Modelling Internal Wave Dynamics Using Unstructured Grids

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July 28, 2010

Overview of the talk

- Introduction to the problem.
- A suitable mathematical model for internal wave dynamics in lakes.
- Past Work:
  - Numerical solutions with pseudospectral methods for simple geometries.
- Current/Future Work:
  - Numerical solutions with Discontinuous Galerkin (DG-FEM) methods for complex geometries.

Internal Wave Modelling in Lakes: What equations to Solve?

In general we have a 3D, rotating, stratified (free-surface) flow with an irregularly shaped boundary.

- Solutions to the full 3D equations are becoming more within reach as parallel computing becomes more powerful and accessible.
- Free surface flows in the full equations are very difficult: Moving boundary. Most 3D models that exist today (e.g. MITgcm) linearize the free surface or "cheat" in some other way.
- Past models have taken 2D slices, rigid lid or assumed hydrostatic flow.
- Shallow water models (SWMs) can address the free surface, and can crudely handle stratification, so perhaps they are the most realistic choice at present.

Non-Hydrostatic Shallow Water Model

The traditional SWM assumes $(H/\lambda) \ll 1$, and thus is only an appropriate model of sufficiently long waves.

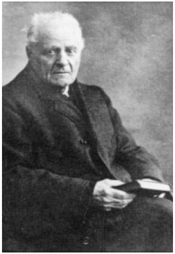
To address dispersive short-wave phenomena, we consider the dispersion-modified SWM of Brandt et. al. (1997)

$$
\begin{aligned}
\frac{\partial h}{\partial t} + \nabla \cdot (h\mathbf{u}) &= 0\,, && (1)\\
\frac{\partial (uh)}{\partial t} + \nabla \cdot ((uh)\mathbf{u}) &= -gh\frac{\partial \eta}{\partial x} + fvh + \frac{H^2}{6}\frac{\partial}{\partial x}\left(\nabla \cdot \frac{\partial (\mathbf{u}h)}{\partial t}\right)\,, && (2)\\
\frac{\partial (vh)}{\partial t} + \nabla \cdot ((vh)\mathbf{u}) &= -gh\frac{\partial \eta}{\partial y} - fuh + \frac{H^2}{6}\frac{\partial}{\partial y}\left(\nabla \cdot \frac{\partial (\mathbf{u}h)}{\partial t}\right)\,. && (3)
\end{aligned}
$$

Q: Where do these mysterious new terms come from?

A: "Boussinesq" equations

- There is an overwhelming number of models in the literature referred as the Boussinesq equations.
- All derivations rely on the principle of (approximately) retaining the dispersion that ensues from the vertical momentum equation, while at the same time removing any dependence on z (vertical structure).
- Original idea can be traced back to Boussinesq's (1872) response to J.S. Russel's observation of solitary waves.



Joseph Boussinesq

Boussinesq's Idea

Consider a fluid lying over a flat bottom at $z = -H$ in the (x,z)-plane. If we assume an irrotational flow then $(u, w) = (\varphi_x, \varphi_z)$ for some potential φ. If we expand in a Taylor series about $z = -H$, we obtain

$$\varphi = \varphi(x, -H) + (z + H)\left[\frac{\partial \varphi}{\partial z}\right]_{z=-H} + \frac{1}{2}(z + H)^2\left[\frac{\partial^2 \varphi}{\partial z^2}\right]_{z=-H} + \cdots .$$

Incompressible $(\nabla \cdot \mathbf{u} = 0) \Rightarrow \varphi_{zz} = -\varphi_{xx}$. Substituting and assuming an impermeable bottom ($\varphi_z = 0$ at $z = -H$) yields

$$\varphi = \varphi(x, -H) - \frac{1}{2}(z + H)^2\left[\frac{\partial^2 \varphi}{\partial x^2}\right]_{z=-H} + \frac{1}{24}(z + H)^4\left[\frac{\partial^4 \varphi}{\partial x^4}\right]_{z=-H} + \cdots .$$

The Boussinesq equations are derived by truncating this series, substituting it into the Navier-Stokes equations, and depth-integrating as with the traditional SWM.

Numerical Concerns: How to Time-Step the Model Equations

Our PDEs contain mixed time/space derivatives. How should we discretize in time to allow for a stable and efficient scheme?

