Dynamical PC scheme for NH kernel of AAA models

Part 1: Theoretical considerations and implementation of LSETTLS residual extrapolation into LPC_CHEAP scheme.

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***Abstract*—We present simplified derivation of second-order accurate SL schemes in the sense of [1]. We further generalize approach to residual computed from explicit guess. We also analyze shortly the stability of proposed set of schemes. We show that schemes proposed in this note are theoretically much more stable than standard SETTLS or NESC scheme for SL advection problem.**

I. Introduction

In [1] is described the complete set of SL schemes that are second-order accurate in time, using information at time levels t and $t-\Delta t$ and spatial location at arrival and departure point. Such approach is effective in NWP, because there is only one location to interpolate per grid point and time step. However, [1] did not include in its analysis the possibility to use also values at time instant $t+\Delta t$ at arrival point. This is possible when $t+\Delta t$ quantities are computed using explicit scheme with SETTLS approach. This ensures that explicit guess is second order accurate in time as shown by [1] and that ensured that whole scheme is second order accurate.

We present in part 1 simplified approach sufficient to reproduce results in [1]. We reproduce results that the most stable scheme from proposed schemes is SETTLS scheme. We further include $t+\Delta t$ quantities into analysed SL approach. We show in part 3 that the schemes with explicit $t+\Delta t$ are even more stable than SETTLS scheme. We hope this approach will work in the context of full spectral NWP model as there are some limitation of practical implementation.

The implementation in spectral model like ALADIN did not allow to compute effectively horizontal derivatives of prognostic quantities of explicit guess. This requires going into spectral space and back and this is something we want to avoid due to effectivity of the scheme. Therefore NL residual at explicit guess can not be fully evaluated at $t+\Delta t$. We are using prognostic quantites at explicit $t+\Delta t$ and their derivatives at t. This is the same approach used in ND4SYS=2 to compute evolution of X-term.

II. Simplified approach to formulate second-order accurate SL scheme in time

We want to solve equation $\frac{df(t,x)}{dt} = N(t,x)$. We use explicit centered scheme and SL approach.

We have adopted traditional SL notation in which the supersript '-','m','0' and '+' stand for the $t-\Delta t$, $t-\frac{\Delta t}{2}$, t and $t+\Delta t$ time levels respectively ($t+\Delta t$ being the forecasted one) and the subscripts 'D','M' and 'A' stand for the departure $(x-\Delta x)$, middle $(x-\frac{\Delta x}{2})$ and arrival (x) points of the SL trajectory.

The second-order time centered scheme is

$$\frac{f_A^+ - f_D^0}{\Delta t} = N_M^m + O\left(\Delta t^2\right). \tag{1}$$

We have to approximate N_M^m. We look for second order approximation in the form

$$a_1 N_A^0 + a_2 N_A^- + a_3 N_D^0 + a_4 N_D^- = N_M^m + O\left(\Delta t^2\right) \tag{2}$$

We use polynomial series expansion around the state N_A^0. We assume advection by constant wind U. The expansion gives

$$\begin{aligned} N(t+a\Delta t, x+b\Delta x) = N(t+a\Delta t, \Delta x + bU\Delta t) = \\ N_A^0 + \Delta t\left(a\frac{\partial N}{\partial t} + Ub\frac{\partial N}{\partial x}\right)_A^0 + O\left(\Delta t^2\right). \end{aligned} \tag{3}$$

We expand all quantities in Eq. 2. We obtain

$$\begin{aligned} N_A^0(a_1+a_2+a_3+a_4-1)+ \\ \frac{1}{2}\Delta t U\left(\frac{\partial N}{\partial x}\right)_A^0(-2a_3-2a_4+1)- \\ \frac{1}{2}\Delta t\left(\frac{\partial N}{\partial t}\right)_A^0(2a_2+2a_4+1) = O\left(\Delta t^2\right) \end{aligned} \tag{4}$$

We require all terms at LHS to dissapear. This leads to the same solution as in [1], $a_1 = \frac{3}{4}-\alpha$, $a_2 = \alpha - \frac{1}{4}$, $a_3 = \alpha + \frac{3}{4}$ and $a_4 = -\frac{1}{4} - \alpha$.

