|v\|^2 = \sum_i |(u_i, v)|^2$

(Bessels inequality, with the equals sign)

→ infinite dimensional (function) spaces are more difficult in particular, when we represent $f(x)$ by a series of $\phi_n(x)$

as in $$f(x) = \sum_{n=0}^{\infty} \phi_n A_n$$

we might mean

i) the r.h.s. converges to $f(x)$ at all x (pointwise or uniform convergence) (close analogy to finite dimensional spaces)

or

ii) Convergence in the mean

e.g. $$\lim_{N \to \infty} \int_a^b \left| f(x) - \sum_{n=0}^{N-1} A_n \phi_n(x) \right|^2 dx = 0$$

the latter, weaker convergence is just the statement that

$$\lim_{N \to \infty} \| f - f_N \|^2 = 0$$

where f_N is the sequence of least squares approximations

(3) ⇒ Where do complete orthonormal sets of $\{\phi_n\}$ come from?

Start with any second order linear differential operator, and its eigenvalue problem, on the interval $a \le x \le b$

$$\mathcal{L} u = \lambda u$$

where $\mathcal{L} u = a(x) u'' + b(x) u' + c(x) u = \lambda u$

define the inner product as

$$(u, v) = \int_a^b u^* v \, w(x) \, dx$$

$\mathcal{L}$ can be shown to be self-adjoint (Hermitian) $\left\{ \begin{array}{l} \text{real eigenvalues} \\ \phi \end{array} \right.$

i.e. $(u, \mathcal{L} v) = (\mathcal{L} u, v)$

provided that

① $w(x)$ is chosen to be the solution to $(wa)' = wb$

and

② $\left[wa \left(u^* v' - v u^{*\prime} \right) \right]_a^b = 0$

which holds for a number of cases including

e.g. Dirichlet: $u = v = 0$ at $x = a$ and $x = b$

Neumann bc's: $u' = v' = 0$ at $x = a$ and $x = b$

The differential equation can be rewritten in Sturm-Liouville form

$$\boxed{\frac{d}{dx}\left[p(x) \frac{du}{dx} \right] - s(x) u + \lambda w(x) u = 0}$$

where $p = wa$ and $s = wc$

or $\mathcal{L}' u = \lambda w(x) u$

For S.L. problem (with proper boundary condition). $\mathcal{L}'\phi_n = \lambda_n w \phi_n$.

- Self adjoint $\begin{cases} \lambda \text{ is real} \\ (\phi_n, \phi_\ell) = 0 \text{ unless } n = \ell. \end{cases}$

- orthonormal set

- Completeness
  - Fourier Series
  - Bessel functions
  - Various polynomials $\left\{ \begin{array}{l} \text{Jacobi} \\ \text{Gegenbauer} \\ \text{Chebychev} \\ \text{Legendre} \\ \text{Hermite} \\ \text{Laguerre.} \end{array} \right.$

NB/4 on the finite interval the S-L $\{\phi_n\}$ are complete whenever $\lambda_n \to \infty$ as $n \to \infty$.
[characteristic scale $\ell_n = \frac{1}{\sqrt{\lambda_n}} \to 0$ as $n \to \infty$]

- Rate of convergence of $f(x) \simeq \sum_{\ell=0}^{N-1} A_\ell \phi_\ell$.

→ always at least algebraic

$$A_\ell \sim \frac{1}{\lambda_\ell} \quad \text{as } \ell \to \infty$$

often $\sim \frac{1}{\ell^3}$

→ NON singular S-L problem $p(x) > 0$ $w(x) > 0$
in $a \le x \le b$

algebraic convergence except when special conditions are satisfied at the boundaries

$\longrightarrow$ singular S.L problem, e.g. $p(a) = 0$
relaxes the convergence conditions so the order
of convergence rate depends on the
smoothness of $f(x)$ near $x = a$,
not on the boundary conditions

(6) Fourier series $\quad f(x) \approx \sum_{-K}^{+K} a_k e^{ikx} \Big\}$ least squares approximation

- $f(x)$ smooth and periodic (no discontinuities)
  uniform convergence.
- $f(x)$ nonperiodic or has an interior discontinuity
  $\Rightarrow$ Gibbs phenomenon near region of
  x near x_0 of size $\sim \frac{1}{K}$ as $K \to \infty$

- rate of convergence

$$a_k = \frac{1}{2\pi} \int_0^{2\pi} f(x)\, e^{-ikx}$$

suppose f is periodic and has continuous derivatives
up to order $n-1$ and $\frac{d^n f(x)}{dx^n}$ is integrable.

then, integrating by parts

$$a_k = \frac{1}{2\pi} \frac{1}{(ik)^n} \int_0^{2\pi} \frac{d^n f(x)}{dx^n} e^{-ikx} dx$$

then $\displaystyle\int_0^{2\pi} \frac{d^n f}{dx^n} e^{-ikx} dx \ll 1$ as $k \to \infty$

and $\quad |a_k| \ll \frac{1}{|k|^n}$ as $|k| \to \infty$

Therefore if f is infinitely differentiable

$|a_k| \to 0$ faster than any power of k
as $k \to \infty$

f continuous, f' integrable $\quad a_k << 1/k \quad k \to \infty$

f' piecewise continuous $\quad a_k \sim 1/k^2 \quad k \to \infty$

- estimates of convergence of least squares approximation with K the maximum wavenumber

If $a_k \to \frac{1}{k^n}$ as $k \to \infty$ but not faster

then $\frac{d^{n-1} f}{dx^{n-1}}$ is discontinuous

Therefore

$$f_K - f = O(K^{-n}) \quad \text{away from the discontinuity}$$

$$= O(K^{-n+1}) \quad \text{when } x - x_{\text{discontinuity}} = O(1/K)$$

$$\boxed{\text{IF } f \text{ is infinitely differentiable and periodic} \quad f_K \to f \text{ faster than any power of } 1/K}$$

⑦ Chebychev series

$$f(x) = \sum_{n=0}^{\infty} A_n T_n(x) \qquad -1 \le x \le +1$$

is closely related to Fourier series since

$$T_n(\cos\theta) = \cos n\theta$$

$\Rightarrow$ if $f(x)$ is infinitely differentiable, $f_N = \sum_{n=0}^{N-1} A_n T_n(x)$ converges to f faster than any power of $1/N$

$\Rightarrow$ No Gibbs phenomenon at $x = \pm 1$ (singular S-L problem)

$\Rightarrow$ Gibbs phenomenon at interior discontinuities

$\Rightarrow$ Minimax property: Maximum of the remainder is minimum, with respect to all polynomials of degree N and leading term 1

B. TYPES OF SPECTRAL METHODS

① Galerkin ("Spectral") METHOD

$$u_N = \sum_{n=1}^{N} A_n(t)\, \phi_n(x). \qquad (1)$$

is an approximation to $u(t)$, satisfying

$$\frac{\partial u}{\partial t} = H(u) \qquad H = \text{nonlinear differential operator} \qquad (2)$$

[where the $\{\phi_n\}$ each satisfy the boundary conditions on u]

Assume that u is "exact" at some time t

i) work with the best (least squares) approximation to u, of the form (1); i.e. u_N

ii) calculate the best (least squares) approximation to $H(u_N)$, of the form (1).

$$\left(\frac{\partial u}{\partial t}\right)_N = \sum_{i=1}^{N} B_i \phi_i \qquad u_N = \sum_{n=1}^{N} A_n \phi_n.$$

ze $\left(\left(\frac{\partial u}{\partial t}\right)_N - H(u_N), \left(\frac{\partial u}{\partial t}\right)_N - H(u_N)\right)$ by setting $\frac{\partial}{\partial B_i} = 0 = \frac{\partial}{\partial B_i^*}$

results in $B_e = (\phi_e, H(u_N))$

or since $B_e = \frac{\partial}{\partial t} A_e$

$$\boxed{\frac{\partial A_e}{\partial t} = \left(\phi_e(x), H\left(\sum_{i=1}^{N} A_i \phi_i(x)\right)\right)}$$

where $(\phi_e, \phi_m) = \delta_{em}$ has been used (orthonormal basis)

This prescription can also be written using projection operators P_N

> Recall: projection operators satisfy
>
> $$P_N^2 u = P_N u$$
>
> $$(P_N^2 - P_N)\, u = 0$$
>
> $$\Rightarrow \quad P_N u = \lambda u \quad \text{has solution for } \lambda = 0 \text{ or } 1$$
>
> $(\mathbb{I} - P_N)$ is a projection onto a space orthogonal to the space projected onto by P_N

the spectral equations in terms of P_N's are

$$\frac{\partial u_N}{\partial t} = P_N H (P_N u_N)$$

calculate inner product with $(\phi_\ell, \ )$, on (2)

~~Here we won't assume $(\phi_\ell, \phi_m) = \delta_{\ell m}$~~

$$\cancel{\sum_{n=1}^{N} (\phi_\ell, \phi_n) \frac{\partial A_n}{\partial t}} = \cancel{\left(\phi_\ell, H\left(\sum_{m=1}^{N} \phi_m\right.\right.}$$

$$\cancel{\text{consider} \quad \left(\phi_\ell, \sum_{n=1}^{N} \phi_n C_n\right) = \sum_{n=1}^{N} (\phi_\ell, \phi_n) C_n}$$

$$\sum_n (\phi_\ell, \phi_n) \frac{\partial A_n}{\partial t} = \left(\phi_\ell, \left(H\left(\sum_{i=1}^{N} \phi_i A_i\right)\right)\right)$$

$$\frac{\partial A_\ell}{\partial t} = \left(\phi_\ell, H\left(\sum_i^N A_i \phi_i\right)\right)$$

can be easily generalized for linearly independent but non orthogonal $\{\phi_n\}$

② Collocation (Method of Selected Points, pseudospectral).

(1) $$u_N = \sum_{\ell=1}^{N} A_\ell \phi_\ell.$$ $\{\phi_\ell\}$ each satisfy boundary conditions on u.