- Assume we have discretized in space so that $\partial_x \to D_x$ (method of lines), and what remains is to numerically solve the resulting system of ODEs.
- The most obvious approach is to apply the same time-stepping formula to all instances of ∂_t.
- This results in a 2×2 block system for $((uh)^{n+1}, (vh)^{n+1})$ that can be quite expensive to invert ("coupled approach" Eskilsson & Sherwin (2005)):

$$\begin{pmatrix} I - \frac{H^2}{6} D_{xx} & -\frac{H^2}{6} D_{xy} \\ -\frac{H^2}{6} D_{xy} & I - \frac{H^2}{6} D_{yy} \end{pmatrix} \begin{pmatrix} (uh)^{n+1} \\ (vh)^{n+1} \end{pmatrix} = \begin{pmatrix} RHS^{(n,n-1,\dots)} \\ RHS^{(n,n-1,\dots)} \end{pmatrix}$$

Auxiliary Variable Approach

Eskilsson & Sherwin (2005) noted that the following approach results in a linear system half the size of that in the coupled approach.

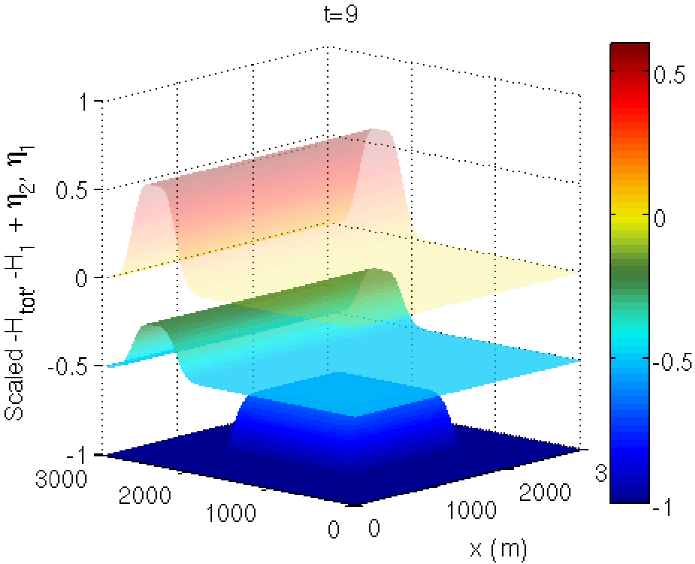
- Let $z = \nabla \cdot (\mathbf{u}h)_t$.
- Momentum equations become: $(\mathbf{u}h)_t = \mathbf{a} + \frac{H^2}{6}\nabla z$.
- Take $\nabla \cdot$, get an elliptic problem: $\nabla \cdot \left(\frac{H^2}{6}\nabla z\right) - z = -\nabla \cdot \mathbf{a}$.
- Momentum equations are now effectively decoupled.
- Now have to invert a Helmholtz problem with spatially-dependent diffusivity at each time-step.
- Reminiscent of how one solves for pressure in the full N-S equations.

Previous Work: Pseudospectral Modelling

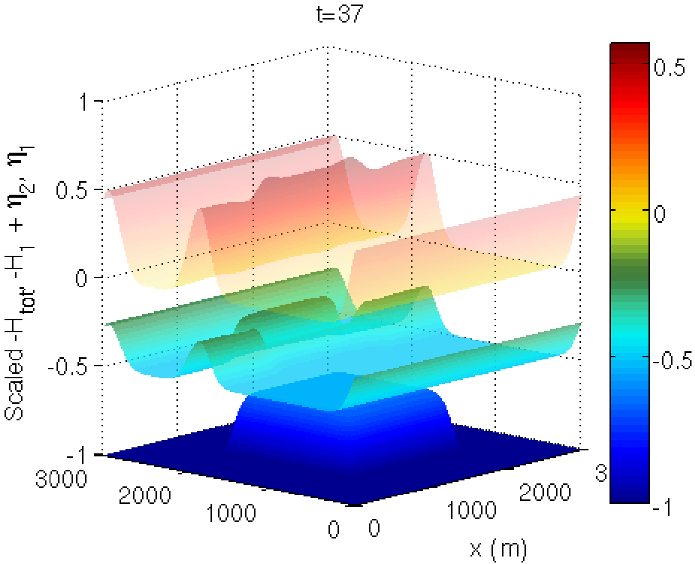
Psedospectral methods provide a good benchmark for simple geometries due to their excellent resolution characteristics and small amounts of inherent dissipation. The basics:

- Periodic boundary conditions $\Rightarrow$ Fourier basis. Differentiate in spectral space (FFT). Perform any products in physical space.
- Impermeable boundary $\Rightarrow$ Chebyshev basis. Again, differentiate in spectral space (DCT implemented with FFT).
- Remove energy pile-up from small scales with low-pass wavenumber filter in spectral space.
- Solve Helmholtz problem iteratively (GMRES preconditioned with LU/LU-inc).
- 2D pseudospectral codes thus far:
  - Doubly periodic (1-layer or 2-layer & bottom topography), MATLAB
  - Periodic channel (1-layer & bottom topography), MATLAB
  - Circular geometry (1-layer & bottom topography), MATLAB
  - Doubly periodic (1-layer & flat bottom), C++ with MPI

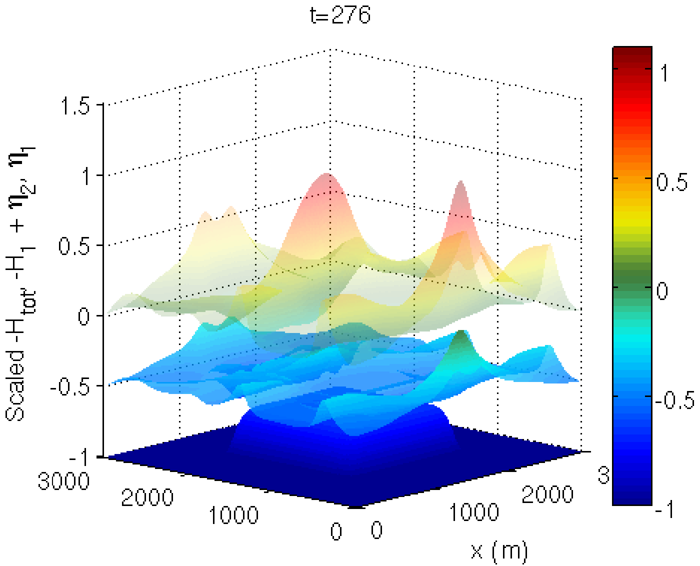
Results: Internal Wave Generation with the 2-layer Model



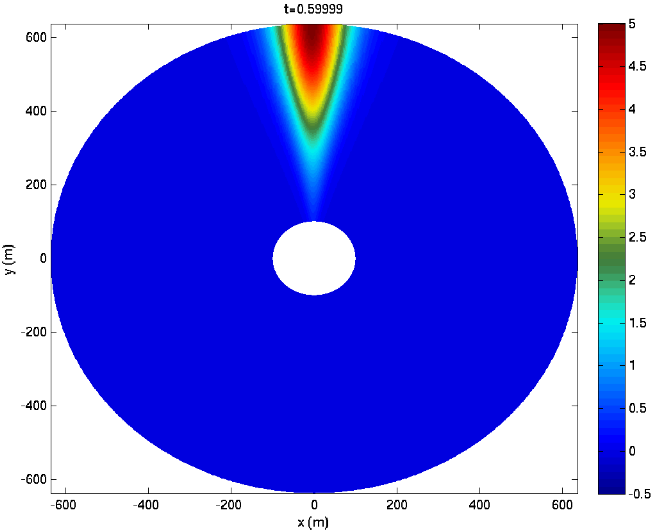
Results: Internal Wave Generation with the 2-layer Model



Results: Internal Wave Generation with the 2-layer Model



Results: Nonlinear Kelvin Wave on Donut Lake



Onto more complicated geometries: Why DG-FEM?

- DG-FEM was originally intended as a high-order extension of FVM for complex geometries.
- FVM methods are typically constrained to low orders of accuracy, since making the reconstruction problem high-order destroys geometric flexibility.
- DG-FEM attains high-order accuracy in complex geometries by adding more degrees of freedom (DoFs) to a cell.
- This allows DG-FEM to mimick FEM formulations whilst removing the need for global operators by addressing inter-cell coupling with an appropriate numerical flux (same idea as FVM).

Why DG-FEM? (cont'd)

	complex geometries	high-order accuracy	expl. semi-discrete form	conserv. laws	elliptic problems
FDM	X	X	✓	✓	✓
FVM	✓	X	✓	✓	(✓)
FEM	✓	✓	X	(✓)	✓
PSM	X	✓	✓	(✓)	✓
DG-FEM	✓	✓	✓	✓	(✓)

Table annotated from Hesthaven & Warburton (2008).

- Main Drawback: To ensure the locality of the scheme, interfacial element nodes must be duplicated. $\Rightarrow$ More memory/processor intensive.

