

Report from RC LACE stay

Topic: VFE descretisation of NH dynamics of AAA system
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Introduction

The stay was dedicated to cleaning of existing code, phasing the development made on cy36t1 into cy40. I worked together with Petra Smolikova and we cooperated with HIRLAM colleagues from Spain, Alvaro Subias and Juan Simmaro. Concerning code issues we have been cooperating with Karim Yessad from METEO France.

The following topics were covered:

1. definition of eta levels in the maximas of splines
2. definition of knots from the predefined full levels (the splines have maximas close to full levels for computed knots sequence)
3. definition of invertible operators (derivative and integral) (LVFE_FIX_ORDER)
4. implementation of invertible operators into the model (LVFE_GW key) with gw on model full levels
5. implementation of invertible operators into the model (LFE_GW_HALF) with gw on model half levels
6. cleaning if the code and optimization
7. 3D idealized tests (1km resolution ALP domain)
8. 2D idealized tests
9. study of pure VFE definition of laplacian operator (up to now we are obliged to use top boundary condition (TBC) and bottom boundary condition (BBC) in VFE manner)

9. Study of pure VFE definition

The traditional SI resp. ICI scheme are formulated with linear model L^* . This model is traditionally obtained via linearization of nonlinear model M around determined hydrostatically balanced resting background state X^* . The purpose of L^* is purely numerical, in order to stabilize time stepping procedure via semi-implicit treatment of linear part of gravity and acoustic waves. But it was shown (Benard) that such L^* is not optimal for gravity and acoustic waves in spectral models at the same time. The stability condition for gravity waves yields $T^* > T$ and for acoustic waves $T^* < 0$. Therefore Benard proposed to introduce two reference temperature profiles. This stabilized the SI (ICI) time stepping scheme. This showed that the L^* must be formulated with respect to required stability conditions and not with respect to “physically” correct solution.

This leads us to idea that also the boundary conditions in L^* can be freely chosen with respect to stability conditions. The stability of time stepping requires that laplacian term has real and negative eigenvalues (this was not shown yet, but it is the statement consistent with our experience, this probably somehow relates to the fact that the eigenvalues must be purely imaginary as shown later in this report). Up to know we have tested many possible formulations using VFE discretisation without success. The proper eigenvalues were obtained

only when BCs treatment of VFE scheme was replaced by FD treatment (we replaced upper and bottom row in our linear laplacian operator by FD solution). The problem lied in the fact that the laplacian is applied on pressure departure $p - \pi$ in the moded and the natural boundary TBC is therefore $(p - \pi)_{top} = 0$. However, this was found to be the reason for unstable behaviour of our scheme. But this conditions does not need to be satisfied in the linear mode L^* as this is not the model that described the physical solution, but rather L^* is operator to stabilize the time stepping procedure. Therefore we implemented TBC condition $\frac{\partial \pi^*}{\partial \eta} = 0$. The continuous laplacian term is

$$L^*(p - \pi) = \frac{\partial}{\partial \eta} \left(\frac{\pi^{*2}}{m^*} \right) \frac{\partial(p - \pi)}{\partial \eta} + \left(\frac{\pi^*}{m^*} \right)^2 \frac{\partial^2(p - \pi)}{\partial \eta^2}$$

The “new” VFE discretisation of this term gives

$$L^*(p - \pi) = \mathbf{D}_1 \left(\frac{\pi^{*2}}{m^*} \right) \mathbf{D}_1(p - \pi) + \left(\frac{\pi^*}{m^*} \right)^2 \mathbf{DD}(p - \pi)$$

