Understanding the rational approximation of the exponential integrator (REXI)

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This document serves as the basis for implementing the rational approximation of the exponential integrator (REXI). Here, we purely focus on the linear part of the shallow-water equations (SWE) and show the different steps to approximate solving this linear part with an exponential integrator. This paper mainly summarises previous work on REXI.

1 Problem formulation

We use the advective formulation of the SWE with a full linearization with perturbation (see [1]) with $U := (h, u, v)^T$, yielding

$$L(U) := \begin{pmatrix} & H\delta_x & H\delta_y \\ g\delta_x & & -f \\ g\delta_y & f & \end{pmatrix} U$$

Here, we neglect all non-linear terms, assume only small perturbations (hence negligible ones) around the average surface height and negligible non-linear terms.

Then, the time evolution of the PDE with the subscript t denoting the derivative in time is given by

$$U_t := L(U).$$

We continue writing the linear operator in matrix-style L and applying L on U as $L.U$.

$$U_t := L.U$$

It is further worth noting, that this system describes an oscillatory system, hence the operator L has imaginary eigenvalues.

2 Exponential integrator

Linear systems of equations are well known to be solvable with exponential integrators for arbitrary time step sizes via

$$U(t) := e^{Lt} U(0),$$

see e.g. [5]. However, this is typically quite expensive to compute and analytic solutions only exist for some simplified system of equations, see e.g. [1] for f-plane shallow-water equations. These exponential integrators can be approximated with rational functions and this paper is on giving insight into this approximation.

3 Underlying idea of rational approximation

Terry et. al. developed a rational approximation of the exponential integrator, see [2]. First, we like to get more insight into it with a one-dimensional formulation before applying REXI to a rational approximation of a linear operator. Our main target is to find an approximation of an operator with an *exponential shape*, in our case e^{ix}, which (in one-dimension) is given by a function $f(x)$. We will end up in an approximation given by the following rational approximation:

$$e^{ix} \approx \sum_{n=-N}^{N} \frac{\beta_n}{ix - \alpha_n}$$

with complex coefficients α_n and β_n.

3.1 Step A) Approximation of solution space

First, we assume that we can use Gaussian curves as basis functions for our approximation and they are somehow naturally related to this problem (Gaussians are given by exponential functions). So first, we find an approximation of one of our underlying Gaussian basis function

$$\psi_s(x) := (4\pi)^{-\frac{1}{2}} e^{-x^2/(4s^2)}$$

In this formulation, s can be interpreted as the horizontal "stretching" of the basis function. Note the similarities to the Gaussian distribution, but by dropping certain parts of the vertical scaling as it is required for probability distributions. We can now approximate our function $f(x)$ with a superposition of basis functions $\psi_s(x)$ by

$$f(x) \approx \sum_{m=-M}^{M} b_m \psi_s(x + ms)$$

with M controling the interval of approximation (~size of "domain of interest") and s the accuracy of integration (~resolution in "domain of interest"). The s

value depends on the max. frequency of the oscillations generated by the linear operator. To compute the coefficients b_m, we rewrite the previous equation in Fourier space with

$$\frac{\hat{f}(\xi)}{\hat{\psi}_h(\xi)} := \sum_{m:=\infty}^{\infty} b_m e^{2\pi i m h \xi},$$

see [2], page 11. We can rearrange this equation which allows us to directly compute the desired coefficients

$$b_m := h \int_{-\frac{1}{2h}}^{\frac{1}{2h}} e^{-2\pi i m h \xi} \frac{\hat{f}(\xi)}{\hat{\psi}_h(\xi)} d\xi.$$

Since we are only interested in approximating $f(x) := e^{ix}$, we can simplify the equation by using the response in frequency space $\hat{f}(\xi) := \delta(\xi - \frac{1}{2\pi})$:

$$b_m := h\, e^{-2\pi i m h \frac{1}{2\pi}} \frac{\hat{f}(\frac{1}{2\pi})}{\hat{\psi}_h(\frac{1}{2\pi})} = h\, e^{-imh} \hat{\psi_h}(\frac{1}{2\pi})^{-1}.$$

