



# Design of a Runge-Kutta based time-stepping algorithm

# for the NEMO ocean model

Nicolas Ducousso

Florian Lemarié, Gurvan Madec, Laurent Debreu

NEMO solves the non-linear, hydrostatic, primitive equations

since the 80's :

- finite-difference approach
- C-grid staggering on the horizontal, Lorenz-grid staggering on the vertical
- Leapfrog time stepping + Robert-Asselin time filtering -> LFRA scheme

more recently :

- non-linear free-surface, with z\* (and z tilde) vertical coordinates
- fast free surface dynamics treated with a mode-splitting algorithm
- high-order (possibly non linear and adaptive implicit) advection schemes

# Context



#### revise the time-stepping algorithm to improve the model stability/accuracy/efficiency

LFRA alternatives : AB3 (Durran), LF-AM3 Pred-Cor (Shchepetkin McWilliams), one step, forward-in-time, Runge-Kutta family (Hundsdorfer, Wicker Skamarock)...

RK3 scheme (Wicker Skamarock, 2002) has been favored in several NWP models :

- accurate,
- low storage,
- good stability properties for centered and upwind-biased advection,
- allow a stable time-splitting procedure.

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#### in the following, I investigate the relevancy of RK3 for use in an OGCM

- the analysis framework : normal mode decomposition
- von Neumann linear stability analysis of time-stepping schemes
  - Shallow Water equations
  - Hydrostatic Primitive equations with mode-splitting algorithm
- an idealized numerical experiment

Starting from the inviscid, adiabatic, hydrostatic primitive equations, in a 2d (x,z) plane, linearized about a resting state, and in absence of rotation :



$$\begin{cases} \partial_t u + \frac{1}{\rho_0} \partial_x p &= 0\\ \partial_z p &= -\rho g\\ \partial_x u + \partial_z w &= 0\\ \partial_t \rho + w \frac{d\overline{\rho}}{dz} &= 0 \end{cases}$$

$$w(z = 0) = \partial_t \eta$$
$$p(z = 0) = \rho_0 g \eta$$
$$w(z = -H) = 0$$

The solution can be decomposed using the vertical normal modes

(Gill 1982, Demange et al. 2019)

$$\begin{cases} u(x,z,t) &= \sum_{q=0}^{\infty} u_q(x,t) M_q(z) \\ p(x,z,t) &= g\rho_0 \sum_{q=0}^{\infty} h_q(x,t) M_q(z) \end{cases}$$

$$\begin{aligned} \rho(x,z,t) &= -\rho_0 \sum_{q=0}^{\infty} h_q(x,t) \frac{dM_q}{dz}(z) \\ w(x,z,t) &= -\sum_{q=0}^{\infty} \partial_x u_q(x,t) \int_{-H}^{z} M_q(s) ds \\ \eta(x,t) &= \sum_{q=0}^{\infty} h_q(x,t) M_q(0) \end{aligned}$$

The vertical modes are the eigenfunctions of the Sturm-Liouville problem :

$$\begin{cases} \Lambda M_q(z) &= c_q^{-2} M_q(z) \text{ with } \Lambda = -\frac{d}{dz} \left( N^{-2} \frac{d}{dz} \right) \\ \frac{dM_q}{dz}(z=0) &= -\frac{N^2(0)}{g} M_q(0) \\ \frac{dM_q}{dz}(z=-H) &= 0 \end{cases}$$

All vertical modes are depth dependent, including the barotropic/external mode :

with 
$$N^2 = \text{cste}$$
,  

$$\begin{cases}
c_0 = \alpha_0 \sqrt{gH}, \text{ with } \alpha_0 = 1 + \frac{\varepsilon}{6} + \mathcal{O}(\varepsilon^2) \\
M_0(z) = 1 - \varepsilon \left[ \frac{1}{2} \left( \frac{z}{H} \right)^2 + \left( \frac{z}{H} \right) + \frac{1}{3} \right] + \mathcal{O}(\varepsilon^2) \quad \varepsilon = \frac{N^2 H}{g} = \mathcal{O}(10^{-2} - 10^{-4})
\end{cases}$$