(2) $$\frac{\partial u}{\partial t} = H(u)$$

i) select a set of points X_i $i = 1, 2, \ldots N$

ii) require that $u_N(X_i) = u(X_i)$
to determine A_ℓ $\Rightarrow$ $\sum_{\ell=1}^{N} A_\ell \phi_\ell(X_i) = u(X_i)$

point of view 1:
Eq. (2) is solved in (x, t) at the points $\{X_i\}$, using the interpolating function $$u_N = \sum_{\ell=1}^{N} A_\ell \phi_\ell$$
to evaluate all derivatives, by differentiating ϕ_ℓ numerically or analytically

Point of view 2:
$\{A_\ell\}$ coefficients are advanced in time, with the operations, especially nonlinear ones in $H(u)$ evaluated by forming $u_N(X_i)$ and doing them in $\{X_i\}$ space.

properties i) and ii) serve to define P_N

(3) TAU Method

$$u_N = \sum_{n=1}^{N+k} A_n(t)\,\phi_n(x)$$

ϕ_n do NOT satisfy boundary conditions separately but they are orthonormal.

i) the first N terms $A_1, A_2 \ldots A_N$ satisfy a least squares approximation

ii) the last k terms are chosen to satisfy k boundary constraints

then for $\dfrac{\partial u}{\partial t} = H(u)$

$$\frac{\partial A_n}{\partial t} = (\phi_n, H(u_N)) \qquad n = 1, 2 \ldots N$$

$$\sum_{n=1}^{N+k} A_n \mathcal{B} \phi_n = 0$$

determines $A_{N+1}, \ldots A_{N+k}$ where $\mathcal{B}$ is an operator evaluating u_N at the boundaries in the proper way.

C ADVANTAGES (and some DISADVANTAGES) OF SPECTRAL METHODS

① lack of phase errors

suppose you have $\quad u_N = \sum_{n=1}^{N} A_n \phi_n$.

and you want $\quad u_N' = \sum_{n=1}^{N} A_n \phi_n'$

If you can calculate ϕ_n' exactly, the derivative is exact, up to roundoff.

<u>Fourier series</u>

$$u_N = \sum A_n e^{inx}$$

$$u_N' = \sum A_n in e^{inx}$$

$$= \sum B_n e^{inx}$$

$$B_n = in A_n$$

<u>Chebychev series</u>

$$u_N = \sum A_n T_n(x)$$

$$u_n' = \sum B_n T_n(x)$$

$$= \sum A_n T_n'(x)$$

Directly From ~~[illegible]~~

$T_n(x) = \cos(n \cos^{-1} x)$

$T_0' = 0$

$T_1' = T_0$

$T_2' = 4T_1$

for $n \geq 2$ $\quad \dfrac{T_{n+1}'}{n+1} = 2T_n(x) + \dfrac{T_{n-1}'(x)}{n-1}$

thus (B_n) is obtainable from (A_n) by a matrix multiply.

-or- for finite N you could just numerically evaluate $T_n'(x)$ for the needed points (psuedospectral) once

This is in contrast to the phase errors that are sometimes substantial in finite difference schemes!

e.g.

$$\Delta u_j = \frac{u_{j+1} - u_{j-1}}{2\Delta} \quad \text{applied to } u \sim e^{inx}$$

gives

$$\Delta u_j = \frac{e^{inx_{j+1}} - e^{inx_{j-1}}}{2\Delta} = \frac{e^{inx_j}}{2\Delta}\left(e^{in\Delta} - e^{-in\Delta}\right)$$

$$= iu\,\frac{\sin n\Delta}{\Delta}$$

$$\approx \frac{iu}{\Delta}\left(n\Delta - \frac{(n\Delta)^3}{6} + \cdots\right) = \left(1 - \frac{n^2\Delta^2}{6} + \cdots\right) iu$$

need $n\Delta \ll 1$ for accuracy

error is order $(n\Delta)^2$.

... etc for u'', though gets better for higher order methods

② Closely related ... Algebraic differentiation

→ less operations

→ less subtractions

③ HANDLING of BOUNDARY CONDITION.

Galerkin and pseudo spectral : exact!

but restricted in which boundary conditions can be handled.

(4) High order convergence of the approximations
- infinite order in some cases

(5) Global nature
- can slide collocation points around for local effects

(6) Control over resolution

D Simple Examples

(Hussaini, Street and Zang, ICASE 172248)

① $$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0$$ periodic in x, $0 \le x \le 2\pi$

INITIAL CONDITION

$$u(x,0) = \sin(\pi \cos x)$$

exact solution is

$$u(x,t) = \sin(\pi \cos(x-t))$$

Fourier expansion of exact $u(x,t)$

$$u(x,t) = \sum_k A_k(t)\, e^{ikx}$$

$$A_k(t) = \frac{1}{2\pi}\int_0^{2\pi} \sin[\pi \cos(x-t)]\, e^{-ikx}\, dx$$

Using the generating function for Bessel function

$$e^{\frac{z}{2}(t-1/t)} = \sum_{m=-\infty}^{\infty} J_m(z)\, t^m$$

evaluated at $t = ie^{i\theta}$

$$e^{iz\cos\theta} = \sum_{m=-\infty}^{\infty} J_m(z)\, e^{im\theta}\, i^m$$

let $z = \pi$, $\theta = x-t$

$$e^{i\pi\cos(x-t)} = \sum_{m=-\infty}^{\infty} J_m(\pi)\, e^{im(x-t)}\, i^m$$

then calculate the related integral

$$I_K = \frac{1}{2\pi}\int_0^{2\pi} \sum_{m=-\infty}^{\infty} i^m J_m(\pi)\, e^{im(x-t)} e^{-ikx}$$

$$I_K = \sum_m i^m J_m(\pi)\, e^{-imt}\, \delta_{mk}$$

$$I_K = i^K J_K(\pi)\, e^{-ikt}$$

use $J_{-K} = (-1)^K J_K$

$$\text{then } A_K = \frac{I_K - I_{-K}^*}{2} = \frac{i^K - (-i)^{-K}(-1)^K}{2} J_K(\pi)\, e^{-ikt}$$

$$\boxed{A_k = \sin\left(\frac{\pi k}{2}\right) J_k(\pi)\, e^{-ikt}}$$

Notice several things

- $|A_k(t)|^2 = \sin^2\left(\frac{\pi k}{2}\right) J_k^2(\pi)$ independent of time

  its a linear wave equation, phases of modes change, but "energy" doesn't undergo spectral transfer

- for large k $\quad J_k(\pi) \longrightarrow \frac{1}{\sqrt{2\pi k}}\left(\frac{e\pi}{2k}\right)^{+k}$

  thus
  $$k^p A_k \to \sin\left(\frac{\pi k}{2}\right) \frac{k^{p-1/2}}{\sqrt{2\pi}} k^{-k} (\quad)$$
  $$\doteq k^{p-1/2} e^{-k \ln k} (\quad)$$
  $$\to 0 \quad \text{for all fixed } p \text{ when } k \to \infty$$

  "infinite order"

numerical methods. $\quad \dfrac{\partial u}{\partial t} + \dfrac{\partial u}{\partial x} = 0$

Galerkin $\quad \dfrac{\partial A_k}{\partial t} = -ik\,A_k$

pseudo spectral $\quad$ choose $\quad x_j = \dfrac{2\pi j}{N} \qquad j = 0, 1 \ldots N-1$

$$\frac{\partial u(x_j)}{\partial t} = -\left.\frac{\partial \hat{u}}{\partial x}\right|_{x=x_j}$$

$\hat{u} =$ interpolating function $= \displaystyle\sum_{k=-N/2+1}^{N/2} A_k\, e^{ikx}$

where A_k is calculated from the numerical solution in x-space by $\quad A_k = \dfrac{1}{N}\displaystyle\sum_{j=0}^{N-1} u(x_j)\, e^{-ikx_j}$

Numerical Results (4th order Runge-Kutta time step)
at $t = 1$

N	Galerkin	Pseudospectral	Finite Diff. 2nd order	Finite Diff. 4th order
8	9.8×10^{-2}	1.62×10^{-1}	1.11	$9.62\ 10^{-1}$
16	2.55×10^{-4}	4.97×10^{-4}	6.13×10^{-1}	2.36×10^{-1}
32	1.05×10^{-11}	1.03×10^{-11}	1.99×10^{-1}	2.67×10^{-2}
64	6.22×10^{-13}	9.55×10^{-12}	5.42×10^{-2}	$1.85 \times 10^{-}$
128	—	—	1.37×10^{-2}	$1.18 \times 10^{-}$

② An analytically solvable problem in 2D Kinematic MHD

2D periodic geometry

$$\frac{\partial a}{\partial t} + \underset{\sim}{V} \cdot \nabla a = 0$$

$a = a(x,y,t)$ $\quad \underset{\sim}{V} = \underset{\sim}{K}(x,y)$ independent of time

$$\begin{cases} a(x,y,0) = -\sin 2y - \frac{1}{10}\sin 2x \\ \underset{\sim}{V}(x,y) = -2\sin x\,\hat{y} \end{cases}$$

Solution is

$$a(x,y,t) = a(x,\, y + 2t\sin x,\, 0)$$

$$= -\frac{1}{10}\sin 2x - \sin\left[2(y + 2t\sin x)\right]$$

<u>some conserved quantities</u>

$$\int a^{2n}\, d^2x = \text{const.} \qquad n = 1, 2, 3 \ldots \infty$$

but can't conserve all of them <u>exactly</u> with any numerical scheme.

$$A \equiv \int a^2\, d^2x = \text{mean square vector potential in 2D MHD}$$

other exactly known properties:

$$\frac{1}{2}\int (\nabla a)^2 d^2x = \text{"magnetic energy"} = \mathcal{E}_B = 1.01 + 2t^2$$

$$\frac{1}{2}\int (\nabla^2 a)^2 d^2x = \text{"mean square current"} = J = 4.04 + 18t^2 + 24t^4$$

→ Method of solution: Galerkin $N = 64$ "64×64" method.