We finally require to compute $\hat{\psi_h}(\xi)$ which we derive in the following part:

$$\hat{\psi_h}(\xi) := \int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi}} e^{-\left(\frac{x}{2h}\right)^2} e^{-2\pi i x \xi} dx$$

$$= \frac{1}{\sqrt{4\pi}} \int_{-\infty}^{\infty} e^{-\left(\left(\frac{x}{2h}\right)^2 + 2\pi i x \xi + (2h\pi i \xi)^2 - (2h\pi i \xi)^2\right)} dx$$

$$= \frac{1}{\sqrt{4\pi}} e^{-(2h\pi\xi)^2} \int_{-\infty}^{\infty} e^{-\left(\frac{x}{2h} + 2h\pi i \xi\right)^2} dx$$

$$= \frac{1}{\sqrt{4\pi}} e^{-(2h\pi\xi)^2} \int_{-\infty}^{\infty} e^{-\left(\frac{x}{2h}\right)^2} dx$$

Then, evaluting the integral yields $\int_{-\infty}^{\infty} e^{-\left(\frac{x}{2h}\right)^2} dx = h\sqrt{4\pi}$ and specialising on the case $\xi := \frac{1}{2\pi}$, we get

$$\hat{\psi_h}(\xi) := \frac{1}{\sqrt{4\pi}} e^{-(2h\pi\frac{1}{2\pi})^2} h\sqrt{4\pi} = h\, e^{-h^2}.$$

Finally, one can obtain the equation

$$b_m := h\, e^{-imh} \frac{1}{h\, e^{-h^2}} = e^{-imh} e^{h^2}$$

to compute the coefficients b_m for $f(x) := e^{ix}$.

3.2 Step B) Approximation of basis function

The second step is the approximation of the basis function $\psi_s(x)$ itself with a rational approximation, see [6]. Our basis function is given by

$$\psi_s(x) := (4\pi)^{-\frac{1}{2}} e^{-x^2/(4s^2)}$$

and a close-to-optimal approximation of $\psi_1(x)$ with a sum of rational functions is given by

$$\psi_1(x) \approx Re\left(\sum_{l=-L}^{L} \frac{a_l}{ix + (\mu + i\,l)}\right)$$

with the μ and a_l given in [6], Table 1. We can generalise this approximation to arbitrary choosen s via

$$\psi_s(x) \approx Re\left(\sum_{l=-L}^{L} \frac{a_l}{i\frac{x}{s} + (\mu + i\,l)}\right)$$

3.3 Step C) Approximation of the approximation

We then combine the approximation (B) of the approximation (A), yielding

$$f(x) \approx \sum_{m=-M}^{M} c_m \psi_s(x + ms) = \sum_{m=-M}^{M} b_m Re\left(\sum_{l=-L}^{L} \frac{a_l}{i\frac{x+ms}{s} + (\mu + i\,l)}\right)$$

$$= \sum_{m=-M}^{M} b_m Re\left(\sum_{l=-L}^{L} \frac{a_l}{ix + s(\mu + i(m+l))}\right).$$

We further like to simplify this equation and we observe, that for $n := n+l$, the denominator is equal. We can hence express parts of the denomiator in terms of $n := n + l$ by

$$\alpha_n := s(\mu + in).$$

Now, we merge the b_m and a_l coefficients and first have a look at the b_m which is complex values. We observe the following property: Assuming that we want to compute the real value of $f(x)$, only the real value of b_m has to be merged with the sum, since the imaginary component would be dropped afterwards. This allows us to move the $Re(b_m)$ values inside the $\sum_L$:

$$Re(f(x)) := Re\left(\sum_{m=-M}^{M} \sum_{l=-L}^{L} \frac{Re(b_m)\, a_l}{ix + s(\mu + i(m+l))}\right).$$

Now we can collect all nominators with equivalent denominator (if $n = m + l$), yielding

$$\beta_n^{Re} := \sum_{m=-M}^{M} \sum_{l=-L}^{L} Re(b_m) a_l \delta(n = m + l)$$

for real values $f(x)$ and

$$\beta_n^{Im} := \sum_{m=-M}^{M} \sum_{l=-L}^{L} Im(b_m) a_l \delta(n = m + l)$$

for complex values of $f(x)$. This finally leads us to the REXI approximation

$$e^{ix} \approx \sum_{n=-N}^{N} Re\left(\frac{\beta_n^{Re}}{ix - \alpha_n}\right) + i\, Re\left(\frac{\beta_n^{Im}}{ix - \alpha_n}\right)$$

for the complex-valued function e^{ix}.