Case Study: Testing DG on a Nonlinear Dispersive Problem

Consider the nonlinear KdV equation in standard form on a periodic domain

$$u_t + 6uu_x + u_{xxx} = 0\ , \tag{4}$$

Exact 2-soliton solution (cf. Johnson (2001))

$$u(x,t) = 12\frac{3 + 4\cosh(2x-8t) + \cosh(4x-64t)}{(3cosh(x-28t) + \cosh(3x-64t))^2}\ . \tag{5}$$

The main difficulty: $\Delta t \propto \Delta x^3$.

Q: How do:

- increasing the number of elements (h-refinement)
- increasing the order of basis function (p-refinement)

improve the accuracy of the numerical solution?

Nonlinear KdV Equation: DG Formulation

Re-write as a first-order system of conservation laws

$$u_t + (f(u) + q)_x = 0 \; , \tag{6}$$

$$q = p_x \; , \tag{7}$$

$$p = u_x \; , \tag{8}$$

where $f(u) = 6u^2/2$. Form local solution with a nodal approach.
$x \in \mathbf{D}^k = [x_l^k, x_r^k]$:

$$u_h^k = \sum_{i=1}^{N_p} u_h^k(x_i^k, t)\ell_i^k(x), \; p_h^k = \sum_{i=1}^{N_p} p_h^k(x_i^k, t)\ell_i^k(x), \; q_h^k = \sum_{i=1}^{N_p} q_h^k(x_i^k, t)\ell_i^k(x).$$

The strong form is obtained by multiplying equations (6)–(8) by a member of the space of local test functions (9) and integrating by parts twice.

$$V_h^k = \{\ell_j^k\}_{j=1}^{N_p} \; . \tag{9}$$

Nonlinear KdV Equation: Strong Form DG Formulation

We obtain the $3N_p$ Galerkin equations on each element k

$$
\begin{aligned}
\mathcal{M}^k \frac{d\mathbf{u}_h^k}{dt} + \mathcal{S}^k\left(\mathbf{f}_h^k + \mathbf{q}_h^k\right) &= \left[\boldsymbol{\ell}^k(x)(f_h^k - f^*)\right]_{x_l^k}^{x_r^k} + \left[\boldsymbol{\ell}^k(x)(q_h^k - q^*)\right]_{x_l^k}^{x_r^k}, \\
\mathcal{M}^k \mathbf{q}_h^k - \mathcal{S}^k \mathbf{p}_h^k &= -\left[\boldsymbol{\ell}^k(x)(p_h^k - p^*)\right]_{x_l^k}^{x_r^k}, \\
\mathcal{M}^k \mathbf{p}_h^k - \mathcal{S}^k \mathbf{u}_h^k &= -\left[\boldsymbol{\ell}^k(x)(u_h^k - u^*)\right]_{x_l^k}^{x_r^k},
\end{aligned}
$$

where $\mathbf{v}_h^k = [v_1^k, \cdots, v_{N_p}^k]^\mathsf{T}$,

and $\mathcal{M}_{ij}^k = \int_{\mathbf{D}^k} \ell_i^k(x)\ell_j^k(x)dx$, $\mathcal{S}_{ij}^k = \int_{\mathbf{D}^k} \ell_i^k(x)\frac{d\ell_j^k}{dx}dx$ are the $N_p \times N_p$ local mass and stiffness matrices.

Appropriate Numerical Fluxes (f^*, p^*, q^*, u^*)

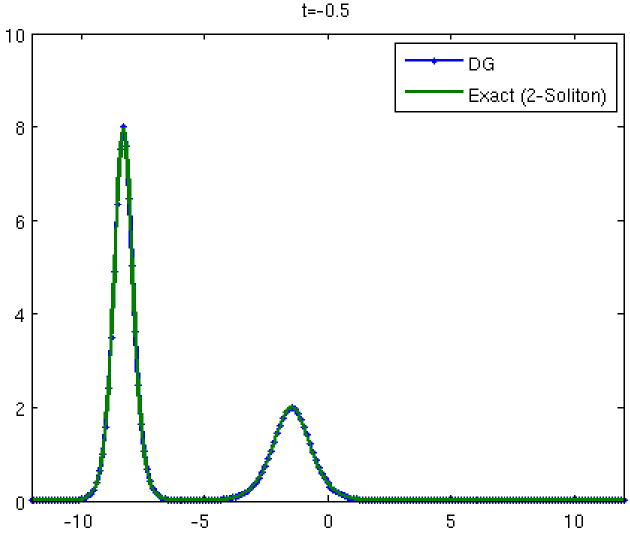
- The DG method shows its flexibility by allowing for choice of numerical flux.
- Often, simple averaging of interface node values (a central flux) works well.
- The best choices "mimic the flow of information in the underlying PDE." For the KdV equation, we choose