The operators are defined as

| Operator | TBC IN | BBC IN | TBC OUT | BBC OUT |
|--|--|---|---------|---------|
| $\mathbf{D}_1 \left(\frac{\pi^{*2}}{m^*} \right)$ | $\frac{\partial}{\partial \eta} \left(\frac{\pi^{*2}}{m^*} \right)_0 = 0$ | $\left(\frac{\partial}{\partial \eta} \frac{\pi^{*2}}{m^*} \right)_1 = 2\pi_s$ | - | - |
| $\mathbf{D}_1(p - \pi)$ | $\frac{\partial}{\partial \eta} (p - \pi)_0 = 0$ | $\frac{\partial}{\partial \eta} (p - \pi)_1 = 0$ | - | - |
| $\mathbf{DD}(p - \pi)$ | $\frac{\partial}{\partial \eta} (p - \pi)_0 = 0$ | $\frac{\partial}{\partial \eta} (p - \pi)_1 = 0$ | - | - |

The boundary conditions of $\frac{\partial}{\partial \eta} \left(\frac{\pi^{*2}}{m^*} \right)$ term are derived from

$$\frac{\partial}{\partial \eta} \left(\frac{\pi^{*2}}{m^*} \right) = \pi^* \left[2 - \frac{\frac{\partial^2 \pi^*}{\partial \eta^2}}{\left(\frac{\partial \pi^*}{\partial \eta} \right)^2} \right].$$

This fully depends on the choice of A and B as $\pi(\eta) = A(\eta) + B(\eta)\pi_s$. Due to simplicity (and due to fact that we are free to do that) in linear model L^* we assume $\frac{\partial^2 \pi^*}{\partial \eta^2} = 0$ on BCs.

This leads to boundary conditions $\frac{\partial}{\partial \eta} \left(\frac{\pi^{*2}}{m^*} \right)_0 = 0$ and $\left(\frac{\partial}{\partial \eta} \frac{\pi^{*2}}{m^*} \right)_1 = 2\pi_s$. One shall realize that

the BBC is not of great importance at this place as the term is multiplied by factor $\frac{\partial}{\partial \eta}(p - \pi)_1 = 0$. What matters are the eigenvalues of linear laplacian operator as they determine the eigenvalues of the whole linear model.

The BC condition of terms $\frac{\partial}{\partial \eta}(p - \pi) = 0$ and $\frac{\partial^2(p - \pi)}{\partial \eta^2}$ must be consistent. The BBC is determined with respect to stability. The BBC is determined from linearized vertical momentum equation

$$\left(\frac{\partial w}{\partial t} \right)_1 = \frac{g}{m^*} \left(\frac{\partial(p - \pi)}{\partial \eta} \right)_1$$

At the surface the material boundary conditions is used $gw_1 = v_1 \nabla \phi$. But there is flat orography background $\nabla \phi = 0$ and therefore the vertical velocity at the surface is always $w_1 = 0$. This leads to BBC

$$\left(\frac{\partial(p - \pi)}{\partial \eta} \right)_1 = 0.$$

However, one must realize that BCs in the nonlinear model M must satisfy the physical conditions as our time numerical scheme converges towards it as time step converges to zero. Therefore the vertical momentum equation in nonlinear model M is discretized as

$$\frac{dw}{dt} = \frac{g}{m} \mathbf{D}_2 \frac{\partial(p - \pi)}{\partial \eta}$$

With BCs summarized in the following table

| Operator | TBC IN | BBC IN | TBC OUT | BBC OUT |
|--|-------------------|--|---------|---------|
| $\mathbf{D}_2 \frac{\partial(p - \pi)}{\partial \eta}$ | $(p - \pi)_0 = 0$ | $\left(\frac{\partial}{\partial \eta}(p - \pi) \right)_1 = 0$ | - | - |

The BBC is consistent with condition $(p - \pi)_L = (p - \pi)_U$ used in FD discretisation. But the VFE formulation is more elegant, as the interpolating spline $(p - \pi)(\eta) = \sum a_i B_i(\eta)$ is constant just in the infinitesimal distance from model surface, rather than in the whole layer between surface and the first bottom full model level. But other reasonable BBC can be applied at this place. The VFE allows us to determine that shape of interpolating spline with BBC. This must be determined with respect to accuracy and the stability of our model.