This means that for any α we approximate N_M^n with second-order of accuracy in time.

The LSETTLS scheme is obtained for $\alpha = \frac{1}{4}$.

When we introduce control parameter β into LSETTLS scheme we can write it as departure from LNESC scheme

$$\frac{f_A^+ - f_D^0}{\Delta t} = \frac{1}{2}\left(N_A^0 + N_D^0\right) + \frac{\beta}{2}\left(N_D^0 - N_D^-\right). \tag{5}$$

Setting $\beta = 0$ we obtain LNESC scheme that is $O\left(\Delta t\right)$.

III. Second-order accurate SL scheme in time with explicit guess at $t + \Delta t$

We assume we have available some guess $\tilde{f}_A^+$. For example explicit guess computed using LSETTLS scheme

$$\tilde{f}_A^+ = f_D^0 + \frac{\Delta t}{2}\left(N_A^0 + N_D^0\right) + \Delta t \frac{1}{2}\left(N_D^0 - N_D^-\right). \quad (6)$$

We can compute $\tilde{N}_A^+$ and we could search for approximation of N_M^m using

$$e_1 N_A^0 + e_2 \tilde{N}_A^+ + e_3 N_D^0 + e_4 N_D^- = N_M^m + O\left(\Delta t^2\right). \quad (7)$$

We replaced N_A^- by explicit guess N_A^+ in Eq. 7. Following procedure described in previous section we obtain solution $e_1 = \frac{1}{4} + \alpha$, $e_2 = \frac{1}{4} - \alpha$, $e_3 = \alpha + \frac{3}{4}$ and $e_4 = -\frac{1}{4} - \alpha$.

The final scheme

$$\frac{f_A^+ - f_D^0}{\Delta t} = (\frac{1}{4} + \alpha) N_A^0 + (\frac{1}{4} - \alpha)\tilde{N}_A^+ + (\alpha + \frac{3}{4}) N_D^0 + (-\frac{1}{4} - \alpha) N_D^- \quad (8)$$

is second order accurate for any value of α.

IV. Analysis of stability of SI SETTLS/NESC scheme

Analysis of stability is performed as in [2]. We analyse the stability of system

$$\frac{df(t,x)}{dt} = N(t,x) = (\lambda + i\omega)\, f(t,x). \quad (9)$$

We consider only $\lambda \leq 0$ to avoid solutions that are exponentially growing already in analytical form.

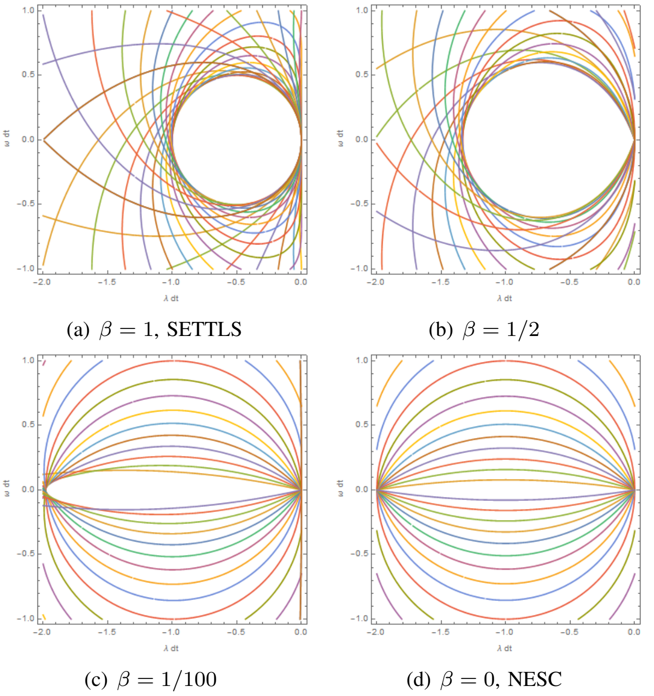
We analyze the stability of single fourier component $f(n\Delta t, j\Delta x) = A^n e^{ikj\Delta x}$ advected using constant wind U. When we introduce CFL $\theta = Uk\Delta t$ we could write fourier components as $f(n\Delta t, j\Delta x) = A^n e^{ij\theta}$.