The vertical modes are orthonormal w.r.t. the scalar product  $\langle f,g
angle=rac{1}{H}\int_{-H}^{0}fg\,dz$ 

$$u_q = \langle u, M_q \rangle, \ h_q = \frac{1}{\rho_0 g} \langle p, M_q \rangle$$

$$\begin{cases} \partial_t u_q + g \,\partial_x h_q &= 0\\ \\ \partial_t h_q + \frac{c_q^2}{g} \partial_x u_q &= 0 \end{cases}$$

$$\begin{cases} \partial_t \tilde{h} + c \,\partial_x u &= 0\\ \partial_t u + c \,\partial_x \tilde{h} &= 0 \end{cases} \qquad \tilde{h} = \frac{g}{c} \,h \\ \end{cases}$$
von Neumann analysis : 
$$\begin{aligned} \tilde{h}(t) \, e^{ikx}\\ u(t) \, e^{ikx} &\longrightarrow \begin{cases} \partial_t \tilde{h} + c \, i \, k \, u &= 0\\ \partial_t u + c \, i \, k \, \tilde{h} &= 0 \end{aligned}$$

$$\begin{cases} \partial_t h + c \partial_x u &= 0\\ \partial_t u + c \partial_x \tilde{h} &= 0 \end{cases} \qquad \tilde{h} = \frac{g}{c} h$$
  
von Neumann analysis : 
$$\begin{array}{c} \tilde{h}(t) \, e^{ikx}\\ u(t) \, e^{ikx} \end{array} \longrightarrow \begin{cases} \partial_t \tilde{h} + c \, i \, k \, u &= 0\\ \partial_t u + c \, i \, k \, \tilde{h} &= 0 \end{cases}$$

LFRA scheme with Brown-Campana pressure averaging :

$$\begin{cases} \tilde{h}^{n+1,*} &= \tilde{h}^{n-1} - 2\Delta t \, c \, i \, k \, u^{n,*} \\ u^{n+1,*} &= u^{n-1} - 2\Delta t \, c \, i \, k \, ((1-2\gamma)\tilde{h}^{n,*} + \gamma(\tilde{h}^{n+1,*} + \tilde{h}^{n-1})) \\ \tilde{h}^n &= (1-2\epsilon)\tilde{h}^{n,*} + \epsilon(\tilde{h}^{n+1,*} + \tilde{h}^{n-1}) \\ u^n &= (1-2\epsilon)u^{n,*} + \epsilon(u^{n+1,*} + u^{n-1}) \end{cases}$$

3-time-level scheme, with a single rhs evaluation per time step

$$\begin{cases} \partial_t \tilde{h} + c \,\partial_x u &= 0\\ \partial_t u + c \,\partial_x \tilde{h} &= 0 \end{cases} \qquad \tilde{h} = \frac{g}{c} \,h$$
  
von Neumann analysis : 
$$\begin{aligned} \tilde{h}(t) \, e^{ikx}\\ u(t) \, e^{ikx} & \longrightarrow \end{aligned} \qquad \begin{cases} \partial_t \tilde{h} + c \, i \, k \, u &= 0\\ \partial_t u + c \, i \, k \, \tilde{h} &= 0 \end{aligned}$$

RK3 scheme (Wicker Skamarock, 2002) with Forward-Backward feedback :

$$\begin{cases} \tilde{h}^{n+1/3} &= \tilde{h}^n - \frac{1}{3} \Delta t \, c \, i \, k \, u^n \\ u^{n+1/3} &= u^n - \frac{1}{3} \Delta t \, c \, i \, k \, \tilde{h}^n \\ \tilde{h}^{n+1/2} &= \tilde{h}^n - \frac{1}{2} \Delta t \, c \, i \, k \, u^{n+1/3} \\ u^{n+1/2} &= u^n - \frac{1}{2} \Delta t \, c \, i \, k \, \tilde{h}^{n+1/3} \\ \tilde{h}^{n+1} &= \tilde{h}^n - \Delta t \, c \, i \, k \, u^{n+1/2} \\ u^{n+1} &= u^n - \Delta t \, c \, i \, k \, ((1-2\gamma)) \tilde{h}^{n+1/2} + \gamma (\tilde{h}^{n+1} + \tilde{h}^n)) \end{cases}$$