(~~[illegible]~~ = ~~[illegible]~~ $k_{max} = 30.5$

Time stepping 2^{nd} order accurate explicit, $\Delta t = \frac{1}{256}$

$$\text{Error} \equiv \frac{1}{8\pi^2}\int (a_{exact} - a_{numerical})^2 d^2x = E(t)$$

$E(t) \sim$ roundoff (10^{-8}) up until $t > 4$

$\Delta A < 0.1\%$ up until $t > 6$

$\Delta J \sim 6 \times 10^{-4}$ at $t = 6$

$\Delta \mathcal{E}_B \sim 6.4 \times 10^{-4}$ at $t = 6$

(A few graphs...)

the exact solution had.

$$A(\ell, m, t) = \frac{i}{2} J_\ell(4t) \left[(-1)^\ell \delta_{m,-2} - \delta_{m,2} \right]$$

with $$\sum_{\underset{\sim}{k}} |A_{\underset{\sim}{k}}|^2 = \frac{1}{4} \left[\underbrace{J_0^2 + 2J_1^2 + 2J_2^2 + \cdots}_{=1} \right]$$

$$= \text{const.}$$

∴ there is a considerable amount of <u>spectral transfer</u> in this problem

⟹ Galerkin method has very high accuracy for linear problems, and very high accuracy for nonlinear problems provided that <u>spectral transfer</u> does not try to push excitation out past k_{max}

E. Evaluation of Nonlinear Terms (transform methods, aliasing, etc.)

$$\frac{\partial u}{\partial t} = u(x)\, v(x).$$

(1) Convolution theorems

a) 'continuous, infinite domain' $\Rightarrow$ Fourier xform

$$f(x) = \int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk \qquad g(x) = \int_{-\infty}^{\infty} G(k)\, e^{ikx}\, dk.$$

let $h(x) = f(x) g(x) = \int_{-\infty}^{\infty} H(k)\, e^{ikx}\, dk$

then $H(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} h(x)\, e^{-ikx}\, dx$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} \int_{-\infty}^{\infty} F(p)\, e^{ipx}\, dp \int_{-\infty}^{\infty} G(q)\, e^{iqx}\, dq\, dx$$

$$= \frac{1}{2\pi} \iint dp\, dq\; F(p)\, G(q) \int_{-\infty}^{\infty} e^{i(p+q-k)x}\, dx$$

$$= \iint dp\, dq\; F(p)\, G(q)\, \delta(k-q-p)$$

$$H(k) = \int dp\; F(k-p)\, G(p) \qquad \text{convolution integral}$$

product in x space $\longrightarrow$ convolution in k space

product in k space $\longrightarrow$ convolution in x space.

⇒ Fourier series instead
x form

b) finite domain, CONTINUOUS x, infinite # discrete k's $0 \le x \le 2\pi$

$$f(x) = \sum_k F(k)\, e^{ikx} \qquad g(x) = \sum_k G(k)\, e^{ikx}.$$

$$h(x) = f(x)\, g(x) = \sum_k H(k)\, e^{ikx}$$

$$H(k) = \frac{1}{2\pi} \int_0^{2\pi} dx\, e^{-ikx} h(x)$$

$$= \frac{1}{2\pi} \int_0^{2\pi} dx\, e^{-ikx} \sum_p F(p)\, e^{+ipx} \sum_q G(q) e^{iqx}$$

$$= \sum_p \sum_q F(p)\, G(q)\, \underbrace{\frac{1}{2\pi} \int_0^{2\pi} dx\, e^{i(p+q-k)x}}_{\delta_{q,\,k-p}}$$

$$H(k) = \sum_p F(p)\, G(k-p)$$

c) same as b) but N discrete x's ⇒ $x_i = \frac{2\pi(i-1)}{N}$

$$h(x_i) = f(x_i)\, g(x_i)$$

$$\frac{1}{2\pi} \int_0^{2\pi} dx \rightarrow \frac{1}{2\pi} \sum_{i=1}^{N} \Delta x_i = \frac{1}{N} \sum_{i=1}^{N}$$

$$e^{i\frac{2\pi(i-1)}{N}} \stackrel{?}{=} \quad H(k) = \frac{1}{N} \sum_{i=1}^{N} e^{-ik\frac{2\pi(i-1)}{N}} \sum_{p=-\infty}^{\infty} F(p)\, e^{ip\frac{2\pi(i-1)}{N}} \sum_{q=-\infty}^{\infty} G(q)\, e^{iq\frac{2\pi(i-1)}{N}}$$

$$= \sum_p \sum_q F(p)\, G(q)\, \underbrace{\frac{1}{N} \sum_{i=1}^{N} e^{i\frac{2\pi(i-1)}{N}(p+q-k)}}_{?}$$

c) finite number of degrees of freedom in a finite interval

$0 \le x \le 2\pi$, $\quad x_i = \frac{2\pi(i-1)}{N}$, $\quad i = 1, 2 \ldots N$

$k = -N/2+1, \ldots\ldots 0, 1 \ldots N/2$ [or, if you like: $0, 1 \ldots N-1$]

Discrete Fourier series (formally periodic in x_i and k)

$$f(x_i) = \sum_k F(k)\, e^{ikx_i} \qquad F(k) = \frac{1}{N}\sum_{i=1}^{N} e^{-ikx_i} f(x_i)$$

Note e^{ikx_i} is orthogonal to $e^{ik'x_i}$ unless $k = k'$

$$f(x_i) = \sum_k e^{ikx_i} \frac{1}{N}\sum_{j=1}^{N} e^{-ikx_j} f(x_j)$$

$$= \sum_{j=1}^{N} f(x_j) \frac{1}{N} \underbrace{\sum_{k=0}^{N-1} e^{ik(x_i - x_j)}}_{\sum_k e^{i k\frac{2\pi}{N}(i-j)}}$$

$$\left[\sum_{k=0}^{N-1} e^{kz} = \frac{1 - e^{Nz}}{1 - e^{z}}\right]$$

$$= \frac{1 - e^{2\pi i (k)(i-j)}}{1 - e^{2\pi i (i-j)/N}}$$

$\longleftarrow$ numerator $\equiv \emptyset$

$\longleftarrow$ denominator $\frac{i-j}{N} \neq 0$ unless $i = j$

$$\left.\begin{aligned} &= 0 \text{ when } i \neq j \\ &= \sum_{k=0}^{N-1} 1 = N \text{ when } i = j \end{aligned}\right\} N\delta_{ij}$$

for $i \in \{1, 2 \ldots N\}$, $j \in \{1, 2 \ldots N\}$

$$f(x_i) = f(x_i)$$

Now form convolution

$$h(x_i) = f(x_i)\, g(x_i)$$

$$h(x_i) = \sum_{k=0}^{N-1} H(k)\, e^{ikx}$$

$$H(k) = \frac{1}{N}\sum_{j=1}^{N} h(x_j)\, e^{-ik2\pi j/N}$$

$$= \frac{1}{N}\sum_{j=1}^{N} e^{-i2\pi kj/N} \sum_{p=0}^{N-1} F(p)\, e^{i2\pi jp/N} \sum_{q=0}^{N} G(q)\, e^{i2\pi jq/N}$$

$$= \sum_{p=0}^{N-1}\sum_{q=0}^{N-1} F(p)G(q)\ \underbrace{\frac{1}{N}\sum_{j=1}^{N} e^{i\frac{2\pi j}{N}(p+q-k)}}_{}$$

$p+q$ may be outside the interval $1, 2, \dots N$

$$\sum_{j=1}^{N} \frac{1}{N}\, e^{i\frac{2\pi j}{N}(\ell-k)} = ? \qquad \text{let} \quad k = KN + k' \quad \ell = LN + \ell'$$

$$\sum_{j=1} \underbrace{e^{i\frac{2\pi j}{N}(L-K)N}}_{\equiv 1}\, e^{i\frac{2\pi j}{N}(\ell'-k')}$$

$$= \frac{1}{N}\ \frac{1 - e^{i2\pi j(\ell'-k')}}{1 - e^{i2\pi j(\ell'-k')/N}} = \begin{cases} 0 & \text{if } k' \neq \ell' \\ 1 & \text{if } k' = \ell' \end{cases}$$

but this is the same as

$$\frac{1}{N}\sum e^{i\frac{2\pi j}{N}(\ell-k)} = \left\{\begin{matrix} 1 & \text{if } k \equiv \ell \mod N \\ 0 & \text{otherwise} \end{matrix}\right\} \equiv \delta_{\ell,k}(N)$$

$k \equiv \ell \mod N$ means $\ell = QN + R$

for some Q integer, when $k < N$

therefore

$$H(k) = \sum_{p=0}^{N-1} \sum_{q=0}^{N-1} F(p)\, G(q)\, \left(\delta_{p+q,k}(N)\right) \quad = 1 \text{ when } \begin{array}{l} p+q = k \\ p+q = k+N \\ p+q = k-N \end{array}$$

$$= \sum_p F(p)\, G(k-p)$$

$$+ \sum_p F(p)\, G(k+N-p)$$

$$+ \sum_p F(p)\, G(k-N-p)$$

Second two terms are "aliases" of the convolution

② Aliasing errors

Note in galerkin approximation to

$$~~~~ \quad \frac{\partial f}{\partial t} = fg$$

the spectral equations are

$$\frac{\partial F(k)}{\partial t} = \sum_{p+q=k} F(p)\, G(q)$$

$$\left[\begin{array}{l} p \in \{-N/2+1, +N/2\} \\ q \in \{ \qquad \} \\ k \in \{ \qquad \} \end{array}\right] \quad -\tfrac{N}{2}+1 \text{ to } \tfrac{N}{2}-1$$

$$\equiv H^s(k) \qquad \text{"s" for spectral spa}$$

therefore, instead of the usual convolution theorem, the transform method gives

$$H(k) = \frac{1}{N}\sum_{j=1}^{N} f(x_j)\, g(x_j)\, e^{-ik2\pi j/N}$$

$$= H^g(k) + \underbrace{H^g(k+N) + H^g(k-N)}_{\text{aliasing errors}} \qquad \text{"g" for galer}$$

this is what you get with a pseudo spectral method.