We analyze the stability of time stepping described by Eq. 5. We substitute N by our prototype Eq. 9. We obtain quadratic equation for evolution of amplitude A

$$-2A^2 e^{i\theta} + A\left[2 + \left(1 + \beta + e^{i\theta}\right)(\lambda + i\omega)\right] - \beta(\lambda + i\omega) = 0 \quad (10)$$

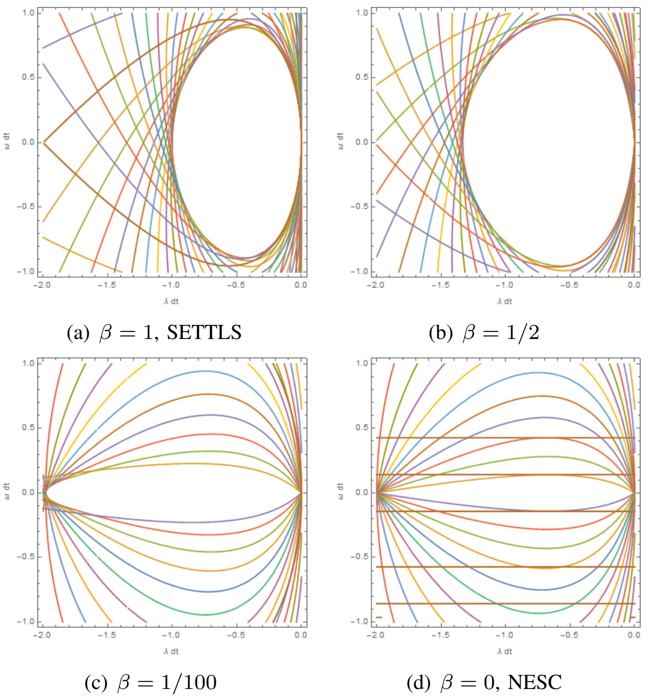
Since equation is periodic with respect to θ (because expression $e^{i\theta}$ represents circle in complex plane) we limit ourself to domain $\theta \in (-\pi, \pi]$. We plot contour line $A = 1$ for each θ in the set of values $[-9\pi/10, -8\pi/10, \ldots, 0, \ldots, \pi]$. The domain of stabilty in $(\omega\Delta t, \lambda\Delta t)$ plane for four values of β scheme is plotted on Fig. 5. The stability of SETTLS is identical to one presented at Fig. 1 in [2]. We enlarge stability in $\lambda\Delta t$ domain with decreasing β.

We know that NESC scheme is stable for all values of λ in the case of $\omega = 0$ only. However, this is not practical problem, because SI scheme is applied to stabilize time stepping with respect to processes represented by ω in our system. We introduce linear model $L(t,x) = i\delta\omega f(t,x)$. Here δ is tuning parameter. Setting $\delta = 1$ the wave modes are treated in fully implicit manner. The time stepping than follows traditional SI SL scheme written with nonlinear residual $R(t,x) =$



(a) $\beta = 1$, SETTLS (b) $\beta = 1/2$ (c) $\beta = 1/100$ (d) $\beta = 0$, NESC

Figure 1: Stability of SETTLS/NESC scheme for various values of β.



(a) $\beta = 1$, SETTLS (b) $\beta = 1/2$ (c) $\beta = 1/100$ (d) $\beta = 0$, NESC

Figure 2: Same as on Fig. 5, but we implement semi-implicit scheme with $\delta = 3/4$.

