Fluid Dynamics — Numerical Techniques

MATH5453M Numerical Exercises 3, 2023

Due date: December 2023

1 Introduction

The finite-element method (FEM) is explained and explored for systems of partial differential equations for wave dynamics in several ways:

- by employing how the space-time dynamics arises from a variational principle (VP), yielding the Ritz-Galerkin FEM with continuous-Galerkin finite elements (CGFEM), in which the weak forms derive directly from the VP; and,
- by deriving the weak or integral formulations using multiplication of each equation by appropriate test functions, integration (by parts), resulting in (leading- or first-order) discontinous Galerkin or finite-volume schemes (DG0, DGFEM or FV0). TBD.

The time discretisation will be implemented explicitly either by using an appropriate time-discrete VP or by using a Euler-forward or a higher-order variation-diminishing time-stepping scheme[1].

2 Shallow-water equstions –potential flow

The VP for the scaled shallow-water equations, expressed in terms of a velocity potential $\phi(x,y,t)$ and deviation $\eta(x,y,t)$ of the free surface from a scaled (unit) rest level, is as follows

$$0 = \delta\mathcal{F} \equiv \delta \int_0^T \iint_{\Omega_h} \eta\partial_t\phi + \frac{1}{2}(1+\epsilon\eta)|\nabla\phi|^2 + \frac{1}{2}\eta^2 \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t \tag{1}$$

in a horizontal domain $(x,y) \in \Omega_h$, for a time interval $t \in [0,T]$. Herein, the horizontal gradient operator reads $\nabla = (\partial_x, \partial_y)^T$. Observe that the middle term is the kinetic energy (density) and the last term the

[1] A FEM for the Poisson equation and its Firedrake implementation is provided as a first example, to be considered for self-study. Work through this on-line GitHub example first.

potential energy (density). The total scaled water depth over a flat bottom is then given by $h(x,y,t) = 1+\epsilon\eta(x,y,t)$ with $\epsilon = a_w/H_0$ a nonlinearity parameter, which is the ratio of a typical dimensional wave height a_w over the dimensional water depth H_0. The definition of the *functional* derivative for a functional $\mathcal{F}[\phi,\eta]$, here an integral of the functions $\phi(x,y,t)$ and $\eta(x,y,t)$, is the following

$$\delta\mathcal{F}[\phi,\eta] = \lim_{\epsilon_v\to 0}\frac{\mathcal{F}[\phi+\epsilon_v\delta\phi,\eta+\epsilon_v\delta\eta]-\mathcal{F}[\phi,\eta]}{\epsilon_v} = \frac{\mathrm{d}}{\mathrm{d}\epsilon_v}\mathcal{F}[\phi+\epsilon_v\delta\phi,\eta+\epsilon_v\delta\eta], \tag{2}$$

in which $w_\phi = (\delta\phi), w_\eta = (\delta\eta)$ are the arbitrary variations or "test functions" $w_\phi(x,y), w_\eta(x,y)$. See Van der Kan et al. (2005) –please study the relevant sections on minimization problems and arbitrary variations therein. Note that the "δ-symbol" in front of the space-time integral constitutes the variational-derivative operation or operator, defined above in (2). In the VP (1), we used the functional $\mathcal{F}$ as defined above. Its variations yield the equations of motion

$$0 = \int_0^T\iint_{\Omega_h}\left(\partial_t\phi+\frac{1}{2}\epsilon|\nabla\phi|^2+\eta\right)\delta\eta - \left(\partial_t\eta+\nabla\cdot((1+\epsilon\eta)\nabla\phi)\right)\delta\phi\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t \tag{3a}$$

$$+\int_0^T\int_{\partial\Omega_h}(1+\epsilon\eta)\hat{\mathbf{n}}\cdot\nabla\phi\,\delta\phi\mathrm{d}s\,\mathrm{d}t + \iint_{\Omega_h}\eta\delta\phi|_0^T\mathrm{d}x\,\mathrm{d}y \tag{3b}$$

with a boundary integral $\int_{\partial\Omega_h}$ and a boundary line element $\mathrm{d}s$ as well as outward normal $\hat{\mathbf{n}}$ thereon. After using the end-point (in time) conditions/restrictions on $\delta\phi(x,y,0) = \delta\phi(x,y,T)$, no flow at the solid boundary, and the aribitrariness of variations $\delta\phi,\delta\eta$, the Bernoulli and continuity equations emerge from (3b) as

$$\delta\eta: \qquad \partial_t\phi+\frac{1}{2}\epsilon|\nabla\phi|^2+\eta = 0, \tag{4a}$$

$$\delta\phi: \qquad \partial_t\eta+\nabla\cdot((1+\epsilon\eta)\nabla\phi) = 0. \tag{4b}$$

Exercise-I: Prove (3) using (2). Prove (3) and argue why arbitrariness of variations applied to (3) yields (4).