③ Eliminating Aliasing errors in

$$\frac{\partial f}{\partial t} = f(x_j)\, g(x_j)$$

where $x_j = 2\pi(j-1)/N$

a) extended grid

suppose that we form

$$F(k) = \frac{1}{N}\sum_{j=1}^{N} f(x_j)\, e^{-ikx_j} \qquad \text{as before}$$

but now define the extended transform F^e as

$$F^e(k) = F(k) \qquad k = 0, 1, \ldots N-1$$

$$= 0 \qquad k = N, N+1 \ldots 2N-1$$

thus F^e is a $2N$ point transform, with exactly the same information as $F(k)$

Also do the same for $G \rightarrow G^e(k)$ $k = 0, 1 \ldots 2N-1$

Now form

$$H^e(k) = \frac{1}{2N}\sum_{j=1}^{2N} h^e(x_j)\, e^{-ik2\pi j/2N}$$

$$= \frac{1}{2N}\sum_{p=0}^{2N-1}\sum_{q=0}^{2N-1} F^e(p)\, G^e(q) \sum_{j=1}^{2N} e^{i\frac{2\pi j}{2N}(p+q-k)}$$

$$H^e(k) = \sum_{p=0}^{2N-1}\sum_{q=0}^{2N-1} F^e(p)\, G^e(q) \underbrace{\delta_{p+q,k}(2N)}_{0 \text{ unless}}$$

$p+q = Q2N + k$

for some integer Q

but the biggest that $p+q$ can be, for nonzero F^e and G^e is $N+N-2$ since

$F^e(k) \neq 0$ only for $|k| < N/2$, so only nonzero term is for $Q = 0$ and

$H^e(k) = H^g(k)$ for $|k| < N/2$ which is the Galerkin convolution

b) shifted grid

still looking at

$$\frac{\partial f}{\partial t} = f(x)\, g(x)$$

suppose we have already calculated

$$H(k) = \underbrace{H^g(k) + H^g(k+N) + H^g(k-N)}_{\text{aliasing errors}}$$

Now form the shifted grid convolution

$$H^S(k) = \frac{1}{N}\sum_{j=1}^{N} f(X_{j+1/2})\, g(X_{j+1/2})\, e^{-ik2\pi j/N}$$

where
$$f(X_{j+1/2}) = \sum_{k=0}^{N-1} F(k)\, e^{i2\pi k(j+1/2)/N}$$
$$g(X_{j+1/2}) = \sum_{k=0}^{N-1} G(k)\, e^{i2\pi k(j+1/2)/N}$$

$$H^S(k) = \sum_{p=0}^{N-1}\sum_{q=0}^{N-1} F(p)\, G(q)\, \underbrace{\frac{1}{N}\sum_{j=1}^{N} e^{i2\pi j(p+q-k)/N}}_{\delta_{p+q,k}(N)}\ \underbrace{e^{i\pi\frac{(p+q)}{N}}}_{\text{New Term.}}$$

$$= \sum_{p=0}^{N-1} F(p)\, G(k-p)\, e^{i\pi k/N}$$
$$+ \sum_{p=0}^{N-1} F(p)\, G(k+N-p)\, e^{i\pi k/N} e^{i\pi N/N}$$
$$+ \sum_{p=0}^{N-1} F(p)\, G(k-N-p)\, e^{i\pi k/N} e^{-i\pi N/N}$$
$$= e^{i\pi k/N}\left\{ H^G(k) - H^G(k+N) - H^G(k-N)\right\}$$

Therefore

$$H^G(k) = \frac{1}{2}\left\{ H(k) + e^{-i\frac{\pi k}{N}} H^S(k) \right\}$$

gives the exact galerkin convolution

ordinary transform method convolution

transform method on the shifted grid

II SIMULATION OF Turbulence in MHD (and Hydrodynamics)

A. Incompressible MHD

(1) $$\frac{\partial \underset{\sim}{V}}{\partial t} + \underset{\sim}{V}\cdot\nabla\underset{\sim}{V} = -\nabla p + \underset{\sim}{J}\times\underset{\sim}{B} + \nu\nabla^2\underset{\sim}{V}$$

(2) $$\frac{\partial \underset{\sim}{B}}{\partial t} = \nabla\times\underset{\sim}{V}\times\underset{\sim}{B} + \mu\nabla^2\underset{\sim}{B}$$

(3) $$\nabla\cdot\underset{\sim}{V} = 0$$

(4) $$\nabla\cdot\underset{\sim}{B} = 0$$

from (3) and (1), if $\frac{\partial}{\partial t}\nabla\cdot\underset{\sim}{V} = 0$ then.

(3*) $$\nabla^2 p = \nabla\cdot\left(\underset{\sim}{J}\times\underset{\sim}{B} - \underset{\sim}{V}\cdot\nabla\underset{\sim}{V}\right)$$

- Nonlinear Terms $\Rightarrow$ convolutions in $\underset{\sim}{k}$ space
  (i.e.) amplitude in $\underset{\sim}{k}$ changed by all $\underset{\sim}{p}, \underset{\sim}{q}$ such that $\underset{\sim}{p}+\underset{\sim}{q}=\underset{\sim}{k}$
  & i.e. get spectral Transfer.
- linear Terms $\nu\nabla^2\underset{\sim}{V}$, $\mu\nabla^2\underset{\sim}{B}$ damp each fourier mode.

$$\underset{\sim}{V}(\underset{\sim}{x},t) = \sum_{\underset{\sim}{k}} \underset{\sim}{V}(\underset{\sim}{k},t)\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{x}}$$

$$\frac{\partial \underset{\sim}{V}(\underset{\sim}{k})}{\partial t} \sim -\nu k^2 \underset{\sim}{V}(\underset{\sim}{k}) \underset{\text{only thing}}{\Longrightarrow} \underset{\sim}{V}(k,t) = \underset{\sim}{V}(k,0)\, e^{-\nu k^2 t}$$

B. Spectral equations: 3D MHD

using $\underset{\sim}{J} \times \underset{\sim}{B} = (\nabla \times B) \times B = -\nabla \frac{B^2}{2} + B \cdot \nabla B$

and defining $p^* = p + B^2/2$.

$$\rightarrow \quad \frac{\partial \underset{\sim}{V}}{\partial t} + \underset{\sim}{V} \cdot \nabla \underset{\sim}{V} = -\nabla p^* + \underset{\sim}{B} \cdot \nabla \underset{\sim}{B} + \nu \nabla^2 \underset{\sim}{V}$$

let $\underset{\sim}{V} = \sum_{\underset{\sim}{k}} \underset{\sim}{V}(\underset{\sim}{k}, t)\, e^{+i \underset{\sim}{k} \cdot \underset{\sim}{x}}$ $\qquad \underset{\sim}{B} = \sum_{\underset{\sim}{k}} \underset{\sim}{B}(k, t)\, e^{i \underset{\sim}{k} \cdot \underset{\sim}{x}}$

$$e^{i \underset{\sim}{k}' \cdot x} \frac{\partial \underset{\sim}{V}(\underset{\sim}{k}')}{\partial t} = \sum_{\underset{\sim}{q}} -i \underset{\sim}{q} P_{\underset{\sim}{q}}\, e^{i \underset{\sim}{q} \cdot \underset{\sim}{x}} + \sum_{\underset{\sim}{p}, \underset{\sim}{q}} e^{i(\underset{\sim}{p} + \underset{\sim}{q}) \cdot \underset{\sim}{x}}\, \underset{\sim}{V}(\underset{\sim}{p}) \cdot i \underset{\sim}{q}\, \underset{\sim}{V}(\underset{\sim}{q})$$

$$+ \sum_{\underset{\sim}{p}, \underset{\sim}{q}} e^{i(\underset{\sim}{p} + \underset{\sim}{q}) \cdot \underset{\sim}{x}}\, \underset{\sim}{B}(\underset{\sim}{p}) \cdot i \underset{\sim}{q}\, \underset{\sim}{B}(\underset{\sim}{q}) - \sum_{\underset{\sim}{k}'} \nu k^2 \underset{\sim}{V}(\underset{\sim}{k})$$

multiply by $e^{-i \underset{\sim}{k} \cdot \underset{\sim}{x}}$ and $\frac{1}{V} \int_0^{2\pi}\!\!\iint d^{(n)} x$

$$\frac{\partial \underset{\sim}{V}(\underset{\sim}{k})}{\partial t} = -i \underset{\sim}{k}\, P^*_{\underset{\sim}{k}} + i \sum_{\underset{\sim}{p} + \underset{\sim}{q} = \underset{\sim}{k}} - \underset{\sim}{V}(\underset{\sim}{p}) \cdot \underset{\sim}{q}\, \underset{\sim}{V}(\underset{\sim}{q}) + \underset{\sim}{B}(p) \cdot \underset{\sim}{q}\, \underset{\sim}{B}(\underset{\sim}{q}) - \nu k^2 \underset{\sim}{V}(\underset{\sim}{k})$$

Note $\nabla \cdot \underset{\sim}{V} = 0 \Rightarrow \underset{\sim}{k} \cdot \underset{\sim}{V}(\underset{\sim}{k}) = 0$ but $\underset{\sim}{p} + \underset{\sim}{q} = \underset{\sim}{k}$ so $\underset{\sim}{q} \cdot \underset{\sim}{V}(p) = \underset{\sim}{k} \cdot \underset{\sim}{V}(\underset{\sim}{p})$.

and $\nabla^2 p^* = \nabla \cdot (\underset{\sim}{B} \cdot \nabla \underset{\sim}{B} - \underset{\sim}{V} \cdot \nabla \underset{\sim}{V}) \Rightarrow$

$$-k^2 P^*_{\underset{\sim}{k}} = i\,\underset{\sim}{k} \cdot \sum_{\underset{\sim}{p} + \underset{\sim}{q} = \underset{\sim}{k}} \left[\underset{\sim}{B}(p) \cdot \underset{\sim}{q}\, \underset{\sim}{B}(\underset{\sim}{q}) - \underset{\sim}{V}(p) \cdot \underset{\sim}{q}\, \underset{\sim}{V}(\underset{\sim}{q}) \right]$$

or $\quad P^*_{\underset{\sim}{k}} = +\frac{1\underset{\sim}{k}}{k^2} \cdot \sum \left[\qquad\qquad\qquad \right]$

$\underset{\sim}{V}(\underset{\sim}{p}) \cdot \underset{\sim}{q} \equiv \underset{\sim}{V}(\underset{\sim}{p}) \cdot (\underset{\sim}{k} - \underset{\sim}{p})$

$$\frac{\partial V_i(\underset{\sim}{k})}{\partial t} = i k_e \sum_{p+q=k} -V_e(p)\,V_i(q) + B_e(p)\,B_i(q)$$

$$- i \frac{k_i k_n k_e}{k^2} \sum_{p+q=k} -V_e(p) V_n(q) + B_e(p)\,B_n(q)$$

$$- \nu\, k^2 V_i(k)$$

$$= \left(i k_e \delta_{in} - i \frac{k_e k_i k_n}{k^2}\right) \sum_{\underset{\sim}{p}+\underset{\sim}{q}=\underset{\sim}{k}} \underset{\sim}{B_e}(\underset{\sim}{p})\, \underset{\sim}{B_n}(\underset{\sim}{q}) - \underset{\sim}{V_e}(\underset{\sim}{p})\, \underset{\sim}{V_n}(\underset{\sim}{q})$$

$$- \nu k^2 V_i(\underset{\sim}{k})$$

$$(5) \quad \boxed{\frac{\partial V_i(\underset{\sim}{k})}{\partial t} = i k_e \left(\delta_{in} - \frac{k_i k_n}{k^2}\right) \sum_{\underset{\sim}{p}+\underset{\sim}{q}=\underset{\sim}{k}} \underset{\sim}{B_e}(p)\, \underset{\sim}{B_n}(q) - \underset{\sim}{V_e}(p)\, \underset{\sim}{V_n}(q) - \nu k^2 \underset{\sim}{V}(\underset{\sim}{k})}$$

project onto k-direction

project perpendicular to $\underset{\sim}{k}$ (Transverse projection operator)

Similarly

$$(6) \quad \boxed{\frac{\partial \underset{\sim}{B}(\underset{\sim}{k})}{\partial t} = i \underset{\sim}{k} \cdot \sum_{\underset{\sim}{p}+\underset{\sim}{q}=\underset{\sim}{k}} \left(\underset{\sim}{B}(p)\, \underset{\sim}{V}(q) - \underset{\sim}{V}(p)\, \underset{\sim}{B}(q)\right) - \mu k^2 \underset{\sim}{B}(\underset{\sim}{k})}$$

(5) and (6) are exact ~~equations~~, ~~Galerkin and pseudospectral methods~~ representation of (1)–(4).