$N(t,x) - L(t,x) = [\lambda + i(1-\delta)\omega]\, f(t,x)$ as

$$\frac{f_A^+ - f_D^0}{\Delta t} = \frac{1}{2}\left(R_A^0 + R_D^0\right) + \frac{\beta}{2}\left(R_D^0 - R_D^-\right) + \frac{1}{2}\left(L_A^+ + L_D^0\right). \tag{11}$$

When we again analyze the stability of single fourier mode, the equation 10 now takes the form

$$\begin{aligned} & iA^2 e^{i\theta}(\delta\omega\Delta t + 2i) \\ & + A\left[-i\omega\Delta t\left[\tau_1(\beta + e^{i\theta}) - 1\right] + \lambda\Delta t\left(\beta + e^{i\theta} + 1\right) + 2\right] \\ & -\beta\left[\lambda\Delta t - i\tau_1\omega\Delta t\right] = 0 \end{aligned} \tag{12}$$

The stability for $\delta = 3/4$ (major part of waves is treated implicitly) is shown on Fig. 2. We see stabilisation effect in direction along $\omega\Delta t$ axes.

V. Analysis of stability of SI scheme with explicit guess

We add SI treatment to equation 8. This yields

$$\begin{aligned} \frac{f_A^+ - f_D^0}{\Delta t} &= (\frac{1}{4} + \alpha)R_A^0 + (\frac{1}{4} - \alpha)\tilde{R}_A^+ \\ &+ (\alpha + \frac{3}{4})R_D^0 + (-\frac{1}{4} - \alpha)R_D^- \\ &+ \frac{1}{2}\left(L_A^+ + L_D^0\right). \end{aligned} \tag{13}$$

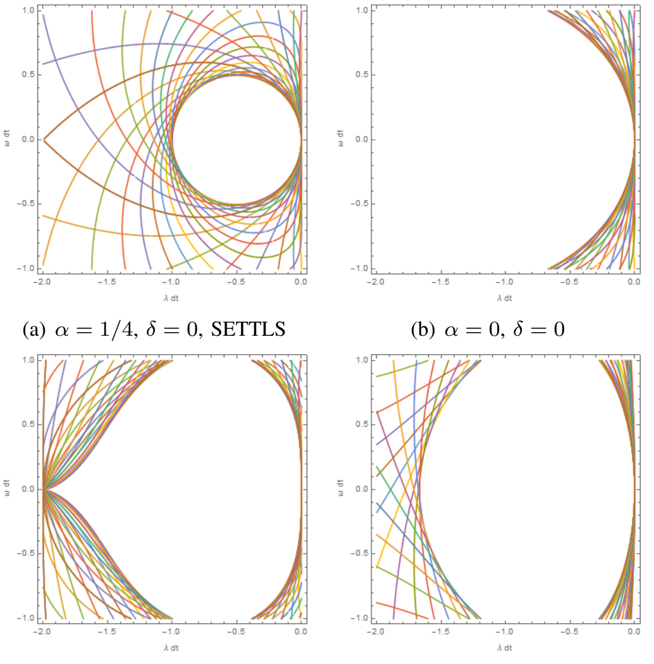
The relation for amplitude A in this case is very complex (we do not put it into report). We present the results for various values of α and δ on Fig. 3. The region of stability of SL scheme is greatly enhanced by Fig. 3. The stability regions is enlarged in λ, so the scheme has similar property as NESC scheme, but the stability in ω directions if preserved.

The problem arises in implementation of proposed scheme in spectral model. Horizontal derivatives are needed to evalues $\tilde{R}^+$. However, they are not availaible at the end of SL advection (LAPINEB). We want to avoid going to spectral space and back, because in such case we have PC scheme option that is sufficient to stabilize model. We would like our scheme to remain semi-implicit, therefore we evaluate $\tilde{R}^+ = \tilde{R}^+(\tilde{f}+, \vec{\nabla} f^0)$. Such scheme is apparently not second order accurate, but the framework of our analysis do not allow us to study this aspect.

Practical implementation of the scheme is very simple under LPC_CHEAP and LSETTLS scheme, beceuse the division of linear and nonlinear terms allow effective computation of explicit guess $\tilde{f}^+$.