A time-discrete version of (1) reads

$$0 =\delta\iint_{\Omega_h}\eta^{n+1/2}\frac{(\phi^{n+1}-\phi^n)}{\Delta t}-\phi^{n+1/2}\frac{(\eta^{n+1}-\eta^n)}{\Delta t}+\frac{1}{2}(1+\epsilon\eta^{n+1/2})|\nabla\phi^{n+1/2}|^2+\frac{1}{2}(\eta^{n+1/2})^2\,\mathrm{d}x\,\mathrm{d}y \tag{5}$$

with time step Δt, previous-future-and-mid-point time levels $\phi^n, \phi^{n+1}, \phi^{n+1/2}$, et cetera; combined with definitions of these future time levels as

$$\eta^{n+1} =2\eta^{n+1/2}-\eta^n \quad \text{and} \quad \phi^{n+1} = 2\phi^{n+1/2}-\phi^n. \tag{6}$$

That implies that $\eta^{n+1/2}$ and $\phi^{n+1/2}$ are the average or mid-point levels of η and ϕ in a time slab $t\in[t_n,t_{n+1}]$. It is a so-called second-order modified mid-point (MMP) time discretisation.

Exercise-II: Show that variations of (5) with respect to $\phi^{n+1/2}, \eta^{n+1/2}$ (only) yield the following time-discrete system of equations:

$$\delta\eta^{n+1/2}: \qquad \frac{(\phi^{n+1}-\phi^n)}{\Delta t} + \frac{1}{2}\epsilon|\nabla\phi^{n+1/2}|^2 + \eta^{n+1/2} = 0, \tag{7a}$$

$$\delta\phi^{n+1/2}: \qquad \frac{(\eta^{n+1}-\eta^n)}{\Delta t} + \nabla\cdot\Big((1+\epsilon\eta^{n+1/2})\nabla\phi^{n+1/2}\Big) = 0, \tag{7b}$$

which are completed or closed off with relations (6). Note that when $\epsilon \to 0$, we obtain the time-discrete linear shallow-water equations.

2.1 Finite-element method

Partial variation of (5) such that the highest-appearing spatial derivatives remain low, i.e. first-order, yields the weak formulation used in a particular finite-element discretisation, provided that suitable finite-element expansions and functions spaces for both variables and test functions are defined. This partial variation gives

$$\begin{aligned} 0 = \iint_{\Omega_h} & \delta\eta^{n+1/2}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t} + \frac{1}{2}\epsilon|\nabla\phi^{n+1/2}|^2 + \eta^{n+1/2}\right) \\ & - \delta\phi^{n+1/2}\frac{(\eta^{n+1}-\eta^n)}{\Delta t} + (1+\epsilon\eta^{n+1/2})\nabla\phi^{n+1/2}\cdot\nabla(\delta\phi^{n+1/2})\,\mathrm{d}x\,\mathrm{d}y, \end{aligned} \tag{8}$$

wherein $\delta\eta^{n+1/2}$ and $\delta\phi^{n+1/2}$ appear as the test functions. In a continuous Galerkin finite-element discretisation (CGFEM) the function spaces for variables $\{\eta^{n+1/2}, \phi^{n+1/2}\}$ and test functions are (nearly) the same and chosen to be continuous. In CGFEM, both variables and test functions are expanded in terms of the same basis functions $\varphi_k(x,y)$, as follows

$$\phi^{n+1/2}(x,y) = \phi_k^{n+1/2}\varphi_k(x,y), \qquad \delta\phi^{n+1/2}(x,y) = (\delta\phi_k)^{n+1/2}\varphi_k(x,y), \quad k = 1,2\ldots,N_{dof}, \tag{9}$$

with N_{dof} the number of degrees-of-freedom and summation of repeated indices k implied (Einstein summation convention). Note that $\phi_k^{n+1/2}, (\delta\phi_k)^{n+1/2}$ are scalar coefficients. E.g., for first-order CG1 these basisfunctions equal the tent functions with N_{dof} the number of nodes involved in the problem, in which there may be fewer degrees-of-freedom for the test functions involved or otherwise said some of these variations may be zero. A fully space-time algebraic VP arises when (9) is substituted into (5), since in that case the integrals over the test functions can be evaluated explicitly. However, the *automated system for the solution of partial differential equations using the finite element method (FEM)* "Firedrake" performs this step internally.