Galerkin and Pseudospectral 3D MHD

B. Galerkin Approx to (5) and (6) in 3D, let $(k_i)_{max} = N/2$, an N^3 simulation

interpret all the fields as truncated series
interpret the convolution in the same way

$$\sum_{\substack{p+q=k \\ k_i, p_i, q_i \in S}}$$

set S: $\{\underset{\sim}{k}$ with $|k_i| \le N/2\}$

Implementation is more difficult

- Multidimensional transform methods
  $\Rightarrow$ pseudo spectral
- Multidimensional De-aliasing (we'll get to that)
  $\Rightarrow$ Combination of shifted grid and grid extension
- Compact Representations

  (5) and (6) preserve $\underset{\sim}{k} \cdot \underset{\sim}{B}(\underset{\sim}{k}) = \underset{\sim}{k} \cdot \underset{\sim}{V}(\underset{\sim}{k}) = 0$

  but can you get away with 2 components for each vector?

  in principle, yes

  $$\underset{\sim}{B}(\underset{\sim}{k}) = i\, \underset{\sim}{k} \times \hat{z}\; b_1(\underset{\sim}{k}, t) + \underset{\sim}{k} \times (\underset{\sim}{k} \times \hat{z})\; b_2(\underset{\sim}{k}, t).$$

  but it gets complicated.

  [in other geometries (Turner, Christensen function)

  $$\underset{\sim}{B}(\underset{\sim}{x}) = \nabla \times \hat{z}\, b_1 + \nabla \times (\nabla \times b_2 \hat{z}).]$$

Pseudospectral 3D MHD

2 approaches

1) solve (1)–(4) along with (3′)

- using fourier representation to calculate all derivatives, transform back to $\underline{x}$-space to form nonlinear products
- $\nabla^2 p$ equation can be solved using transform method
- dissipation can be handled in either $\underline{x}$ or $\underline{k}$ space

2) Solve in $\underline{k}$ space, but dont dealiase the convolutions

~~C. Conservation Laws in MHD Turbulence~~

C. 2D MHD in periodic geometry

— widely studied.

let $\underset{\sim}{B} = \underset{\sim}{B}(x, y, t)$

$\underset{\sim}{V} = \underset{\sim}{V}(x, y, t)$

periodic in 2π in x and y direction

then $\underset{\sim}{B} = \nabla \times \hat{z}\, a(x, y, t)$ — z component vector potential

$\underset{\sim}{V} = \nabla \times \hat{z}\, \psi(x, y, t)$ — streamfunction ψ

the current density $\underset{\sim}{J} = \underset{\sim}{\nabla} \times B = -\nabla^2 a\, \hat{z} \equiv j\, \hat{z}$

the vorticity $\underset{\sim}{\Omega} = \nabla \times \underset{\sim}{V} = -\nabla^2 \psi\, \hat{z} \equiv \omega\, \hat{z}$

then $\nabla \cdot \underset{\sim}{B} = \nabla \cdot \underset{\sim}{V} = 0$ automatically and

$$\frac{\partial \omega}{\partial t} + \underset{\sim}{V} \cdot \nabla \omega = \underset{\sim}{B} \cdot \nabla j + \nu \nabla^2 \omega$$

$$\frac{\partial a}{\partial t} + \underset{\sim}{V} \cdot \nabla a = \mu \nabla^2 a .$$

the Fourier representation of these are

$$\frac{\partial \omega(\underset{\sim}{k})}{\partial t} = i\underset{\sim}{k} \cdot \sum_{\underset{\sim}{q}+\underset{\sim}{p}=\underset{\sim}{k}} \left(\underset{\sim}{B}(q)\, j(p) - \underset{\sim}{V}(\underset{\sim}{q})\, \omega(p) \right)$$

$$- \nu k^2 \omega(\underset{\sim}{k})$$

$$\frac{\partial a(\underset{\sim}{k})}{\partial t} = -i\underset{\sim}{k} \cdot \sum_{\underset{\sim}{q}+\underset{\sim}{p}=\underset{\sim}{k}} \underset{\sim}{V}(\underset{\sim}{q})\, a(\underset{\sim}{p}) - \mu k^2 a(k)$$

The Galerkin approximation is obtained directly by restricting all wave numbers to lie in the N^2 space with $|k_i| \leq N/2$

The Transform method is typically used and is de-aliased.

D. Conservation Laws in ideal MHD : $\boxed{\text{exact equation with } \nu = \mu = 0}$

3D define $\langle \dots \rangle$ as the volume average.
over a Volume fixed in time., volume V, surface S

energy $= \langle V^2 + B^2 \rangle / 2 = E$

$$\frac{dE}{dt} = 0 \quad \text{for} \quad \begin{cases} \text{periodic boundaries} \\ \hat{n} \cdot \underline{B} = \hat{n} \cdot \underline{V} = 0 \text{ on surface } S \\ \underline{V} = 0 \text{ on surface } S \\ \text{and others} \end{cases}$$

cross helicity

$$H_c = \langle \underline{V} \cdot \underline{B} \rangle / 2 \qquad \frac{dH_c}{dt} = 0 \quad \begin{cases} \text{periodic} \\ \hat{n} \cdot \underline{B} = \hat{n} \cdot \underline{V} = 0 \text{ on } S \\ \underline{B} = 0 \text{ on } S \end{cases}$$

Magnetic Helicity

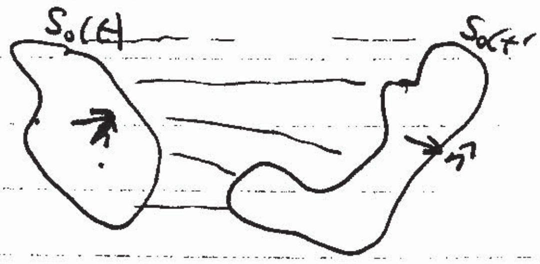
$$H_M = \langle \underline{A} \cdot \underline{B} \rangle / 2 \qquad \frac{dH_M}{dt} = 0 \quad \begin{cases} \text{periodic} \\ \hat{n} \cdot \underline{B} = \hat{n} \cdot \underline{V} = 0 \text{ on } S \\ \underline{B} = 0 \text{ or } \underline{V} = 0 \text{ along} \\ \text{with electrostatic } \underline{E} = 0 \text{ ...} \end{cases}$$

$$\underline{B} = \nabla \times \underline{A}$$

$$\nabla \cdot \underline{A} = 0$$

Many others
e.g. Alfven flux invariants

$$\frac{d}{dt} \int_{S_0(t)} \underline{B} \cdot \hat{n} \, da = 0$$



2D MHD.

$E = \langle v^2 + B^2 \rangle / 2$ is constant

$H_c = \langle \underset{\sim}{v} \cdot \underline{B} \rangle / 2$ is constant

$H_M \equiv 0$

but $A \equiv \langle a^2 \rangle / 2$ is constant for periodic b.c.'s and others.

others

equivalents of Alfven invariants

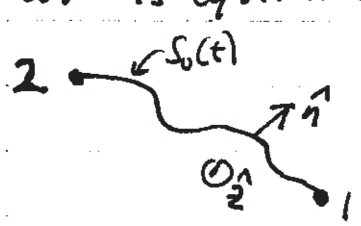
$$\frac{\partial a}{\partial t} + v \cdot \nabla a = 0 = \frac{Da}{Dt} \qquad \text{convective derivative}$$

every material element maintains a constant value of a as it moves around...

an infinite number of invariants

implies that
$$\frac{d}{dt}\int a^{2m} d^2x = \int a^{2m-1} \frac{\partial a}{\partial t} d^2x$$
$$= -\int a^{2m-1} \underset{\sim}{v} \cdot \nabla a \, d^2x = \int \nabla \cdot \underline{v} a^{2m} d^2x$$
$$\equiv 0$$

and is equivalent to the Alfven flux invariants



$$\frac{d}{dt}\int_{S_0(t)} B \cdot \hat{n} \, dl = \frac{d}{dt}\int (\nabla \times \hat{z} a) \cdot \hat{n} \, dl$$
$$= \frac{d}{dt}\int^2 (\hat{z} \times \hat{n}) \cdot \nabla a \, dl = \frac{\partial a(2)}{\partial t} - \frac{\partial a(1)}{\partial t} \equiv 0$$

E Rugged Invariants

$E \quad H_c \quad H_M$ in 3D

$E \quad H_c \quad A$ in 2D

($E \quad \langle \Omega^2 \rangle$ in 2D Navier Stokes)

these are invariants in time for any (ideal) Galerkin approximation, in fact they are invariants for any triad of wave vectors satisfying

$$\underset{\sim}{k} + \underset{\sim}{p} + \underset{\sim}{q} = 0$$

example rugged conservation of $A \equiv \langle a^2 \rangle / 2$.
in 2D MHD with $\mu = 0$

$$\frac{\partial a(\underset{\sim}{k})}{\partial t} = -i\underset{\sim}{k} \cdot \sum_{\underset{\sim}{p}+\underset{\sim}{q}=\underset{\sim}{k}} \underset{\sim}{v}(\underset{\sim}{p})\, a(\underset{\sim}{q})$$

$$\frac{\partial a(-\underset{\sim}{k})}{\partial t} = i\underset{\sim}{k} \cdot \sum_{\underset{\sim}{p}+\underset{\sim}{q}+\underset{\sim}{k}=0} \underset{\sim}{v}(\underset{\sim}{p})\, a(\underset{\sim}{q}) \qquad \text{sum on } \underset{\sim}{p}, \underset{\sim}{q}$$

$$a(k)\frac{\partial a(-k)}{\partial t} = i\underset{\sim}{k} \cdot \sum_{\underset{\sim}{p}+\underset{\sim}{q}+\underset{\sim}{k}=0} \underset{\sim}{v}(\underset{\sim}{p})\, a(\underset{\sim}{q})\, a(\underset{\sim}{k})$$

$$= \frac{1}{2}\frac{\partial}{\partial t} |a(\underset{\sim}{k})|^2$$

$$= -i \sum_{\substack{\underset{\sim}{p}+\underset{\sim}{q}+\underset{\sim}{k}=0 \\ \underset{\sim}{p},\underset{\sim}{q}}} \underset{\sim}{v}(\underset{\sim}{p}) \cdot \underset{\sim}{q}\, a(\underset{\sim}{q})\, a(\underset{\sim}{k})$$