VI. Analysis of stability of PC scheme with SETTLS/NESC predictor

PC scheme requires solution of SI solver in both steps predictor and corrector. Therefore is more expensive than the



(a) $\alpha = 1/4$, $\delta = 0$, SETTLS (b) $\alpha = 0$, $\delta = 0$

(c) $\alpha = -1/4$, $\delta = 0$ (d) $\alpha = 1/10$, $\delta = 3/4$

Figure 3: Stability of scheme with $\tilde{N}{+}_A$ term for various values of α.

schemes mentioned in previous paragraphs. Nevertheless, it is used in operational practice of NH model as it is robust and stable. (PC scheme belongs to class of schemes called linear multistep method class Adams-Moulton methods).

The predictor scheme is performed using SETTLS/NESC scheme as

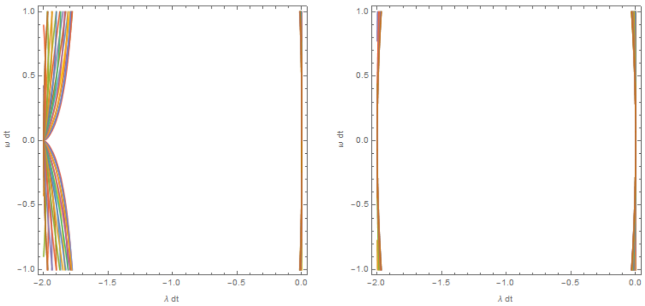
$$\begin{aligned} \frac{f_A^{+(0)} - f_D^0}{\Delta t} =& \frac{1}{2}\left(R_A^0 + R_D^0\right) + \frac{\beta}{2}\left(R_D^0 - R_D^-\right) \\ &+ \frac{1}{2}\left(L_A^{+(0)} + L_D^0\right), \end{aligned} \tag{14}$$

and corrector is

$$\frac{\tilde{f}_A^{+(n)} - f_D^0}{\Delta t} = \frac{1}{2}\left(R_A^{+(n-1)} + R_D^0\right) + \frac{1}{2}\left(L_A^{+(n)} + L_D^0\right). \tag{15}$$

The notation " $+(n)$" represents state at $t + \Delta t$ after n-th corrector step. In the model n is represented by variable NSITER.

We analyzed the stability for $\delta = 3/4$ with respect to β parameter. The results are on Fig. 4. We confirmed that PC scheme is very stable and robust. However, we know that PC scheme with SETTLS in predictor is unstable in NH model simulation in some situation. We know that in such situations using NESC scheme will stabilize time stepping. It seems that the source of instability is not in the SL treatment studied in this report, but rather some other process sensitive to time stepping treatment.



(a) $\beta = 1$, SETTLS predictor, NSITER=1 (b) $\beta = 0$, NESC predictor, NSITER=1

Figure 4: Stability of PC for $\delta = 3/4$.

VII. Implementation of PC scheme in model ALADIN

The PC scheme is implemented exactly as described by equations 14 and 15. We have further choice to iterate also trajectories. They are computed during predictor as

$$\frac{\vec{r}_A - \vec{r}_D^{(0)}}{\Delta t} = \frac{1}{2}\left(\vec{v}_A^0 + \vec{v}_D^0\right) + \frac{\beta}{2}\left(\vec{v}^0 - \vec{v}^-\right)_D^{(0)}, \tag{16}$$

and during n-th corrector as

$$\frac{\vec{r}_A - \vec{r}_D^{(n)}}{\Delta t} = \frac{1}{2}\vec{v}_A^{+(n-1)} + \frac{1}{2}\vec{v}_D^{(n)}. \tag{17}$$

Tracectory search algorithm is divided into horizontal and vertical part in the model (see LAVENT). Extrapolation in horizontal part of 16 is controlled by (LSETTLST, LNESCT) keys and vertical part by (LSETTLSV, LNESCV) keys.

It was found that recomputation of trajectories during corrector has detrimental effect on model simulation. Also the CPU costs of such scheme is higher because we have to re-interpolate all quantites at D point every corrector.