2-time-level scheme, with 3 rhs evaluations per time step

with  $\mu = c\,k\,\Delta t$ ,

LFRA+BC scheme :

$$\begin{pmatrix} \tilde{h}^{n+1,*} \\ u^{n+1,*} \\ \tilde{h}^{n} \\ u^{n} \end{pmatrix} = \begin{bmatrix} A & B \\ \epsilon A + (1-2\epsilon)I_2 & \epsilon B + \epsilon I_2 \end{bmatrix} \begin{pmatrix} \tilde{h}^{n,*} \\ u^{n,*} \\ \tilde{h}^{n-1} \\ u^{n-1} \end{pmatrix} \qquad A = \begin{bmatrix} 0 & -2i\mu \\ -2i\mu(1-2\gamma) & -4\gamma\mu^2 \end{bmatrix}$$

RK3+FB scheme :

$$\begin{pmatrix} \tilde{h}^{n+1} \\ u^{n+1} \end{pmatrix} = \left[ A + B * \left( I + \frac{1}{2}C * \left( I + \frac{1}{3}C \right) \right) \right] \begin{pmatrix} \tilde{h}^n \\ u^n \end{pmatrix}$$

$$A = \begin{bmatrix} 1 & 0 \\ -2i\gamma\mu & 1 \end{bmatrix}$$
$$B = \begin{bmatrix} 0 & -i\mu \\ -i\mu(1-2\gamma) & -\gamma\mu^2 \end{bmatrix}$$
$$C = \begin{bmatrix} 0 & -i\mu \\ -i\mu & 0 \end{bmatrix}$$

with  $\mu = c \, k \, \Delta t$ ,

LFRA+BC scheme :

$$\begin{pmatrix} \tilde{h}^{n+1,*} \\ u^{n+1,*} \\ \tilde{h}^{n} \\ u^{n} \end{pmatrix} = \begin{bmatrix} A & B \\ \epsilon A + (1-2\epsilon)I_2 & \epsilon B + \epsilon I_2 \end{bmatrix} \begin{pmatrix} \tilde{h}^{n,*} \\ u^{n,*} \\ \tilde{h}^{n-1} \\ u^{n-1} \end{pmatrix} \qquad A = \begin{bmatrix} 0 & -2i\mu \\ -2i\mu(1-2\gamma) & -4\gamma\mu^2 \end{bmatrix}$$

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$$C = \begin{bmatrix} 0 & -i\mu \\ -i\mu & 0 \end{bmatrix}$$

Compute eigenvalues  $\lambda^{\pm}(\mu)$  and compare with  $e^{\pm i\mu}$ :

$$E^{amp} = \frac{|\lambda^{\pm}(\mu)|}{|e^{\pm i\mu}|} = |\lambda^{\pm}(\mu)|, \quad E^{phase} = \frac{Arg(\lambda^{\pm}(\mu))}{Arg(e^{\pm i\mu})}$$

### 2 - Linear stability analysis : Shallow Water Equations



- both schemes dissipates and accelerates the gravity waves,
- BC and FB feedback extend the schemes stability : +53% and +22%,
- BC improves Leapfrog accuracy at all scales,
- FB feedback improves RK3 phase error but increases dissipation at small scales.

