Notes on Chebyshev solution methods for PDEs

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1. Physics

We may cast every type of system we plan on solving into the following abstract form,

$$\mathbf{M}.\frac{\partial \boldsymbol{u}}{\partial t} + \mathbf{L}.\boldsymbol{u} = \boldsymbol{F}(\boldsymbol{u}), \tag{1}$$

The left-hand side operators are linear differential operators of the form

$$\mathbf{M} \;=\; \mathbf{M}_0(z, \boldsymbol{\nabla}_\perp) + \mathbf{M}_1(z, \boldsymbol{\nabla}_\perp)\partial_z \tag{2}$$

$$\mathbf{L} \;=\; \mathbf{L}_0(z, \boldsymbol{\nabla}_\perp) + \mathbf{L}_1(z, \boldsymbol{\nabla}_\perp)\partial_z \tag{3}$$

where z represents a "vertical" or "radial" coordinate and $\boldsymbol{\nabla}_\perp$ represents derivatives in a *horizontally homogenous* perpendicular space attached to each value of z.

We represent eqs. (1)–(3) as first-order operators with respect to z-direction direction differentiation. This implies that $\boldsymbol{u}$ is a state vector containing what people normally regard as the primitive solution to some differential equation and possibly enough of its derivatives to render the system first-order. We can assume without loss of generality that $\boldsymbol{F}(\boldsymbol{u})$ only requires $\boldsymbol{u}(z)$ and $\partial_z \boldsymbol{u}(z)$, but not higher-order derivatives. Otherwise, we could further enlarge phase space.

Critically, by the term *horizontally homogenous* we mean that eq. (1) simplifies by applying a horizontal transform to give as set of K_{max} left-hand-side decoupled differential equations in z-t space,

$$\hat{\mathbf{M}}(\boldsymbol{k}).\frac{\partial \hat{\boldsymbol{u}}_{\boldsymbol{k}}}{\partial t} + \hat{\mathbf{L}}(\boldsymbol{k}).\hat{\boldsymbol{u}}_{\boldsymbol{k}} = \hat{\boldsymbol{F}}(\boldsymbol{k}, \hat{\boldsymbol{u}}_{\boldsymbol{k}}), \tag{4}$$

The right-hand side of eq. (4) generally couples different $\boldsymbol{k}$-modes — we even may find some flexibility on this down the road, e.g., rotating spherical flow where the couplings are very simple, *just saying*. The $\boldsymbol{k}$-diagonal linear operators on the left-hand side of eq. (4) take the form

$$\hat{\mathbf{M}}(\boldsymbol{k}) \;=\; \mathbf{M}_0(z,\boldsymbol{k}) + \mathbf{M}_1(z,\boldsymbol{k})\partial_z \tag{5}$$

$$\hat{\mathbf{L}}(\boldsymbol{k}) \;=\; \mathbf{L}_0(z,\boldsymbol{k}) + \mathbf{L}_1(z,\boldsymbol{k})\partial_z \tag{6}$$

where $\mathbf{M}_{0,1}$, and $\mathbf{L}_{0,1}$ in eqs. (5) & (6) take the exact same form as those in eqs. (2) & (3) with the parameter $\boldsymbol{k}$ repaving $\boldsymbol{\nabla}_\perp$. For Cartesian geometry $\boldsymbol{k} = (k_x, k_y)$. For spherical geometry $\boldsymbol{k} = (l, m)$

The user must input the four matrices $\mathbf{M}_{0,1}$, and $\mathbf{L}_{0,1}$. These matrices, along with the ability to compute the right-hand side $\hat{\boldsymbol{F}}(\boldsymbol{k}, \hat{\boldsymbol{u}})$ fully encode all the physics of the problem independent of the time-stepping scheme and method for representing vertical derivatives.

2. Time-stepping

We define the standard notation

$$\hat{\boldsymbol{u}}^{(T)} \equiv \hat{\boldsymbol{u}}(t + n\Delta t), \quad \hat{\boldsymbol{F}}^{(T)} \equiv \hat{\boldsymbol{F}}(\hat{\boldsymbol{u}}^{(T)}, t + n\Delta t) \tag{7}$$

Of course, the time-step need not remain constant.