4 Apply REXI with a matrix:

Finally, we like to apply REXI to a formulation such as

$$U(t) := e^{tL} U(0).$$

To see the relationship between the approximation of e^{ix} with REXI, we first rewrite the exponential formulation in terms of $f(x) := e^{itx}$

$$f(L) := e^{tL} = \Sigma \Lambda \Sigma^H = \Sigma \begin{pmatrix} \ddots & & \\ & e^{i\lambda_n t} & \\ & & \ddots \end{pmatrix} \Sigma^H = \Sigma\, f(\lambda_n)\, \Sigma^H$$

with complex-valued exponentials on the eigenvalues. Hence, the accuracy of the exponential integrator on $f(L)$ only depends on the spectrum of the L and allows to be applied in the same way as e^{ix}, but by replacing x with the matrix L. For error bounds, we like to refer to [2].

5 Filtering

todo: explain why this may be required

6 REXI, our little dog

In the following, we use $L := \tau L'$ and assume an a-priori fixed time step size, making a REXI approximation more efficient. Then, the REXI approximation is given by

$$exp(\tau L') \approx \sum_{k=-K}^{K} \beta_k (L - \alpha_k)^{-1} \tag{1}$$

The coefficients α_k (corresponding to $s(\mu + i\,n)$ in step C for the one-dimensional formulation) can be precomputed or computed during program start. μ is based on a one-dimensional approximation, see the paper, and the α_k can be interpreted as shifts of the rational approximations. The coefficients β_k (corresponding to c_n in step C) are describing the scaling of the basis function and are also constant and independent of the solution itself. Note, that for debugging purpose, their *imaginary values have to cancel out.*

Note an important property (see Sec. 3.3 in [2]). There's an anti-symmetry in the α_i coefficients, which avoids computing half of the inverses:

$$\overline{(L - \alpha)^{-1} u_0} = (L - \overline{\alpha})^{-1} u_0$$

7 Computing inverse of $(L - \alpha)^{-1}$

For computing the inverse, arbitrary solvers can be used. However we like to note, that α is a complex number. Hence, also the solvers have to support for solving in complex space. We still have to compute the inverse of $(L - \alpha)$ which can be very expensive if computing it. Here, we consider a specialization on the shallow-water equations given above with

$$L(U) := \begin{pmatrix} & H\delta_x & H\delta_y \\ g\delta_x & & -f \\ g\delta_y & f & \end{pmatrix} U$$

$$U_t := L(U)$$

and we set $g := 1$ and the average height $H := 1$. [TODO (Pedro): Derive dimensional formulation]. For the REXI method, we now have to solve the systems of equations given by

$$(L - \alpha).U = U0$$

with U_0 the initial conditions. According to [4], instead of solving this relatively large system of equations we can split the problem into an elliptic one for the height which then allows to use an explicit formulation for the velocities. We use the abbreviation$\vec{v} := (u, v)$ in the following paragraph. Using the formulation in [2], the height can be computed with the elliptic equation given by

$$(\nabla^2 - (\alpha^2 + f^2))h(\tau) = \frac{\alpha^2 + f^2}{\alpha}(h(0) + H\nabla \cdot (A.v(0)) \tag{2}$$

with

$$A := \frac{1}{\alpha^2 + f^2} \begin{pmatrix} \alpha & -f \\ f & \alpha \end{pmatrix}.$$