One must realize that the TBC is not arbitrary, because our model top lies at $\pi = 0$. This is very high in the atmosphere (vacuum) at the places where the pressure is not well defined. So there is undefined the vertical acceleration of air parcel. Therefore we assume $p = 0$.

Consideration about the construction of linear model

We have the linear problem:

$$\frac{\partial X}{\partial t} = L^* X$$

The prototype of time stepping used in NWP models is

$$\frac{X^+ - X^0}{dt} = L^* \left(\frac{X^+ + X^0}{2} \right)$$

Assuming $X(t+dt, \eta) = \omega X(t, \eta)$ and having $X(t, \eta)$ eigenmode of L^* such that $L^* X = \lambda X$ yields

$$X(t, \eta) \left(\frac{\omega - 1}{dt} \right) = \lambda X(t, \eta) \left(\frac{\omega + 1}{2} \right)$$

With complex eigenvector $\lambda = \lambda_r + i\lambda_i$ and complex coefficient ω . For any non-zero eigenvector this gives

$$\left(\frac{\omega - 1}{dt} \right) = \lambda \left(\frac{\omega + 1}{2} \right)$$

We require the time stepping to be unconditionally stable. The condition $|\lambda| < 1$ gives the restriction on eigenvalues of L^*

$$\lambda_r = -i\lambda_i.$$

This means that the time stepping procedure is stable only when the eigenvalues of L^* are purely imaginary. Therefore our L^* operator must satisfy this condition.

We have the possibility to change the time stepping procedure having L^* with complex eigenvalues but this is out of scope of our work.

Boundary conditions of VFE operator

The following procedure is applied on input vector $\{f\}$ during our implementation of VFE scheme.

- the vector of **data points** $\{\eta_j, f(\eta_j)\}$ sampled at L levels is projected into the FE space in the form $S(\eta) = \{\eta, f(\eta)\} = \sum_{i=1}^L \{\hat{\eta}_i, \hat{f}_i\} B_i^f(\eta)$. The points $\{\hat{\eta}_i, \hat{f}_i\}$ are called **control point** and

the continuous spline curve $S(\boldsymbol{\eta})$ lies within the convex hull of control points. The spline curve is either

- a. interpolating – passing through data points $\{\boldsymbol{\eta}_j, f_j\}$. The control points can be computed from L equations $\{\boldsymbol{\eta}_j, f(\boldsymbol{\eta}_j)\} = \sum_{i=1}^L \{\hat{\boldsymbol{\eta}}_i, \hat{f}_i\} B_i^f(\boldsymbol{\eta}_j)$. This can be written in matrix form as $\{\boldsymbol{\eta}, f\} = \mathbf{T}^f \{\hat{\boldsymbol{\eta}}, \hat{f}\}$ with transformation matrix \mathbf{T}^f with elements $T_{i,j}^f = B_i^f(\boldsymbol{\eta}_j)$. Comment: notice that $\boldsymbol{\eta}_j = \hat{\boldsymbol{\eta}}_i$ only if $B_i^f(\boldsymbol{\eta}_j) = 1$. This holds for linear Chapeau functions only.
- b. approximating – minimizing some property with respect to some measure between approximating curve and data points. For example in variation diminishing approximation method it is valid $\{\hat{\boldsymbol{\eta}}, \hat{f}_i\} = \{\boldsymbol{\eta}, f(\boldsymbol{\eta}_i)\}$. The control points in this case are equal to data points. But here the choice of $\boldsymbol{\eta}$ depends on the construction of basis functions B_i^f as $\boldsymbol{\eta}_i = \frac{\sum_{k=i}^{i+c} t_k}{c}$ with $\{t\}$ is vector of knots used to construct B_i^f splines of order c.