Exercise-II: Prove how (8) arises from (5).

The weak forms in (8) can be derived automatically within Firedrake, which is particularly advantageous in more complicated (three-dimensional) applications with time-varying demains, such as the three-dimensional potential-flow equations modelling water-waves. Regarding a numerical implementation of the above, relevant Firedrake listings (e.g., in *bennylukefbVP.py*) are the following:

```
# Alternatively, define the modified-midpoint time-discrete variational principle (VP) for SWE system;
            \ VP is expression above with mu=0 and q removed:
VPbl = ( inner(etamp,(phi1-phi0)/dt) - inner(phimp, (eta1 - eta0)/dt) \
        + 0.5*mu*inner(grad(etamp),grad((phi1-phi0)/dt)) \
        + 0.5*inner(etamp,etamp) + 0.5*(1.0+epsilon*etamp)*inner(grad(phimp),grad(phimp)) ) * dx
```

containing the definition of the time-discrete VP, followed by a derivation of the two weak formulations

```
# To obtain 3 weak forms, take the 3 functional derivative (no partial integration/divergence
     \ theorem in space) wrt 3 midpoint n+1/2-time variables
# Replace phi1 and eta1 by their expressions ito phi0,eta0, phimp and etamp (mp=midpoint ie at n+1/2 time)
phiexprnl1 = derivative(VPbl, phimp, du=vvmphi)
phiexprnl1 = replace(phiexprnl1, {phi1: 2.0*phimp-phi0})
phiexprnl1 = replace(phiexprnl1, {eta1: 2.0*etamp-eta0})

etaexprnl1 = derivative(VPbl, etamp, du=vvmpeta)
etaexprnl1 = replace(etaexprnl1, {phi1: 2.0*phimp-phi0})
etaexprnl1 = replace(etaexprnl1, {eta1: 2.0*etamp-eta0})
```

resulting in the two separate weak formulations after use of the "du's" which represent the respective test functions $\delta\phi^{n+1/2}, \delta\eta^{n+1/2}$ and after elimination of the future time levels η^{n+1}, ϕ^{n+1}. We note that $\{phi0, phi1, phimp\}$ in the code represent $\{\phi^{n+1}, \phi^{n}, \phi^{n+1/2}\}$. The "derivative" command in Firedrake performs the partial functional derivative of the VP, as described above. For background information, see § 17.5.1 Alneas et al (2021) and § 6.4 in Alnaes et al. (2013). The final weak formulation is then formed by simply adding the above weak forms, since the Unified Form Language (UFL) in Firedrake is "*fully decomposable*". Somewhat simply rephrased this means that our entire mathematical formulation can nearly be typed in verbatim using UFL:

```
# Combine the 2 weak forms and solve as coupled system using a mixed-variable function space
Fexprnl = phiexprnl1 + etaexprnl1
parampsi    = {'ksp_type': 'preonly', 'pc_type': 'lu'}
solparams={ 'pc_type': 'python', 'pc_python_type': 'firedrake.ASMStarPC','star_sub_sub_pc_type': 'lu',
  \ 'sub_sub_pc_factor_mat_ordering_type': 'rcm'}

#  phicombonl = NonlinearVariationalSolver(NonlinearVariationalProblem(Fexprnl, result_mixedmp), solver_parameters=parampsi)
phicombonl = NonlinearVariationalSolver(NonlinearVariationalProblem(Fexprnl, result_mixedmp), solver_parameters=solparams)
```

The final weak formulation collected into "phicombonl" is essentially (8) with $\{\phi^{n+1}, \eta^{n+1}\}$ replaced via relations (6); this final weak formulation is solved for each time slab in the time loop. Notice that the separate weak forms have first been derived in separation and have subsequently been added together.

The relevant (mixed) functions spaces have been defined earlier in the code via the definitions

```
V = FunctionSpace(mesh,"CG",nCG)


eta0 = Function(V, name="eta")
phi0 = Function(V, name="phi")
eta1 = Function(V, name="eta_next")
phi1 = Function(V, name="phi_next"),
```

in which nCG can be raised for higher-order CG-polynomials and with the eta0,eta1 variables representing the currently known time level n and the future time level $n + 1$. The mixed function space is defined by

```
mixed_Vmp = V * V
result_mixedmp = Function(mixed_Vmp)
vvmp = TestFunction(mixed_Vmp)
vvmphi, vvmpeta = split(vvmp)  # These represent "blocks".
```

```
phimp, etamp = split(result_mixedmp)
```

and is used to solve the pair of unknowns $\{\eta^{n+1/2}, \phi^{n+1/2}\}$ in one fell swoop.