Picking a method, any time-derivative scheme takes the general form

$$\frac{\partial \boldsymbol{u}}{\partial t} \;=\; \frac{1}{\Delta t}\left(\alpha_0 \boldsymbol{u}^{(T+1)} + \alpha_1 \boldsymbol{u}^{(T)} + \alpha_2 \boldsymbol{u}^{(T-1)} + \ldots\right) + \mathit{error} \tag{8}$$

Likewise,

$$\hat{\mathbf{L}}.\hat{\boldsymbol{u}} = \hat{\mathbf{L}}.\left(\beta_0 \hat{\boldsymbol{u}}^{(T+1)} + \beta_1 \hat{\boldsymbol{u}}^{(T)} + \beta_2 \hat{\boldsymbol{u}}^{(T-1)} + \ldots\right) + \mathit{error} \tag{9}$$

and

$$\hat{\boldsymbol{F}}(\hat{\boldsymbol{u}}) = \left(\gamma_1 \hat{\boldsymbol{F}}^{(T)} + \gamma_2 \hat{\boldsymbol{F}}^{(T-1)} + \ldots\right) + \mathit{error}. \tag{10}$$

Putting everything together

$$\left(\frac{\alpha_0}{\Delta t}\hat{\mathbf{M}} + \beta_0 \hat{\mathbf{L}}\right).\hat{\boldsymbol{u}}^{(T+1)} \;=\; -\left(\frac{\alpha_1}{\Delta t}\hat{\mathbf{M}} + \beta_1 \hat{\mathbf{L}}\right).\hat{\boldsymbol{u}}^{(T)} + \gamma_1 \hat{\boldsymbol{F}}^{(T)} + \ldots \tag{11}$$

If we define the following quantities

$$\mathbf{A}(z,\boldsymbol{k},\Delta t) \;\equiv\; \frac{\alpha_0}{\Delta t}\hat{\mathbf{M}}_0(z,\boldsymbol{k}) + \beta_0\hat{\mathbf{L}}_0(z,\boldsymbol{k}) \tag{12}$$

$$\mathbf{B}(z,\boldsymbol{k},\Delta t) \;\equiv\; \frac{\alpha_0}{\Delta t}\hat{\mathbf{M}}_1(z,\boldsymbol{k}) + \beta_0\hat{\mathbf{L}}_1(z,\boldsymbol{k}) \tag{13}$$

$$\boldsymbol{f}^{(T)}(z,\boldsymbol{k},T) \;\equiv\; -\left(\frac{\alpha_1}{\Delta t}\hat{\mathbf{M}} + \beta_1\hat{\mathbf{L}}\right).\hat{\boldsymbol{u}}^{(T)} + \gamma_1\hat{\boldsymbol{F}}^{(T)} + \dots \tag{14}$$

then eq. (11) becomes abstracted as solving

$$\mathbf{A}(z).\boldsymbol{u}^{(T+1)}(z) + \mathbf{B}(z).\partial_z\boldsymbol{u}^{(T+1)}(z) \;=\; \boldsymbol{f}^{(T)}(z) \tag{15}$$

for each individual $\boldsymbol{k}$ mode at each time step — subject to boundary conditions of the form

$$\mathbf{c}_{(+1)}.\boldsymbol{u}^{(T+1)}|_{z=+1} + \mathbf{c}_{(-1)}.\boldsymbol{u}^{(T+1)}|_{z=+1} \;=\; \boldsymbol{b}^{(T)}, \tag{16}$$

where $\mathbf{c}_{(\pm1)}$ generally represent time-and-$\boldsymbol{k}$–dependent matrices selecting specific components of $\boldsymbol{u}^{(T+1)}|_{z=\pm1}$, and $\boldsymbol{b}^{(T)}$ represents some possible (linear or nonlinear) boundary forcing – but really it's just a constant vector which may require some complicated computation, just like $\boldsymbol{F}$.

3. Chebyshev scheme

We now focus on solving a z-dependent differential system in the form eqs. (15) & (18). For a start, I simplify the coefficient matrices to z-independent forms. Therefore, consider

$$\mathbf{A}.\boldsymbol{u}(z) + \mathbf{B}.\partial_z\boldsymbol{u}(z) \;=\; \boldsymbol{f}(z) \tag{17}$$

$$\mathbf{c}_{(+1)}.\boldsymbol{u}|_{z=+1} + \mathbf{c}_{(-1)}.\boldsymbol{u}|_{z=+1} \;=\; \boldsymbol{b}, \tag{18}$$

with $\mathbf{A}$, $\mathbf{B}$ representing constant matrices.