Assuming an f-plane approximation (f is constant), we can rearrange this equation by using the abbreviations $\kappa := \alpha^2 + f^2$ and $\gamma := \alpha^{-1}$ in the following way:

$$(\nabla^2 - \kappa)\, h(\tau) = \frac{\kappa}{\alpha}\,(h(0) + H\nabla \cdot (A.v(0))$$

$$(\nabla^2 - \kappa)\, h(\tau) = \frac{\kappa}{\alpha} h(0) + \frac{1}{\alpha} H\nabla \cdot \begin{pmatrix} \alpha & -f \\ f & \alpha \end{pmatrix} .v(0)$$

$$(\nabla^2 - \kappa)\, h(\tau) = \frac{\kappa}{\alpha} h(0) + \frac{1}{\alpha} H \begin{pmatrix} \alpha & -f \\ f & \alpha \end{pmatrix} \nabla \cdot v(0)$$

$$(\nabla^2 - \kappa) h(\tau) = \frac{\kappa}{\alpha} h(0) - \frac{Hf}{\alpha} \nabla \times v(0) + H\nabla \cdot v(0) \tag{3}$$

Here, the α and κ denote the terms with imaginary numbers and this formulation simplifies programming it. As an interpretation, on the right hand side we see an update-like scheme $h(0)$ in the first scheme, then a vorticity-like formulation $\times$, and an advective part ∇. To simplify the notation for solving the system, we rewrite it as

$$(\nabla^2 - \kappa)\, h(\tau) = D \tag{4}$$

with real-and-imaginary-valued D and $\nabla^2 - \kappa$ as well as a real-and-imaginary-valued $h(\tau)$ for which we want to solve.

We like to solve this without operator support for imaginary values in Cartesian space (e.g. in SWEET). To do so, we reformulate the equation by $K := \nabla^2 - \kappa$ operator on D can be written with the standard complex-number division rules and using $Re(K) := -Im(\nabla)^2 - Re(K)$ as well as $Im(K) := -Im(\kappa)$ as

$$denom := Re(K)^2 + Im(\kappa)^2$$

TODO: for sake of simplicity, the following part should be removed later on.

$$Re(DK^{-1}) = \frac{Re(K)Re(D) + Im(K)Im(D)}{denom}$$

$$Im(DK^{-1}) = \frac{Re(K)Im(D) - Im(K)Re(D)}{denom}$$

and further

$$Re(DK^{-1}) = \frac{Re(K)Re(D) - Im(\kappa)Im(D)}{denom}$$

$$Im(DK^{-1}) = \frac{Re(K)Im(D) + Im(\kappa)Re(D)}{denom}$$

Once computed the height, the velocities can be directly computed via

$$\vec{v}(\tau) = -A.\vec{v}(0) + A.\nabla h$$

$$\vec{v}(\tau) = -A.(\vec{v}(0) - \nabla h) \tag{5}$$

giving us our final solution

$$U := (h, v, u)^T.$$

One final scaling has to be done: the exponential is computing $e^{\tau L}$, hence the real-valued τ has to be included in the operator L. There are basically two different ways: The first one is rescaling all parameters by τ:

$$g' := \tau g$$

$$f' := \tau f$$

$$h'_0 := \tau h_0$$

The second way is to factor the τ parameter out:

$$(\tau L - \alpha).U(\tau) = U0$$

$$(L - \frac{\alpha}{\tau}).U(\tau)\tau = U0$$

So instead of solving for $U(\tau)$, we are solving for $U'(\tau) := U(\tau)\tau$ as well as $\alpha' := \frac{\alpha}{\tau}$and have to divide the computed solution by τ in the end.

8 Bringing everything together

Using the spectral methods (e.g. in SWEET), we can directly solve the height Eq. (2) and then solver for the velocity in Eq. (5). Then, the problem is reduced to computing the REXI as given in Eq. (1). We like to note again, that the α_i and β are independent of the system L to solve, and the number of coefficients only depends on the accuracy and the resolution.

9 Notes on HPC

- The terms in REXI to solve are all independent. Hence, for latency avoiding, the communication can be interleaved with computations.

- The iterative solvers are memory bound. Instead of computing $c := a * b$ for the stencil operations, we could compute $\vec{c} := a\vec{b}$ with a one coefficient in the stencil. This allows vectorization over c and b on accelerator cards with strided memory access.
- It is unknown which method is more efficient to solve the system of equations:
  - iterative solvers have low memory access,
  - inverting the system and storing it as a sparse matrix allows fast direct solving but can yield more memory access operations.
- Splitting the solver into real and complex number would store them consecutively in memory. This has a potential to avoid non-strided memory access and using the same SIMD operations (Just a rough idea, TODO: check if this is really the case).

10 Acknowledgements

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References

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