$$
\begin{aligned}
f^* &= \{\{f_h\}\} + \max_{u_h}\left|\frac{df}{du}\right|\frac{\hat{\mathbf{n}}}{2}\cdot[\![u]\!]\,, && \text{(Lax-Friedrichs)} && (10)\\
u^* &= \{\{u_h\}\} + \hat{\mathbf{n}}\cdot[\![u_h]\!]\,, && \text{(LDG-Upwinding)} && (11)\\
q^* &= \{\{q_h\}\} - \hat{\mathbf{n}}\cdot[\![q_h]\!]\,, && \text{(LDG-Upwinding)} && (12)\\
p^* &= \{\{p_h\}\}, && \text{(Central)} && (13)
\end{aligned}
$$

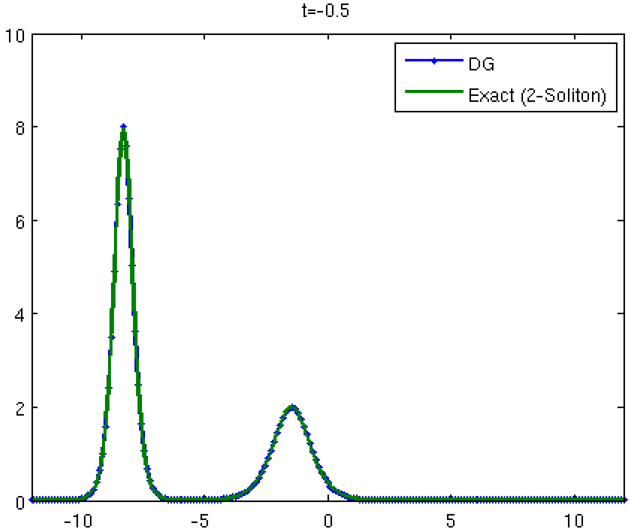
where $\{\{v\}\} = (v^+ + v^-)/2$, $[\![v]\!] = \hat{\mathbf{n}}^- \cdot v^- + \hat{\mathbf{n}}^+ \cdot v^+$.

Element-wise energy considerations reveal a stable scheme.

KdV Solver Animation (N=1, K=200)



KdV Solver Animation (N=3, K=100)



Results

The following table outlines the effects of h and p-refinement for the nonlinear KdV equation integrated from $t_i = -0.5$ to $t_f = 0.5$ with a 5-stage 4th-order low-storage RK method.

N	K	DoF	$\|u(t_f) - u_h(t_f)\|_2$	Run-time (s)
1	100	200	22.1	65.8
1	200	400	8.31	580
3	100	400	0.0364	3165

Q: If same number of DoF's, why is Run #3 over 5x more costly than Run #2?

A: Element-Wise Operations Done With a Legendre Basis

Need a way to calculate $\mathcal{M}^k$ and $\mathcal{S}^k$ for arbitrary N. The optimal choice of basis is the orthonormal Legendre Polynomials $\tilde{P}_n$. Consider the standard interval $r \in [-1, 1]$

$$u(r) \approx u_h(r) = \sum_{n=1}^{N_p} \hat{u}_n \tilde{P}_{n-1}(r) = \sum_{i=1}^{N_p} u(r_i)\ell_i(r) \; . \tag{14}$$

The connection between the nodes $\mathbf{u}$ and the modes $\hat{\mathbf{u}}$ is then established by the generalized Vandermonde matrix $\mathcal{V}_{ij} = \tilde{P}_j(r_i)$

$$\mathbf{u} = \mathcal{V}\hat{\mathbf{u}} \; . \tag{15}$$

Element-Wise Operations Done With a Legendre Basis (cont'd)

In order to ensure that $\mathcal{V}$ is well-conditioned (and the interpolating polynomials are well-behaved), we take the r_i's to be the famous Legendre-Gauss-Lobotto (Chebyshev) quadrature points.

$$r_i = \cos\left(\frac{2i-1}{2N_p}\pi\right) \ , \ i = 1, \ldots, N_p \tag{16}$$

The price: Introduces much smaller Δr's than on a uniform grid.