We expand the right-hand side and solution in terms of Chebyshev polynomials

$$\boldsymbol{f} \;=\; \frac{\boldsymbol{f}_0}{2} + \sum_{n=1}^{n=N}\boldsymbol{f}_nT_n(z), \tag{19}$$

$$\boldsymbol{u} = \frac{\boldsymbol{u}_0}{2} + \sum_{n=1}^{n=N} \boldsymbol{u}_n T_n(z). \tag{20}$$

Therefore define the combined Chebyshev-space state vector and right-hand side,

$$\boldsymbol{\mathcal{U}} \equiv (\boldsymbol{u}_0, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_N) \tag{21}$$

$$\boldsymbol{\mathcal{F}} \equiv (\boldsymbol{f}_0, \boldsymbol{f}_1, \ldots, \boldsymbol{f}_N) \tag{22}$$

Now define the Chebyshev preconditioned stencil and differential matrices

$$\mathcal{D}_{n,m} \equiv \begin{cases} n & \text{if} \quad m - n = 1 \\ 0 & \text{otherwise} \end{cases} \tag{23}$$

$$\mathcal{S}_{n,m} \equiv \begin{cases} \frac{\text{sign}(n-m+1)}{2} & \text{if} \quad |n - m + 1| = 1 \ \& \ m < N \\ 0 & \text{otherwise} \end{cases} \tag{24}$$

The boundary row matrix encodes evaluating at $z = \pm 1$ in Chebyshev space

$$\mathcal{Q}^{(\pm)}_{n,m} = \begin{cases} \frac{1}{2} & \text{if} \quad n = N \ \& \ m = 0 \\ (\pm 1)^m & \text{if} \quad n = N \ \& \ 0 < m \leq N \\ 0 & \text{otherwise} \end{cases} \tag{25}$$

and finally the last-element vector in Chebyshev space

$$e_{n,N} \equiv \begin{cases} 1 & \text{if} \quad n = N \\ 0 & \text{otherwise} \end{cases} \tag{26}$$

$$\boldsymbol{\mathcal{P}} \equiv \mathcal{S} \otimes \mathbf{A} + \mathcal{D} \otimes \mathbf{B} + \mathcal{Q}^{(+)} \otimes \mathbf{c}_{(+)} + \mathcal{Q}^{(-)} \otimes \mathbf{c}_{(-)} \tag{27}$$

$$\boldsymbol{\mathcal{R}} \equiv [\mathcal{S} \otimes \mathbf{I}] . \boldsymbol{\mathcal{F}} + e_N \otimes \boldsymbol{b}, \tag{28}$$

where $\mathbf{I}$ represents the identity matrix in the same space as $\mathbf{A}$ and $\mathbf{B}$.

It all boils down to SOLVE:

$$\boldsymbol{\mathcal{P}}.\boldsymbol{\mathcal{U}} \;=\; \boldsymbol{\mathcal{R}}, \tag{29}$$

which provides the information needed to compute $\boldsymbol{u}(z)$. Furthermore, we can compute the z-derivatives via

$$\partial_z \boldsymbol{u}(z) \;=\; \mathbf{B}^{-1}.\left[\boldsymbol{f}(z) - \mathbf{A}.\boldsymbol{u}(z)\right]. \tag{30}$$

Recall that the matrix $\mathbf{B}$ is low-dimensional and fundamentally must be non-singular if we want a well-posed system in the first place.

4. Non-constant coefficients

In the case where the matrices $\mathbf{A}$ and $\mathbf{B}$ depend on z then we represent them by a matrix-valued Chebyshev series

$$\mathbf{A}(z) \;=\; \frac{\mathbf{A}_0}{2} + \sum_{p=1}^{P} \mathbf{A}_p T_p(z) \tag{31}$$

$$\mathbf{B}(z) \;=\; \frac{\mathbf{B}_0}{2} + \sum_{p=1}^{P} \mathbf{B}_p T_p(z) \tag{32}$$

Very often $P \ll N$.