Similarly

$$\frac{\partial a(-q)}{\partial t} = i\,q \cdot \sum_{\substack{q+p+k=0 \\ p,k}} V(p)\, a(k)$$

$$\frac{1}{2}\frac{d}{dt}|a(q)|^2 = -i \sum_{\substack{q+p+k=0 \\ p,k}} V(p)\cdot k\; a(k)\; a(q)$$

since $\frac{d}{dt}\langle a^2\rangle = \frac{1}{2}\sum_{k} (a(k))^* \frac{\partial a(k)}{\partial t}$

$$\frac{d}{dt}\langle a^2\rangle = \frac{1}{2}\left\{ \sum_{q} \frac{1}{2}\frac{d}{dt}|a(q)|^2 + \sum_{k} \frac{1}{2}\frac{d}{dt}|a(k)|^2 \right\}$$

$$= -\frac{i}{2} \sum_{\substack{q+p+k=0 \\ q,p,k}} V(p)\cdot q\; a(q)\, a(k) + V(p)\cdot k\; a(k)\, a(q)$$

$$= -\frac{i}{2} \sum_{\substack{q+p+k=0 \\ q,p,k}} V(p)\cdot (q+k)\; a(q)\, a(k)$$

$$= \frac{i}{2} \sum_{q+p+k=0} V(p)\cdot p\;\; a(q)\, a(k) \;\; \equiv 0 \quad \text{since } V(p)\cdot p = 0$$

This holds for any set of k's p's and q's since it is zero term by term for any $V(p)$ interaction with both $a(q)$ and $a(k)$. That is, if the only non zero modes we considered were $k+p+q=0$

$$\frac{1}{2}\left(\frac{d}{dt}|a(q)|^2 + \frac{d}{dt}|a(k)|^2 \right) = -i\; V(p)\cdot(k+q)\; a(k)\, a(q)$$

$$\equiv 0 \quad \text{since } V(p)\cdot p \equiv 0$$

Similar proofs of "ruggedness" of E, H_c in 2D and E, H_c and H_m in 3D can be written down, some involve writing the time development of 3 modes down and summing

In general rugged invariants are conserved by each triad satisfying

$$\underset{\sim}{k} + \underset{\sim}{p} + \underset{\sim}{q} = 0$$

and therefore are invariant for any Galerkin approximation

What happens if there are some $\underset{\sim}{p} + \underset{\sim}{q}$ that give $\underset{\sim}{k}$ outside $\mathcal{G}$, the retained $\underset{\sim}{k}$'s?

let that $\underset{\sim}{k}$ be $\underset{\sim}{k}_{outside}$

$$\cancel{a(k_{outside}) \frac{\partial a(k)_{outside}}{\partial t}} \; \frac{1}{2} \frac{d}{dt} |a(\underset{\sim}{k}_{outside})|^2 =$$

$$a(-\underset{\sim}{k}_{outside}) \, \frac{\partial a(k_{outside})}{\partial t}$$

but this is $\doteq 0$ in galerkin

this may be non zero (but its not even calculated) the spatial part of the Galerkin codes therefore conserve the rugged invariants "exactly", i.e. up to roundoff and time integration errors

the "shape" of the set of retained wavevectors S is irrelevant, as long as the retained modes are updated according to the Galerkin convolutions, and all modes outside S are always kept $= 0$. In those circumstances the above type of proof guarantees rugged conservation

Dissipation (non zero μ and ν) can and should change the values of the R.I's., although only η affects the magnetic R.I's such as A and H_m.

Non rugged ideal invariants of the continuum (exact) equations are preserved for limited periods of time by Galerkin codes, when $\nu = \eta = 0$, but eventually excitations spread to k_{max}, then Non-rugged "invariants" can change.

Since topological properties, such as connectivity of magnetic field lines depend on non-rugged conservation principles, they will not be conserved by Galerkin codes when $\nu = \eta = 0$ for long times. Thus, e.g. "Numerical reconnection" can occur, even though numerical dissipation of energy, for example cannot occur, when $\nu = \eta = 0$.

this does not mean that numerical reconnection occurs when $\nu \neq 0$ $\eta \neq 0$.

F. MHD Turbulence and accuracy of spectral codes

~~Ideal MHD~~ Nonlinearities cause many modes to become excited, for small or zero ν, η, one may expect "ergodic" behavior.

Ideal MHD: Abs. Eq. Ensemble (Fyfe + Montgomery)

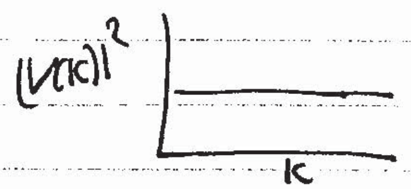
$$D_{eq}\left(\{\underline{V}(\underline{k}), \underline{B}(\underline{k})\}\right)$$

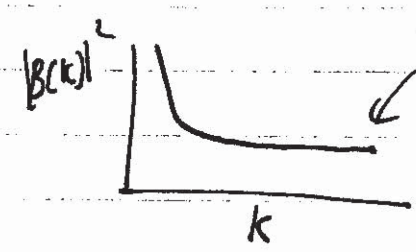
$$\sim \exp\left\{-\alpha E - \beta H_c - \gamma A\right\}$$

can calculate Gibbs ensemble spectrum

$$\langle |\underline{V}(k)|^2 \rangle = f_V(\alpha, \beta, \gamma, k, N)$$

$$\langle |\underline{B}(k)|^2 \rangle = f_B(\alpha, \beta, \gamma, k, N)$$

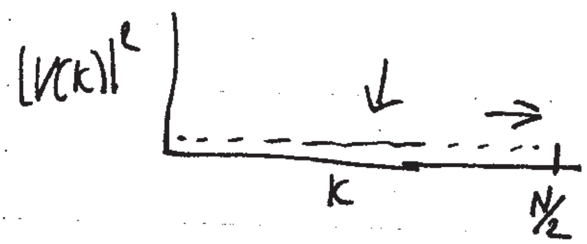


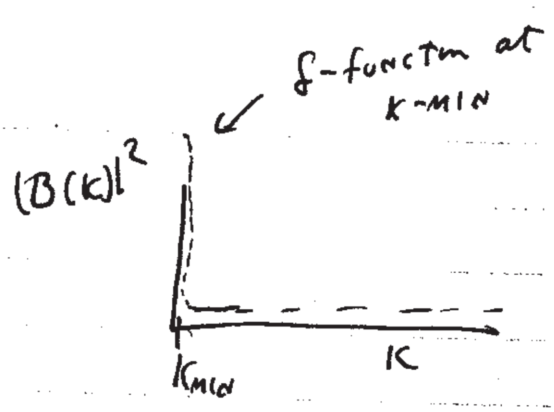


equipartition at high k

$|V(k)|^2 \to$ const as $k \to$ large.

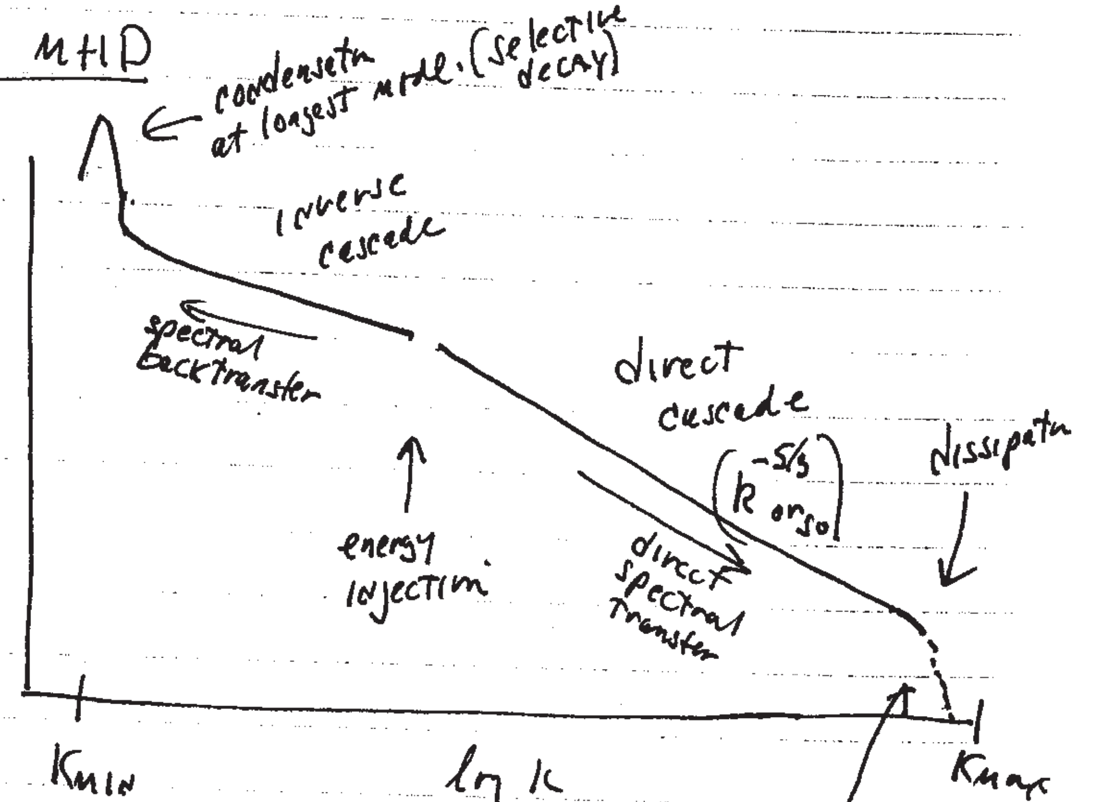
as $N \to \infty$





$\underline{V}$ - excitations spread ergodically to all allowed k.
some magnetic excitatn condense to k_{MIN}, with the rest equipartitioned with $\underset{\sim}{v}$.