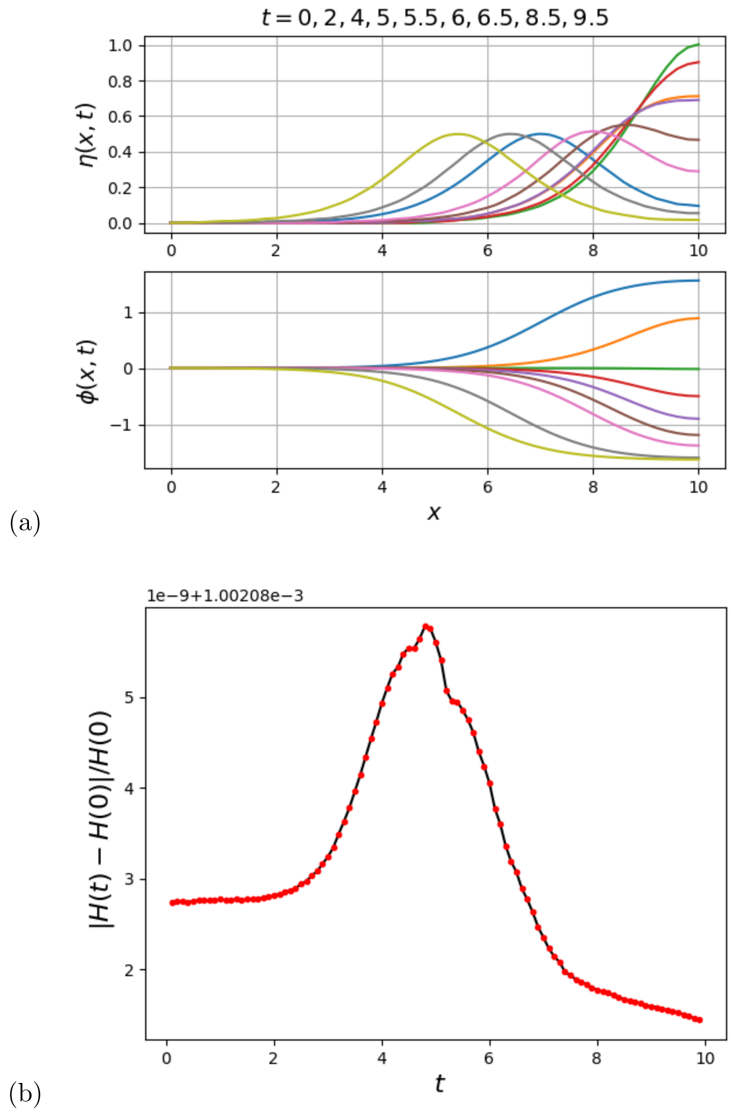

Figure 1: BLE-MMP simulation with 50 elements, $\mu = \epsilon = 0.01$, $\Delta t = 0.005$. (a) Snapshots of free-surface profiles at set times and (b) the relative energy $|H(t) - H(0)|/H(0)$ as function of time.

3 Benney-Luke equations

The VP for the scaled dispersive Benney-Luke water-wave equations (BLE) reads

$$= \delta \int_0^T \int_{\Omega_h} \eta \Phi_t + \frac{\mu}{2} \nabla \eta \cdot \nabla \Phi_t + \frac{1}{2} \eta^2 + \frac{1}{2}(1+\epsilon\eta)|\nabla\Phi|^2 + \mu \left(\nabla q \cdot \nabla \Phi - \frac{3}{4} q^2 \right) \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}t \qquad (10)$$

with dispersion parameter $\mu = H_0/l_0$ and l_0 a typical length scale of a wave. Herein the variables are the velocity potential $\Phi(x, y, t)$ at the flat bottom of the domain, an auxiliary variable $q(x, y, t)$ and again the free-surface deviation $\eta(x, y, t)$.