It is important to realize that at this point the control of boundary properties of $S(\boldsymbol{\eta})$ is simple. We can freely add points at our boundaries and to require $S(\boldsymbol{\eta})$ to fulfill them. For example we can require $\frac{\partial f}{\partial \boldsymbol{\eta}} = 0$ at model surface $\boldsymbol{\eta}=1$. So we simply add one additional point to the vector of data points (the values of the additional values will be {1,0}) and we require the interpolating property at this point

$$\{1,0\} = \sum_{i=1}^{L+1} \{\hat{\boldsymbol{\eta}}_i, \hat{f}_i\} \frac{\partial B_i^f(1)}{\partial \boldsymbol{\eta}}.$$

This we can do anywhere inside our model domain, but practically we do apply this kind of conditions just at the boundaries. This kind of condition are further mentioned as **the explicit BCs**.

2. second step is the projection of control points from 1. into control points of $g(f)$ operator coefficients of the equation

$$g(f(\boldsymbol{\eta})) = \gamma(\boldsymbol{\eta}) \quad \Rightarrow \quad \sum_i \hat{f}_i g(B_i^f) = \sum_i \hat{g}_i B_i^g$$

This projection is performed with Galerkin method with proper chosen weighting functions $\{w(\boldsymbol{\eta})\}$

$$\int_0^1 \sum_i \hat{f}_i g(B_i^f) w_j d\boldsymbol{\eta} = \int_0^1 \sum_i \hat{g}_i B_i^g w_j d\boldsymbol{\eta}$$

or in the matrix form

$$\mathbf{S}\{\hat{f}\} = \mathbf{M}\{\hat{g}\}.$$

With so called stiff matrix \mathbf{S} with elements $S_{i,j} = \int_0^1 g(B_i^f) w_j d\boldsymbol{\eta}$ and mass matrix \mathbf{M} with elements $M_{i,j} = \int_0^1 B_i^g w_j d\boldsymbol{\eta}$.

The first vector of data points $\{\hat{\eta}\}$ is not the subject to projection as it represents the vertical coordinate.

In order to determine the values $\{\hat{g}\}$ the mass matrix \mathbf{M} must be inverted. Due to well posedness of mass matrix we define weighting functions as

$$\{w\} = \{B^g\}.$$

The mass matrix \mathbf{M} is then symmetrix and positive definite and therefore easily invertable. This is thanks to positiveness of splines.

3. evaluation of operator values at given data points

Having coefficients $\{\hat{g}\}$ of $\gamma(\eta) = \sum_i \hat{g}_i B_i^g$ we can evaluate the curve anywhere within our domain. At this point we assume that the curve $\gamma(\eta)$ is interpolating inside whole domain. This can be written in matrix form as $\{\gamma\} = \mathbf{T}^g \{\hat{g}\}$ with transformation matrix \mathbf{T}^g with elements $T_{i,j}^g = B_i^g(\eta_j)$.

As the $\gamma(\eta)$ is solution of the Galerking procedure, there is no method we could ensure its BCs explicitly as in the point 1.. Therefore we have to implement so called implicit conditions build directly into basis function $\{B^g\}$.

For example if $\gamma(\eta)=0$ at model top (the typical property of integral operator when we integrate from model top) then all basis functions must satisfy that property $\{B^g\}_0=0$. This inclusion of BCs into the spline basis we call **the implicit BCs**.

Comment: When the basis functions $\{B^g\}$ of $\gamma(\eta)$ can be expressed as a linear combination of basis functions $\{B^f\}$ of $f(\eta)$, than the Galerking method is not necessary as the solution already lies inside the space of allowed functions and no projection is needed. For example: if function is represented by spline of order C and the derivative is represented by the the spline of order C-1, than the Galerking method gives exactly the same solution as analytical evaluation of derivative of function spline curve. This property is crucial when we want to formulate invertible integral and derivative operator.

Invertible VFE operators

Here the invertible operators is called the couple of derivative operator \mathbf{D} and integral operator \mathbf{I} (numerically formulated with VFE approach) which satisfy

$$I_d = \mathbf{I} \cdot \mathbf{D} = \mathbf{D} \cdot \mathbf{I}$$

Following previous text we can write integral operator as $\mathbf{I} = \mathbf{T}_i^g \cdot \mathbf{M}_i^{-1} \cdot \mathbf{S}_i \cdot \mathbf{T}_i^{f^{-1}}$ and the derivative operator as $\mathbf{D} = \mathbf{T}_d^g \cdot \mathbf{M}_d^{-1} \cdot \mathbf{S}_d \cdot \mathbf{T}_d^{f^{-1}}$.