<u>DISSIPATIVE MHD</u>



spectrum steepens above $k = k_{dissipatn}$

$\tau_{NL} = L/v$

$k_{diss} \approx \left(\langle \omega^2 + j^2 \rangle\right)^{1/4} \sqrt{R}$

either $\frac{1}{\nu}$ or $\frac{1}{\eta}$

- Decreasing the dissipation coefficients just increases k_d and enlarges the range of direct spectral transfer wavenumbers (in steady state the direct cascade powerlaw range).

- but the energy decay rate still should be something like.

$$\frac{dE}{dt} = \frac{E}{\tau} = \frac{U^2}{L/U} = \frac{E^{3/2}}{L}$$

in analogy with laminar dissipation (just looking at energy containing scales)

$$\frac{dE}{dt} \sim \nu_{\text{Turbulent}} \frac{E}{L^2}$$

there is a turbulent dissipation coefficient

$$\nu_{\text{Turbulent}} \sim L E^{1/2} \sim \frac{L^2}{\tau}$$

if you look at the effect of spectral transfer and turbulent dissipation on the small scales

$$\frac{d}{dt} E(k) \sim \frac{V_k^2}{\tau(k)} \sim \frac{V_k^3}{\ell} \qquad \ell \sim 1/k \qquad \tau_k \sim \frac{1}{k V_k}$$

while the small scale turbulent dissipation coefficient is something like that given by

$$\nu_{\text{turb}}(k) \frac{V_k^2}{\ell^2} = \frac{V_k^3}{\ell} \Rightarrow \frac{\ell^2}{\tau_k} = \frac{1}{k^2 \tau_k} = \frac{V_k}{k}$$

(Heisenberg, Yoshizawa, Montgomery)

- The "bottom line" is that the Galerkin approximation handles the spatial couplings within S very well; the only problem for physical dissipative MHD may be inadequate resolution.

k_d can only be well determined experimentally, however 3 estimates are useful (for $\nu = \mu$)

i)

$$k_d = \left(\frac{\left|\frac{d\mathcal{E}}{dt}\right|}{\nu^3} \right)^{1/4} \rightarrow \left(2 \langle \omega^2 + j^2 \rangle\right)^{1/4} \sqrt{R}$$

↑ either $1/\nu$ or $1/\eta$

where $\langle \omega^2 + j^2 \rangle$ is determined from the simulation

ii) when using driving terms, in steady state $\left|\frac{d\mathcal{E}}{dt}\right|$ is the time averaged supply of energy = time averaged dissipation rate

$$k_d = \left|\frac{d\mathcal{E}}{dt}\right|^{1/4} \cancel{R^{3/4}} \left(1/\nu\right)^{3/4}$$

iii) hydrodynamic-like similarity value of k_d. $(\nu = \eta)$

$$\frac{dE}{dt} \sim U^3/L = 2\nu(\Omega + J) \Rightarrow \langle \omega^2 + j^2 \rangle = \frac{U^3}{L} \frac{1}{2\nu}$$

then

$$k_d = \left(\frac{2\nu \langle \omega^2 + j^2 \rangle}{\nu^3} \right)^{1/4} = \left(\frac{U^3}{L \nu^3} \right)^{1/4} = \left(\frac{U^3 L^3}{\nu^3} \frac{1}{L^4} \right)^{1/4}$$

$$= \frac{1}{L} R^{3/4} = k_0 R^{3/4}$$

↑ [illegible]

G. Accuracy and Stability of time integration schemes

Consider $\quad \frac{\partial u}{\partial t} = H(u)$

Often, in implementation of spectral and pseudospectral schemes, 2nd order accurate time integration schemes are used. ⇒ Because, they involve a minimum number of evaluations of $H(u)$, containing nonlinear terms. Higher order explicit schemes and implicit schemes can be costly.

Typically,

$$u^{n+1/2} = u^n + \frac{\Delta t}{2} H(u^n)$$

$$u^{n+1} = u^n + \Delta t\, H(u^{n+1/2})$$

is used, a second order modified Euler method RK2

Consider

$$H(u) = V\frac{\partial u}{\partial x} + \nu \frac{\partial^2}{\partial x^2} u$$

Calculate the growth factor (Von Neumann analysis)

$$u \rightarrow u_k e^{ikx}$$

$$u_k^{n+1} = \underbrace{\left[1 + \Delta t\, Q + \frac{\Delta t^2}{2} Q^2 \right]}_{G} u_k^n$$

where $Q = ikV - \nu k^2$

the growth factor is

$$G^*G = 1 - 2\nu k^2 \Delta t + 2\left[\nu k^2 \Delta t\right]^2$$

$$- \Delta t^3 \left[V^2 \nu k^2 + \nu^3 k^6\right] + \tfrac{1}{4}\Delta t^4 \left[(kV)^2 + \nu^2 k^4\right]^2$$

i) $\nu = 0$ unconditionally ~~un~~stable for pure advection

$$G^*G = 1 + \frac{\Delta t^4}{4}(kV)^4$$

$$|G| = (1+x)^{1/2} \qquad x = \frac{(\Delta t k V)^4}{4}$$

$$|G|^N = (1+x)^{N/2} < e^{Nx/2}$$

$$e^{N\Delta t \frac{x}{2\Delta t}}$$

so $\frac{2\Delta t}{x}$ is ~~an~~ an ~~lower~~ upper bound on the error e-folding time

$$T_{error} < \frac{2\Delta t}{x} = \frac{8\Delta t}{(\Delta t)^4 (kV)^4} = \frac{8}{(\Delta t)^3 (kV)^4}$$

set $V=1$ $k = k_{max}$

$$T_{error} \approx \frac{8}{(\Delta t)^3 (k_{max})^4}$$

but accuracy demands that $\Delta t <<$ shortest timescale $= \frac{1}{k_{max} V}$

$$= \frac{1}{k_{max}} \quad \text{typical}$$

let $\Delta t = \frac{\varepsilon}{k_{max}} \Rightarrow T_{error} = \frac{8}{k_{max}\varepsilon^3}$

this typically has given very long error growth times

e.g. $k_{max} = 32$, $\Delta t = \frac{2}{1000}$ $T_{error} = 953$

$k_{max} = 120$, $\Delta t = \frac{1}{1024}$ $T_{error} \approx 50$

For ideal runs this error can be monitored by following conservation of E and A in 2D
if an ideal run conserves them to better than a fraction of a %, things are OK out to that time.

ii) <u>Dissipative case</u>

ν has stabilizing effect in leading order.

ANALYSIS of the full 4^{th} order growth factor equation indicates that <u>stability</u> is achieved $[|G| < 1]$ for values of $\Delta t = \frac{\varepsilon}{k_{max} V}$ with $\varepsilon \lesssim .3$ or so

For $R = \frac{1}{\nu}$ up to several thousand.

thus for most dissipative cases that we can resolve (in terms of k_d), the codes are stable with the explicit scheme. In a practical sense

ACCURACY $\Longrightarrow$ STABILITY

H. Conservation of "rugged" invariants in collocation (pseudospectral) codes

The arguments leading to conservation of R.I's by the Galerkin method don't hold for pseudospectral algorithms. (ALIASING! in periodic case)

Orszag has given a general criterion for conservation of energy, in terms of projection operators that define the method.

$$\frac{\partial u_N}{\partial t} = H(u_N) \qquad \text{exact} \Rightarrow \frac{\partial}{\partial t}(u,u) = 0$$

energy conservatn

$$\frac{\partial u_N}{\partial t} = P_N H(P_N u_N) \qquad \text{spectral method.}$$

$$\frac{\partial}{\partial t}(u_N, u_N) = (u_N, P_N H(P_N u_N))$$

if P_N is self adjoint $\Rightarrow$ $(P_N u_N, H(P_N u_N)) \equiv 0$

For Navier Stokes flow this implies that, for pseudospectral methods, one must write the NS equatn as

$$\frac{\partial \underset{\sim}{u}}{\partial t} = \underset{\sim}{u} \times (\nabla \times \underset{\sim}{u}) - \nabla p^* + \nu \nabla^2 \underset{\sim}{u}$$

rotation form

$\underset{\sim}{u} \times \underset{\sim}{\omega}$

Let $\mathcal{L}$ be the Laplacian ∇^2 operator $= \mathcal{D} \cdot g$

$\mathcal{D}$ be divergence

g be gradient

(d be $\frac{\partial}{\partial z}$) dont need. (but $d^{+} = -d$.)

then it can be shown that for pseudospectral operators.

$$-\mathcal{D} \text{ is the adjoint of } g^{*}$$

then for

$$\frac{\partial w}{\partial t} = \mathcal{D}(\underline{B}\, j - \underset{\sim}{v}\, w),$$

$$\frac{\partial a}{\partial t} = + v \times B = - v \cdot g\, a.$$

$$w = -\mathcal{L}\psi \qquad g\,\psi = (-v_y, v_x)$$

$$j = -\mathcal{L} a. \qquad g\, a = (-B_y, B_x)$$

Energy

$$\underline{E} = \tfrac{1}{2}(g\psi, g\psi) + \tfrac{1}{2}(ga, ga)$$

$$(g\psi, g\psi) = -(\psi, \mathcal{D} \cdot g\psi) = -(\psi, \mathcal{L}\psi) = -(\psi, w)$$

$$\frac{d}{dt}(\psi, w) = \left(\frac{\partial \psi}{\partial t}, w\right) + \left(\psi, \frac{\partial w}{\partial t}\right) = 2\left(\psi, \frac{\partial w}{\partial t}\right)$$

$$\left(\frac{\partial w}{\partial t}, \psi\right)$$

similarly

$$\frac{1}{2}\frac{d}{dt}(\nabla a, \nabla a) = \left(j, \frac{\partial a}{\partial t}\right)$$

therefore

$$\frac{\partial E}{\partial t} = \left(\psi, \frac{\partial \omega}{\partial t}\right) + \left(j, \frac{\partial a}{\partial t}\right)$$

$$= (\psi, \nabla(\underset{\sim}{B} j - \underset{\sim}{v}\omega)) + (j, -\underset{\sim}{v}\cdot\nabla a)$$

$$= -(\nabla\psi, \underset{\sim}{B} j - \underset{\sim}{v}\omega) + (j, -\underset{\sim}{v}\cdot\nabla a)$$

$$= +\underbrace{(\nabla\psi, \underset{\sim}{v}\omega)}_{0} - (\nabla\psi, \underset{\sim}{B} j) + (j, -v\cdot\nabla a)$$

since $(-v_y, v_x)\cdot \underset{\sim}{v}\omega = 0$

$$-(-v_y B_x, j) + (j, +v_x B_y)$$
$$-(v_x B_y, j) + (j, -v_y B_x)$$

$$= 0$$

A similar proof holds for 3D MHD
the point is that the induction equation, uncurled
must be written as

$$\frac{\partial a}{\partial t} = (\underset{\sim}{v} \times \underset{\sim}{B})_z = -\underset{\sim}{v}\cdot\nabla a.$$

rather than

$$\frac{\partial a}{\partial t} = -\nabla\cdot(\underset{\sim}{v}\, a)$$

when the pseudo spectral nonlinear terms are calculated.
He is conserved by this pseudospectral method
but not A (aliasing!)