$$\begin{cases} \partial_t \tilde{h} + u_0 \,\partial_x \tilde{h} + c \,\partial_x u &= 0\\ \partial_t u + u_0 \,\partial_x u + c \,\partial_x \tilde{h} &= 0 \end{cases}$$
  
von Neumann analysis : 
$$\begin{array}{l} \tilde{h}(t) \,e^{ikx}\\ u(t) \,e^{ikx} \end{array} \longrightarrow \begin{cases} \partial_t \tilde{h} + u_0 \,i \,k \,\tilde{h} + c \,i \,k \,u &= 0\\ \partial_t u + u_0 \,i \,k \,u + c \,i \,k \,\tilde{h} &= 0 \end{cases}$$

$$\begin{cases} \partial_t h + u_0 \,\partial_x h + c \,\partial_x u &= 0\\ \partial_t u + u_0 \,\partial_x u + c \,\partial_x \tilde{h} &= 0 \end{cases}$$
von Neumann analysis :  $\begin{array}{l} \tilde{h}(t) \,e^{ikx} \\ u(t) \,e^{ikx} \end{array} \longrightarrow \begin{cases} \partial_t \tilde{h} + u_0 \,i \,k \,\tilde{h} + c \,i \,k \,u &= 0\\ \partial_t u + u_0 \,i \,k \,u + c \,i \,k \,\tilde{h} &= 0 \end{cases}$ 

Apply LFRA+BC and RK3+FB schemes,

Write in matrix form, which now depends on  $\mu_{gw} = c \, k \, \Delta t, \ \mu_{adv} = u_0 \, k \, \Delta t$ 

Compute eigenvalues  $\lambda^{\pm}(\mu_{gw},\mu_{adv})$  and compare with  $e^{-i(\mu_{adv}\mp\mu_{gw})}$ 



- for pure GW, we recover previous results with BC and FB feedback at play,
- the pure advection has stability properties identical to pure GW without BC and FB feedback,
- in between, smooth transition

$$\begin{cases} \partial_t \tilde{h}_{i-\frac{1}{2}} + u_0 \mathcal{A}[\tilde{h}]_{i-\frac{1}{2}} + c \mathcal{G}[u]_{i-\frac{1}{2}} &= 0 \\ \partial_t u_i + u_0 \mathcal{A}[u]_i + c \mathcal{G}[\tilde{h}]_i &= 0 \end{cases} \xrightarrow{h_{i-\frac{1}{2}}} \begin{pmatrix} h_{i+\frac{1}{2}} \\ 0 \\ 0 \\ u_{i-1} \\ u_i \\ u_i \\ u_{i+1} \\ u_i \\ u_{i+1} \\ u_$$

von Neumann analysis :



$$\begin{split} \mathcal{S}(\mathcal{G}^{C2}) &= 2i\sin(\theta/2) \\ \mathcal{S}(\mathcal{A}^{C2}) &= i\sin\theta \\ \mathcal{S}(\mathcal{A}^{C4}) &= i(8\sin\theta - \sin 2\theta)/6 \\ \mathcal{S}(\mathcal{A}^{UP3}) &= i(8\sin\theta - \sin 2\theta)/6 + 8\sin(\theta/2)^4/6 \\ \mathcal{S}(\mathcal{A}^{UP3}) &= i(8\sin\theta - \sin 2\theta)/6 + 8\sin(\theta/2)^4/6 \\ \mathcal{S}(\mathcal{A}^{UP5}) &= i(\sin 3\theta - 9\sin 2\theta + 45\sin\theta)/30 - (\cos 3\theta - 6\cos 2\theta + 15\cos\theta - 10)/30 \end{split}$$

$$\begin{cases} \partial_t \tilde{h}_{i-\frac{1}{2}} + u_0 \mathcal{A}[\tilde{h}]_{i-\frac{1}{2}} + c \mathcal{G}[u]_{i-\frac{1}{2}} &= 0 \\ \partial_t u_i + u_0 \mathcal{A}[u]_i + c \mathcal{G}[\tilde{h}]_i &= 0 \end{cases} \xrightarrow{\begin{array}{c} h_{i-\frac{1}{2}} & h_{i+\frac{1}{2}} \\ 0 & 0 & 0 & 0 \\ u_{i-1} & u_i & u_{i+1} \end{array}}$$

von Neumann analysis :



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Apply LFRA+BC and RK3+FB schemes, write in matrix form, compute  $\lambda^{\pm}(\theta, \mu_{gw}, \mu_{adv})$ 

### 2 - Linear stability analysis : Shallow Water Equations



- for pure GW, the stability limit is half the limit of the semi-discrete analysis,
- the stability of GW and advection is very sensitive to advection scheme :
  - for both LFRA and RK3, the use of C4 decreases the stability limit w.r.t C2,
  - for LFRA, the stability limit with Split-UP3 and Split-UP5 is even smaller,
  - for RK3, there is a marked 'overshoot' of stability with UP3 and UP5.