Therefore, the ”cheaper” PC scheme scheme was introduced [3] and [4] (LPC_CHEAP). Idea of this scheme is to compute trajectories and carry out interpolation during predictor only. All neccessary quantites evaluated at D points are stored in buffer (see LAPINEB) and used during corrector step. All computations during corrector are perfomed at A points and there is no need for interpolations.

It can be derived from 15 that the quantity needed during corrector at D point is

$$BC_D = \left[x^0 + \frac{\Delta t}{2}R^0 + \frac{\Delta t}{2}L^0\right]_D = \left[x^0 + \frac{\Delta t}{2}N^0\right]_D \tag{18}$$

The quantity must be precomputed during predictor step and store in buffer.

However, we see from eq. 14 that during predictor we compute at D point quantity

$$BS_D = BC_D + \left[\frac{\beta\Delta t}{2}\left(R^0 - R^-\right)\right]_D \tag{19}$$

When $\beta = 0$ (LNESC scheme) than $BS_D = BC_D$. It means that quantity interpolated at D point during predictor is exactly the same is one needed during corrector. When $\beta > 0$ than we have to interpolate quantity $\left[\frac{\beta\Delta t}{2}\left(R^0 - R^-\right)\right]_D$ independently during predictor.

The cheap PC scheme is further complicated when LGWADV is turned on, because N is formulated using different set of prognostic variables than L. Therefore we can not mix them and they have to be separated. We see from eq. 18 that it is independent of L, therefore only relevant part that have to be separated is term with β

$$BP_D = \left[\frac{\beta\Delta t}{2}\left(N^0 - N^-\right)\right]_D + \left[-\frac{\beta\Delta t}{2}\left(L^0 - L^-\right)\right]_D. \tag{20}$$

VIII. Technical implementation of SETTLS with PC_CHEAP

Implementation of SETTLS scheme with LPC_CHEAP requires 4 interpolation buffers for each predicted quantity during predictor step. The names of SL pointers under LATTEX and relevant quantities in them are listed in Table 1. Only quantity needed to be saved after interpolations during predictor is GMV9 buffer in LAPINEB.

Final point buffers remains unchanged and they are independent of extrapolation method and PC scheme version.

The scheme is designed for HY and NH model (HY not tested). Variables in Table 2 are mandatory.

All other consistencies imposed by setup must be fullfilled.

Modified routines with short explanation are in Table 3.

IX. Evaluation of SETTLS PC_CHEAP scheme

We evaluated scheme using Straka test case from [5].

X. Conclusion

We have analyzed the stability of SETTLS/NESC scheme applied on 1D horizontal advection problem. We know from practical experiments that NESC scheme is stable in wider ranges of situations, than SETTLS scheme, but less accurate. We shown in analysis that the reason is probably better control of processes with exponentially decaying character.

We proposed modification of SETTLS scheme in a way that we include explicit guess into evaluation at RHS, whole still keeping $O\left(\Delta t^2\right)$ character of overall scheme. We compared the stability properties of our scheme against results published by [2]. The proposed scheme is theoretically more stable

PB1 pointer	quantity	usage	routine	quantity under lapineb
MSLB1X9_NL	$\lambda \frac{\Delta t}{2}\left(M^t - M^{t-\Delta t}\right)$	SETTLS predictor	lattex_dnt/lattes	GMV9_NL/C9_NL
MSLB1X9_SI	$\lambda \frac{\Delta t}{2}\left(L^t - L^{t-\Delta t}\right)$	SETTLS predictor	lanhsib	GMV9_SI/C9_SI
MSLB1X0	$\frac{\Delta t}{2} M^t$	SETTLS/NESC predictor/corrector	lattex_dnt/lattes	GMV9/C9
MSLB1X9	x^t	SETTLS/NESC predictor/corrector	lattex_dnt/lattes	GMV9/C9