The time-discete VP for the Benney-Luke equations reads

$$\begin{aligned} 0 = \delta \iint_{\Omega_h} & \eta^{n+1/2} \frac{(\Phi^{n+1} - \Phi^n)}{\Delta t} - \Phi^{n+1/2} \frac{(\eta^{n+1} - \eta^n)}{\Delta t} \\ & + \frac{\mu}{2} \nabla \eta^{n+1/2} \cdot \frac{(\nabla \Phi^{n+1} - \nabla \Phi^n)}{\Delta t} - \frac{\mu}{2} \nabla \Phi^{n+1/2} \cdot \frac{(\nabla \eta^{n+1} - \nabla \eta^n)}{\Delta t} \\ & + \frac{1}{2}(1 + \epsilon \eta^{n+1/2}) |\nabla \Phi^{n+1/2}|^2 + \frac{1}{2} (\eta^{n+1/2})^2 + \mu \Big(\nabla q^{n+1/2} \cdot \nabla \Phi^{n+1/2} - \frac{3}{4} (q^{n+1/2})^2 \Big) \mathrm{d}x\, \mathrm{d}y. \end{aligned} \qquad (11)$$

See Bokhove and Kalogirou (2016) and Choi et al. (2023).

Exercise-IV: Complete similar exercises for the BLE as posed for the SWE. See also the BLE-example and description on the Firedrake website and consider the references. Derive the equations of motion, derive the time-discrete equations and derive the finite-element weak forms.

Numerical tasks-V on BLE-SWE:

- Run the SWE-CGFEM code with $nCG = 1, nVP = 2, \epsilon = 0.01$. Make an energy plot by running the Python code for displaying the energy from the directory with data. Also display the fields using Paraview.

- Run the BLE-CGFEM code with $nCG = 1, nVP = 1, \mu = \epsilon = 0.01$ (modified mid-point time-stepping scheme MMP using a VP). Reproduce Fig. 3 in Bokhove and Kalogirou (2016), also shown in Fig. 1. Make an energy plot by running the relevant Python code from the directory with data. Modify the relevant codes by adding kinetic and potential energies to the energy-data file and plot all three energies in one plot. Make a comparison by increasing nCG but decreasing the number of elements such that the degrees-of-freedom stay the same. Figure out how to find and display the degrees-of-freedom. Explain the results.

- Run the BLE-CGFEM code with $nCG = 1, nVP = 0, \mu = \epsilon = 0.01$ (Störmer-Verlet SV time-stepping scheme using weak forms). Make a comparison by increasing nCG but decreasing the number of elements such that the degrees-of-freedom stay the same. Compare results with results of the MMP-scheme. Write out the time-discrete weak formulations for BLE-SV. Derive a time-discrete VP for this BLE-SV.

- Change μ and ϵ including the case with $\mu = 0$ for BLE with both the MMP and SV schemes. Notice how the soliton steepens. What happens when μ is small or zero and ϵ large(r)? Why is a seperate code for the SWE-MMP-VP required required?

3.1 Wave-breaking parameterisation in shallow-water equations

Following Wang et al. (2021) and Smit et al. (2013, page 4), the wave-breaking parameterisation scheme added to the dimensional shallow-water equations reads

$$\partial_t \phi + \frac{1}{2}\epsilon|\nabla\phi|^2 + g\eta = \nabla\cdot(\nu_b\nabla\phi), \tag{12a}$$

$$\partial_t \eta + \nabla\cdot((H+\eta)\nabla\phi) = \nabla\cdot(\nu_b\nabla(H+\eta)) \tag{12b}$$

$$\nu_b = \nu_{bo} max\left(\Theta^{**}(|\nabla\eta|^2 - \beta^2), \Theta^*(\partial_t\eta - \alpha_s\sqrt{H+\eta})\right) \tag{12c}$$

with special Heaviside functions $\Theta^{**}(\cdot)$ and $\Theta(\cdot)$. That is, once the wave-breaking region is switched on by the provided criteria, it is only switched off: for $\Theta^{**}(\cdot)$ when the wave peak has passed and for $\Theta^*(\cdot)$ when the wave peak with $\partial_t\eta > 0$ has passed, i.e. when the sign changes to $\partial_t\eta < 0$. The dimensionless version thereof emerges when we use the following scaling

$$t = H_0\tilde{t}/\sqrt{gH_0}, \quad (x,y) = H_0(\tilde{x},\tilde{y}), \quad \phi = \epsilon H_0\sqrt{gH_0}\tilde{\phi}, \quad \eta = \epsilon H_0\tilde{\eta}, \tag{13}$$

with velocity scale $U_0 = \sqrt{gH_0}$. Upon dropping these tildes on the dimensionless variables and coordinates, we arrive at the following scaled system in extension of (4) and with wave-breaking diffusion