Usual practice in split ocean models : do not integrate the true barotropic mode but

$$\begin{cases} \partial_t \eta + H \partial_x \overline{u} = 0 \\ \partial_t \overline{u} + g \partial_x \eta = -\frac{1}{\rho_0} \partial_x \left( \frac{1}{H} \int_{-H}^0 p_h \, dz \right) \end{cases}$$

- the red term is a "slow" term absent from the normal mode analysis,
- in practice, this term is kept frozen during the barotropic integration,
- but it contains fast contributions -> source of instability for the barotropic integration
- barotropic/baroclinic corrections have to be done to ensure their compatibility
- dissipation within the barotropic mode is necessary to stabilize the integration
- dissipation can be introduced through averaging filter or dissipative time stepping

## 3 - Linear stability analysis : Hydrostatic Primitive Equations

NEMO LFRA-based mode-splitting algorithm (cf NEMO Book)







### RK3-based mode-splitting algorithm : 3rd stage coupled



Demange etal. 2019 proposed a framework to study the stability of mode-splitting algorithms

- express in terms of normal modes the components of the splitting algorithm
- build the step-multiplier matrix for each vertical mode

$$\begin{pmatrix} h_q \\ u_q \end{pmatrix}^{n+1} = A_q^{3d} \begin{pmatrix} h_q \\ u_q \end{pmatrix}^n + C_q \sum_p V_p \left( A_p^{2d} - A_p^{3d} \right) \begin{pmatrix} h_p \\ u_p \end{pmatrix}^n$$

Demange etal. 2019 proposed a framework to study the stability of mode-splitting algorithms

- express in terms of normal modes the components of the splitting algorithm
- build the step-multiplier matrix for each vertical mode
- restricting attention to the barotropic and 1st baroclinic modes

$$\begin{pmatrix} h_0 \\ u_0 \\ h_1 \\ u_1 \end{pmatrix}^{n+1} = \begin{bmatrix} A_0^{3d} + C_0 V_0 \left( A_0^{2d} - A_0^{3d} \right) & C_0 V_1 \left( A_1^{2d} - A_1^{3d} \right) \\ C_1 V_0 \left( A_0^{2d} - A_0^{3d} \right) & A_1^{3d} + C_1 V_1 \left( A_1^{2d} - A_1^{3d} \right) \end{bmatrix} \begin{pmatrix} h_0 \\ u_0 \\ h_1 \\ u_1 \end{pmatrix}^n$$

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- compute the eigenvalues for the split-RK3 :
  - with mode-splitting at the 1st stage,
  - correction at n+1/3 with transport at n,
  - and the 2d integration being integrated without dispersion errors but the dissipation of the dissipative Forward-Backward scheme (cf Demange etal. 2019)

### 3 - Linear stability analysis : Hydrostatic Primitive Equations



the baroclinic time step has not to be reduced from the stability limit of the RK3 scheme



$$N = 2.10-3 \text{ s-1}$$
  
 $H = 4000 \text{ m}$   
 $g = 9.81 \text{ m.s-2}$   
 $c0/c1 = 77.8$ 

4 - An idealized test-case





- the stability analysis of the fully discrete combined GW-advection problem confirms that RK3+FB is an attractive alternative to LFRA,
- the stability analysis of the mode-splitting algorithm indicates that a dissipative 2d integration scheme is able to stabilise the 1st-stage coupled split-RK3 prototype,
- first numerical experiments with the 1st-stage coupled split-RK3 prototype show benefits in term of accuracy/stability w.r.t the split-LFRA