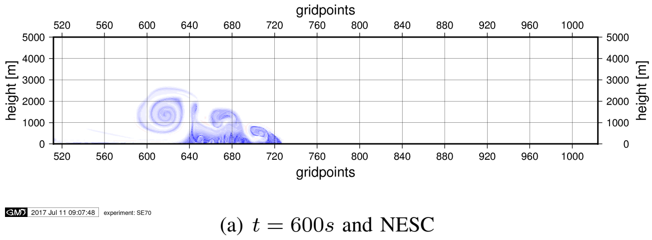
Table I: SL buffers pointers and their content during predictor for LPC_CHEAP scheme

namelist	variable	value
NAMDYNA	LSETTLS	TRUE
NAMDYNA	LPC_CHEAP	TRUE
NAMDYN	N[X]LAG	3

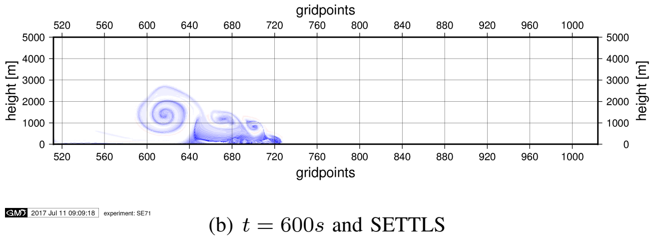
Table II: Namelist parameter for LPC_CHEAP with LSETTLS extrapolation during predictor

routine	modification
ptrslb1.F90	Introduction of pointers MSLB1[x]9_NL
suslb.F90	Initialisation of MSLB1[x]9_NL pointers
lattex.F90	Interface of PB1 buffer to LATTEX_DNT routine
lattex_dnt.F90	SL buffers filled according Table 1; ZEXTRA represents β parameter
lattes.F90	SL buffers filled according Table 1; ZEXTRA represents β parameter
lanhsib.F90	linear part of equation 20; ZEXTRA represents β parameter
lapineb.F90	Interface to LARCINB and LARCINHB; Saving of interpolated buffers into PC_CHEAP buffer during predictor, restoring buffers during corrector; Contruction of RHS from partially interpolated quantities from Table 1
larcinb.F90	Linear interpolation of 3D buffers
larcinhb.F90	Linear interpolation of 3D buffers

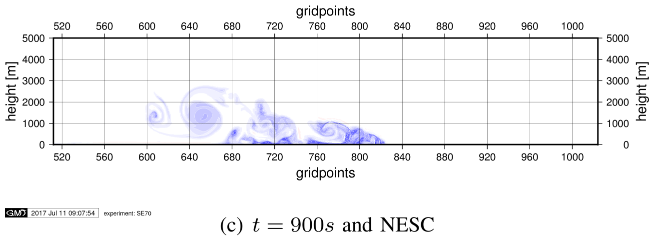
Table III: Modifications in order to implement LSETTLS extrapolation and LPC_CHEAP scheme.



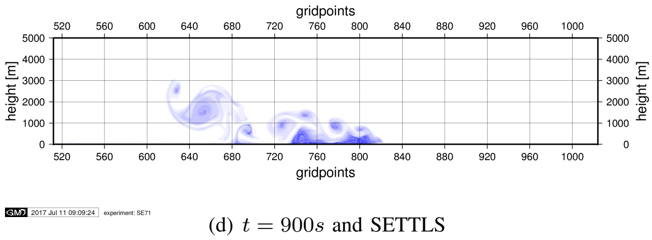
(a) $t = 600s$ and NESC



(b) $t = 600s$ and SETTLS



(c) $t = 900s$ and NESC



(d) $t = 900s$ and SETTLS

Figure 5: Density flow simulation after 600s and 900s. Simulations are performed with $\Delta t = 3s$ and with no diffusion.

and more accurate that NESC scheme. However, the spectral character of our model does not allow us to keep it fully second-order accurate. This aspects must be studied after full implementation of proposed scheme into model ALADIN.

Proposed time stepping is stable with respect to SL advection process. This does not ensure the stability of scheme in vertical direction as published by [6] and [7]. This remain to be studied.

We have implemented SETTLS extrapolation of nonlinear residual terms in LPC_CHEAP. This allow us to control smoothly stability of time stepping via dynamical control of β paramater. This must be done in near future.

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