$$\partial_t \phi + \frac{1}{2}\epsilon|\nabla\phi|^2 + \eta = \nabla\cdot(\nu_b\nabla\phi), \tag{14a}$$

$$\partial_t \eta + \nabla\cdot((1+\epsilon\eta)\nabla\phi) = \nabla\cdot(\nu_b\nabla\eta) \tag{14b}$$

$$\nu_b = \nu_{bo} max\left(\Theta^{**}(|\nabla\eta|^2 - \beta^2), \Theta^*(\partial_t\eta - \alpha_s\sqrt{1+\epsilon\eta})\right) \tag{14c}$$

with scaled $\nu_b = \nu_b^*/(H_0\sqrt{gH_0})$, $\alpha_s = \alpha_s^*/\epsilon$ and $\beta = \beta^*/\epsilon$, wherein $\nu_b^* \approx 1.86\mathrm{m}^2/\mathrm{s}$, dimensionless $\alpha_s^* = 0.6$ and threshold slope $\beta^* = 0.125$. To wit, the formulation (15) above means that diffusive terms are switched on when either $|\nabla\eta|^2 > \beta^2$ or $\partial_t\eta > \alpha_s\sqrt{1+\epsilon\eta}$ holds, or both hold. The accelaration of gravity $g = 9.81\mathrm{m/s}^2$ and $\theta(\cdot)$ is a Heaviside function.

The weak formulations for these extra terms read

$$\iint w_\eta\frac{(\eta^{n+1}-\eta^n)}{\Delta t} + \cdots + \nu_b^{n+1/2}\nabla w_\eta\cdot\nabla\eta^{n+1/2}\,\mathrm{d}x\,\mathrm{d}y = 0, \tag{15a}$$

$$\iint w_\phi\frac{(\phi^{n+1}-\phi^n)}{\Delta t} + \cdots + \nu_b^{n+1/2}\nabla w_\phi\cdot\nabla\phi^{n+1/2} = 0 \tag{15b}$$

$$\nu_b^{n+1/2} = \nu_{bo} max\left(\Theta^{**}(|\nabla\eta^{n+1/2}|^2 - \beta^2), \Theta((\eta^{n+1}-\eta^n))/\Delta t - \alpha_s\sqrt{1+\epsilon\eta^{n+1/2}})\right), \tag{15c}$$

with $\eta^{n+1} = 2\eta^{n+1/2} - \eta^n$. If we focus exclusively on the second wave-breaking scheme for shallow-water regions, then the scheme can be rewritten at every x, y-location:

$$\nu_f^{n+1/2} = \Big(\nu_{bo}\ \Theta((\eta^{n+1} - \eta^n)/\Delta t - \alpha_s\sqrt{1+\epsilon\eta^{n+1/2}}) + \nu_f^{n-1/2}\Theta((\eta^{n+1} - \eta^n)/\Delta t)\Big)\,, \tag{16a}$$

$$\nu_b^{n+1/2} = \nu_f^{n+1/2}, \quad \nu_b^{n+1/2} = \nu_{bo}\text{conditional}(\nu_b^{n+1/2} > \nu_{bo}, \nu_{bo}, \nu_b^{n+1/2}). \tag{16b}$$

To wit, the first term is turned on when at an x, y-location $\partial_t\eta > \beta\sqrt{gh}$ and following the second term stays on till at that location $\partial_t\eta$ changes sign to become negative. Hence, there are four options at every x, y-position: newly-on and old-on with the sum giving outcome $2\nu_{bo}$, newly-on and old-off giving ν_{bo}, newly off and old-on giving ν_{bo}, and newly-off and old-off giving 0. The outcome $2\nu_{bo}$ is not allowed, so the outcome is capped to ν_{bo}. Whether the final diffusion function should be preferably DG0 or CG1 can be decided by trail and error. The weak formulations for these extra terms can be added to the weak forms generated in automated fashion from the VP as is done in the as-yet incomplete sample code provided: bennylukefbwbVP.py

4 Discontinuous Galerkin FEM for (linear) shallow-water equations over topography

TBD. To-be-continued.

In Firedrake, the canonical name for a DG element on a quad is DQ.

See also shallow-water DG-modelling in Flooddrake at: `https://github.com/firedrakeproject/flooddrake/tree/master/flooddrake`

5 Variational Boussinesq model

References

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Onno Bokhove, December 14$^{\text{th}}$ 2023, TBC.