III A 2D MHD Turbulence Code and some results

$$\frac{\partial a(k)}{\partial t} = -i\underset{\sim}{k} \cdot \sum_{\underset{\sim}{r+p=k}}' \underset{\sim}{v}(r)\, a(p) + \mu k^2 a(k)$$

or

$$= \sum_{r+p=k} \underset{\sim}{v}(r) \times \underset{\sim}{B}(p) - \mu k^2 a(k)$$

$$\frac{\partial \omega(k)}{\partial t} = i\underset{\sim}{k} \cdot \sum_{\underset{\sim}{r+p=k}}' \underset{\sim}{B}(r)\, j(p) - \underset{\sim}{v}(r)\,\omega(\underset{\sim}{p}) - \nu k^2 \omega(\underset{\sim}{k})$$

$\sum'$ means spectral interpretation of the convolution.

A. Dealiasing in 2D on an $N \times N$ grid.

$$\frac{\partial a}{\partial t}(\underset{\sim}{k}) = \sum_{r+p=k}' u(\underset{\sim}{r})\, w(\underset{\sim}{p}) \equiv H^G(\underset{\sim}{k})$$

use transform to form $u(\underset{\sim}{x})\, w(\underset{\sim}{x})$
and inverse transform
according to our previous results, slightly generalized this gives

$$\begin{aligned} H(\underset{\sim}{k}) = {} & H^G(k_x, k_y) + H^G(k_x+N, k_y) \\ & + H^G(k_x-N, k_y) + H^G(k_x, k_y+N) + H^G(k_x, k_y-N) \\ & + H^G(k_x+N, k_y+N) + H^G(k_x+N, k_y-N) \\ & + H^G(k_x-N, k_y+N) + H^G(k_x-N, k_y-N) \end{aligned}$$

there are 4 'singly aliased' terms
and 4 'double aliased' terms

In principle several shifted grid steps could be taken, however, Orszag and Patterson have shown that the following works:

i) form the 2D shifted grid convolution.

$$H^S(\underset{\sim}{k}) = \sum_{\underset{\sim}{x}(i,j)} U(x_{i+1/2}, y_{j+1/2})\, W(x_{i+1/2}, y_{j+1/2})\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{x}}$$

ii) correct $H(\underset{\sim}{k})$ by forming a linear combination of $H(\underset{\sim}{k})$ and $H^S(\underset{\sim}{k})$

steps i) and ii) eliminate all 'singly-aliased' errors

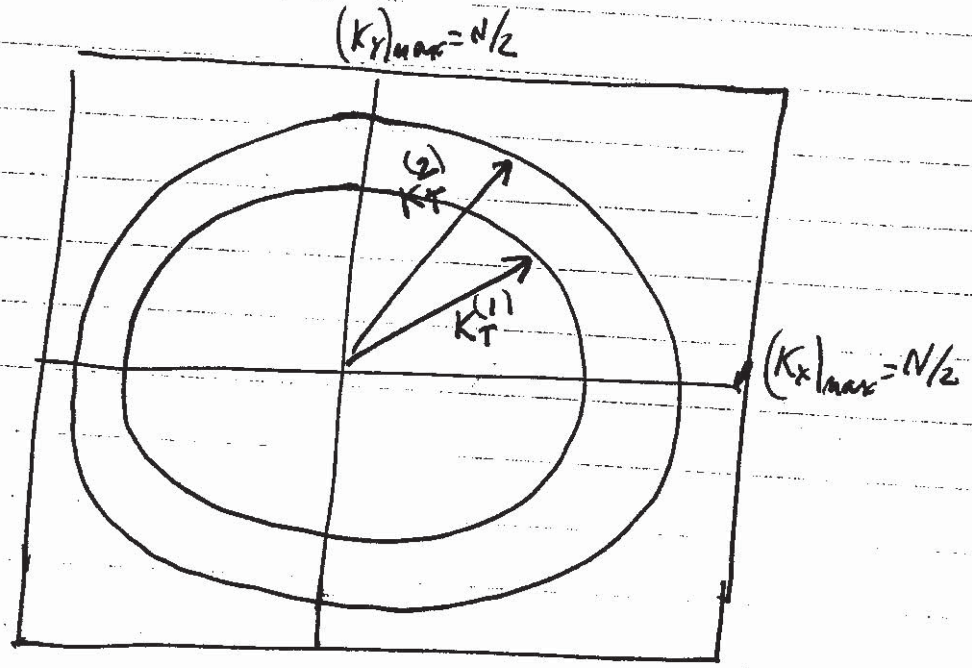
i.e. $$\tfrac{1}{2}\left[H(\underset{\sim}{k}) + e^{-i\pi(k_x+k_y)} H^S(\underset{\sim}{k})\right]$$

$$= H^G(\underset{\sim}{k}) + \text{double aliases}$$

In addition, 'isotropic truncation' is used:

at each half and whole timestep all modes outside a radius K_T are set to zero i.e.

$$a(\underset{\sim}{K}) = 0 \quad \text{for} \quad |\underset{\sim}{K}| > K_T$$



if $K_T = K_T^{(1)} = \frac{2}{3}(K_X)_{max} = \frac{2}{3}\frac{N}{2} = \frac{N}{3}$

then this step removes <u>all</u> aliasing errors

if $K_T = K_T^{(2)} = \sqrt{\frac{8}{9}}\left(\frac{N}{2}\right)$ then this step removes all double aliasing errors, but leaves the single ones.

Therefore

(ii) apply isotropic truncation with $K_T = K_T^{(2)}$ at each half timestep.

$\Longrightarrow$ all aliasing errors are removed.

B. 3D issues, etc.

- The above combination of isotropic truncation (for multiple aliasing errors) and shifted grids (for single aliasing errors) works in 3D as well.

- Pseudospectral will often be used in 3D anyway, for efficiency.

  ? what is the effect of non conservation of H_m by pseudospectral

- How to make use of $\nabla \cdot B = \nabla \cdot V = 0$ to save storage. is this important.

  code size vs code speed.

  memory size vs disk speed.

  execution speed

code timing N^d code. to calculate 1 characteristic time.

$$\frac{1}{\log_2 N} = \underbrace{N}_{\text{time}} \; \underbrace{d}_{\#\ \text{convolutions}} \; \underbrace{dN^{d-1}}_{\#\ \text{1d FFT's}} \; \underbrace{N \log_2 N}_{\text{1d FFT}} = \text{Time.}$$

$$\underbrace{d}_{\text{scaling for \# arrays}} \; \underbrace{N^d}_{\text{each array}} = \text{Size}$$

machine memory limit quickly reached to 3d if machines get faster

C. Aliasing instability, etc.
(Phillips, Roache, etc)

- The "Nonlinear instability" (Phillips) in finite difference algorithms appears to be traceable to aliasing errors. Often they are dealt with by adding dissipation, or high - k filtering..

What we found in Fourier periodic case

pseudosp. = spectral + aliasing errors

aliasing may be stabilized, by writing in correct form, or unstable, if the operators are NOT selfadjoint.

but can stabilize through dissipation.

Never any non conservation of $\underline{E}$ due to aliasing "rugged"

- How can Chebychev pseudospectral be fully or partially de-aliased.

is pseudo sp = spectral + aliasing for Chebychev system ?

- compressible MHD, NS

→ spectral difficult.

$$\rho\left(\frac{\partial v}{\partial t}+v\cdot\nabla v\right) = [\quad]$$

$$\frac{\partial v}{\partial t}+v\cdot\nabla v = \frac{[\quad]}{\rho}$$

Nonlinearities are NOT quadratic! See Ghosh et al

→ there has been some progress for pseudosp. compressible NS
Leorat, Pouquet, Grappin CNRS France.

Nice shocks, Rank. Hug. relations, etc.

SPECTRAL METHODS and MHD TURBULENCE SIMULATIONS

BIBLIOGRAPHY

SPECTRAL METHODS

Patterson and Orszag, Phys Fluids 14, 2538 (1971)

Gottlieb and Orszag, Numerical Analysis of Spectral Methods, SIAM, Philadelphia (1977)

Orszag, Stud. Appl. MATH, 50, 293 (1971)
51, 253 (1972)

Hussaini, Streett and Zang, ICASE Report 172248, NASA/LRC (1983)

Salu and Knorr, J. Comp. Phys. 17, 68 (1975)

Orszag and Israeli, Ann. Rev. FLUID MECH. 6, 281 (1974)

APPLICATIONS

Fyfe and Montgomery, J. Plasma Phys. 16, 181 (1976)

Fyfe, Joyce and Montgomery, J. Plasma Phys 17, 317 (1977)

Fyfe, Montgomery and Joyce, J. Plasma Phys., 17, 369 (1977)

Kraichnan and Montgomery, Rep. Prog. Phys 43, 547 (1980)

Matthaeus and Montgomery, J. Plasma Phys. 25, 11 (1981).

Menneguzzi, Frisch and Pouquet, Phys. Rev. Lett. 47, 1060 (1981)

Matthaeus and Montgomery, Ann. NY Acad. Sci 357, 203 (1980)

Shebalin, Matthaeus and Montgomery, J. Plasma Phys. 29, 525 (1983)

Hossain, Matthaeus and Montgomery, J. Plasma Phys. 30, 479 (1983)

Dahlburg, Montgomery and Matthaeus J. Plasma Phys 34, 1 (1985)

GENERAL

Roache, Computational Fluid Dynamics, Hermosa (1982)

Potter, Computational Physics, John Wiley (1977)

Dahlquist and Bjorck, Numerical Methods, Prentice Hall (1974)