The invertible operators exists under following conditions:

- we use the same sequence of numbers $\{t\}$ to construct the knots of $\{B^g\}$ and $\{B^f\}$. The knots can differ in multiplicity only,
- additive constant is removed from the process by imposing appropriate condition. The integral value is 0 at the **starting point of integration** (so additive constant is 0 automatically). The derivated function is 0 at the starting point of integration as well. This is simply achieved by subtraction of constant from derivated function (this does not change the result as the derivative of constant is zero). **We have to realize that starting point of integration is arbitrary within our domain. This property can be achieved by setting the starting point of integration to be the full level and at the knot at the same time. We require c+1 multiplicity of that knot (??? To be tested).**

Comment: we can chose as a starting point of integration the point somewhere in the middle of our domain where the results reach high accuracy and where the additive constant of derivative is known a priori.. The starting point of integration is not important for the integral is it can be moved to model top resp. bottom simply by subtraction of top resp. bottom value.

- the order of $\{B^g\}$ for derivative operator must be one order lower than the order of derived function $\{B^f\}$,
- the order of $\{B^g\}$ for integral operator must be one order larger than the order of derived function $\{B^f\}$,
- the transformations matrices in both operators must be the same in reverse order. This gives $\mathbf{T}_i^g = \mathbf{T}_d^f$ and $\mathbf{T}_d^g = \mathbf{T}_i^f$. This gives that the explicit BCs and implicit BCs must be consistent for both operators but reverse and the basis splines must satisfy $\{B\}_i^g = \{B\}_d^f$ and $\{B\}_d^g = \{B\}_i^f$.

Definition of A and B on full levels with invertible operators

Having invertible derivative and integral operator we can easily and consistently introduce new definition of full level A and B. It is important to stress that here we consider full levels also the material boundaries. This is necessary for proper BCs treatment.

We use following procedure

1. we define freely A and B on full levels as (for example average on half levels).

$$\begin{aligned} A_0 &= B_0 = 0 \\ A_i &= 0.5(A_{\tilde{i}} + A_{\tilde{i}-1}) \quad B_i = 0.5(B_{\tilde{i}} + B_{\tilde{i}-1}) \\ A_{L+1} &= 0 \quad B_{L+1} = 1 \end{aligned}$$

2. we compute pressure depth of model layers using following expression applied on A and B on full levels

$$\delta\pi_i = \{\mathbf{D}\pi\}_i = \{\mathbf{D}A\}_i + \{\mathbf{D}B\}_i \pi_s$$

3. taking into account the invertibility of operators this expression satisfy for any reasonable choice of full level A and B

$$\{\mathbf{I.D}A\}_{L+1} = 0 \quad \{\mathbf{I.D.B}\}_{L+1} = 1$$

This expression represents integral of depths of A and B over the whole model domain. Due to invertibility and correct BCs this is hold exactly. There is no need to introduce any iterative procedure as is now the case in the ECMWF piece of code for HY model.

We need BCs on both model material boundaries in order to treat BCs correctly. Implicit TBC at model top when we choose the starting point of integration and the explicit BBC (no other way to impose $B_1 = 1$). This requirement leads to operators acting on L+1 levels and the invertibility is fulfilled with respect to L+1 vectors. However, this would require in the model to add one more additional level at model surface. **The complexity of such requirement implementation is enormous and we abandon this direction.**

Definition of knots and model full levels and half levels

Appendix: notation

SI – semi-implicit scheme

ICI – iterative centered implicit scheme

X^+ - model state at $t+dt$

X^0 - model state at t

X^m - model state at $t+dt/2$ (extrapolated quantity)

X^- - model state at $t-dt$

$\{f\}$ - vector of values or functions

TBC – top boundary condition

BBC – bottom boundary condition