We must then define matrices $\mathcal{T}_p$ encoding multiplication by a $T_p(z)$ in Chebyshev-coefficient space,

$$\mathcal{T}_{p;n,m} \;=\; \begin{cases} \frac{1}{2} & \text{if} \quad m = |n \pm p| \\ 0 & \text{otherwise} \end{cases} \tag{33}$$

Then the full matrix to solve becomes

$$\boldsymbol{\mathcal{P}} \;\equiv\; \sum_{p=0}^{P} \left[(\mathcal{T}_p \mathcal{S}) \otimes \mathbf{A}_p + (\mathcal{T}_p \mathcal{D}) \otimes \mathbf{B}_p\right] + \mathcal{Q}^{(\pm)} \otimes \mathbf{c}_{(\pm)} \tag{34}$$

And important note: At this point I'm being a little glib on the definition of $\mathcal{T}_p$. Eq. (33) is correct in a very non-rigourous way. I think we need to weight the entries by the number of degenerate solutions to $m = |n \pm p|$. Furthermore, I haven't worked out how to treat the last few rows and columns — there are unresolved issues with how best to truncate. These issues have answers, and I've worked them out before in the past, I've just lost the details and need to check them again.

5. An example

Consider three-dimensional rotating incompressible flow.

$$\partial_t u - \nu \left(\partial_x^2 + \partial_y^2 + \partial_z^2\right) u - 2\Omega v + \partial_x p \quad = \quad F_x \tag{35}$$

$$\partial_t v - \nu \left(\partial_x^2 + \partial_y^2 + \partial_z^2\right) v + 2\Omega u + \partial_y p \quad = \quad F_y \tag{36}$$

$$\partial_t w - \nu \left(\partial_x^2 + \partial_y^2 + \partial_z^2\right) w + \partial_z p \quad = \quad F_z \tag{37}$$

$$\partial_x u + \partial_y v + \partial_z w \quad = \quad 0 \tag{38}$$

The (F_x, F_y, F_z) represents nonlinear terms and other forcing.

Define:

$$u_z \;\equiv\; \partial_z u, \quad v_z \;\equiv\; \partial_z v, \tag{39}$$

defining a new variable of this type for the z direction is unnecessary since

$$w_z \;\equiv\; \partial_z w = -\partial_x u - \partial_y v \tag{40}$$

Then

$$\boldsymbol{u} \;=\; \begin{pmatrix} u \\ v \\ w \\ p \\ u_z \\ v_z \end{pmatrix}, \quad \boldsymbol{F} \;=\; \begin{pmatrix} F_x \\ F_y \\ F_z \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{41}$$

Now, for example, if

$$F_x \;\propto\; (u\partial_x + v\partial_y + w\partial_z)u \tag{42}$$

then

$$F_x \;\propto\; u\partial_x u + v\partial_y u + w u_z \tag{43}$$

If we know $\boldsymbol{u}$ we can compute $\boldsymbol{F}$ without computing any *vertical* derivatives. Of course horizontal derivatives require using Fourier transforms, and multiplication on grid points requires Chebyshev transforms in our anticipated framework.

No-slip boundary conditions take the form

$$\begin{pmatrix} u|_{z=-1} \\ v|_{z=-1} \\ w|_{z=-1} \\ u|_{z=+1} \\ v|_{z=+1} \\ w|_{z=+1} \end{pmatrix} \;=\; \mathbf{0} \tag{44}$$

Many other possibilities exist. Interesting alternatives could mix variable and their derivatives, or could contain a non-zero (possibly nonlinear) right-hand side to eq. (44). For example, a free surface condition mixes vertical velocity and pressure in a nonlinear manner.

Now in the framework of Section 1 we define $\mathbf{M}_1 = 0$,

$$\mathbf{M}_0 \;=\; \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{45}$$

$$\mathbf{L}_0 = \begin{pmatrix} -\nu\left(\partial_x^2+\partial_y^2\right) & -2\Omega & 0 & \partial_x & 0 & 0 \\ 2\Omega & -\nu\left(\partial_x^2+\partial_y^2\right) & 0 & \partial_y & 0 & 0 \\ 0 & 0 & -\nu\left(\partial_x^2+\partial_y^2\right) & 0 & \nu\partial_x & \nu\partial_y \\ \partial_x & \partial_y & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{46}$$

$$\mathbf{L}_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & -\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & -\nu \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{47}$$

where

$$\mathbf{L} = \mathbf{L}_0 + \mathbf{L}_1\partial_z \tag{48}$$

You can now check that eqs. (35)–(38) are equivalent to

$$\mathbf{M}_0.\partial_t\boldsymbol{u} + (\mathbf{L}_0 + \mathbf{L}_1\partial_z).\boldsymbol{u} = \boldsymbol{F}, \tag{49}$$

Furthermore, for boundary conditions

$$\mathbf{c}_{(+)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{50}$$

$$\mathbf{c}_{(-)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \tag{51}$$

and $\boldsymbol{b} = \mathbf{0}$