If we define the differentiation matrix $\mathcal{D}_{r,(i,j)} = \frac{d\ell_j}{dr}\Big|_{r_i}$ and work out the inner-products, we obtain (Hesthaven & Warburton (2008))

$$\mathcal{M}^k = \frac{h^k}{2}\mathcal{M} = \frac{h^k}{2}\left(\mathcal{V}\mathcal{V}^{\mathsf{T}}\right)^{-1}, \tag{17}$$

$$\mathcal{S}^k = \mathcal{S} = \mathcal{M}\mathcal{D}_r, \tag{18}$$

thus eliminating the need to explicitly calculate inner products numerically.

DG-FEM and the Boussinesq equations

- Single-layer Boussinesq-type equations have already been accurately solved using DG-FEM by Sherwin and Eskilsson (2005) and Ensig-Karup, et. al. (2006).
- My work thus far: 1D single-layer Boussinesq model in MATLAB.
- Short-term goal: 2D single-layer Boussinesq model in MATLAB in complex geometries.
- Long-term goal: 2D 2-layer Boussinesq model in C/C++.

Write mass/momentum equations as a system of conservation laws

$$
\begin{aligned}
\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}(uh) &= 0\,, && (19)\\
\frac{\partial (uh)}{\partial t} + \frac{\partial}{\partial x} f(h,u) &= \frac{H^2}{6}\frac{\partial z}{\partial x} + g\frac{\partial H}{\partial x} h\,, && (20)
\end{aligned}
$$

where $f(h,u) = \left(hu^2 + \frac{1}{2}gh^2\right)$.

For the Non-Hydrostatic pressure equation, let $b(x) = H^2/6$ and $q = \sqrt{b}z_x$. The elliptic problem can be written as

$$
\begin{aligned}
\frac{\partial}{\partial x}(\sqrt{b}q) - z &= -\frac{\partial a}{\partial x}\,, && (21)\\
q &= \sqrt{b}\frac{\partial z}{\partial x}\,. && (22)
\end{aligned}
$$

Strong DG Formulation

- Hyperbolic equations:

$$
\begin{aligned}
\mathcal{M}^k \frac{\partial \mathbf{h}^k}{\partial t} + \mathcal{S}(\mathbf{uh})^k &= \left[\boldsymbol{\ell}(x)((uh)^k - (uh)^*)\right]_{x_l^k}^{x_r^k} , \\
\mathcal{M}^k \frac{\partial \mathbf{uh}^k}{\partial t} + \mathcal{S}\mathbf{f}^k &= \mathcal{B}^k \mathcal{S}\mathbf{z}^k + g\mathcal{H}_x^k \mathcal{M}^k \mathbf{h}^k + \left[\boldsymbol{\ell}(x)(f^k - f^*)\right]_{x_l^k}^{x_r^k} \\
&- \mathcal{B}^k \left[\boldsymbol{\ell}(x)(z^k - z^*)\right]_{x_l^k}^{x_r^k} ,
\end{aligned}
$$

where $\mathcal{B}_{ii}^k = b(x_i^k)$, $\mathcal{H}_{x,ii}^k = \frac{\partial H}{\partial x}(x_i^k)$.

- Elliptic equation:

$$
\begin{aligned}
\mathcal{S}\sqrt{\mathcal{B}}^k \mathbf{q}^k - \mathcal{M}^k \mathbf{z}^k &= \left[\boldsymbol{\ell}(x)(\sqrt{b}q^k - (\sqrt{b}q)^*)\right]_{x_l^k}^{x_r^k} \\
&- \mathcal{S}\mathbf{a} + \left[\boldsymbol{\ell}(x)(a^k - a^*)\right]_{x_l^k}^{x_r^k} , \\
\mathcal{M}^k \mathbf{q}^k &= \sqrt{\mathcal{B}}^k \mathcal{S}\mathbf{z}^k - \left[\boldsymbol{\ell}(x)(\sqrt{b}z^k - (\sqrt{b}z)^*)\right]_{x_l^k}^{x_r^k} ,
\end{aligned}
$$

Numerical Fluxes

- Hyperbolic equations:
  - Advective terms $(f^*, (uh)^*) \Rightarrow$ Lax-Friedrichs flux (in both momentum and mass equations)
  - $z^* = \{\{z\}\}$.
- Elliptic equation:
  - $a^* = \{\{a\}\}$, $(\sqrt{b}z)^* = \{\{\sqrt{b}z\}\}$ (Central fluxes)
  - $(\sqrt{b}q)^* = \{\{\sqrt{b}q\}\} - \tau[\![z]\!]$, $\tau > 0$. (Penalized Central flux)

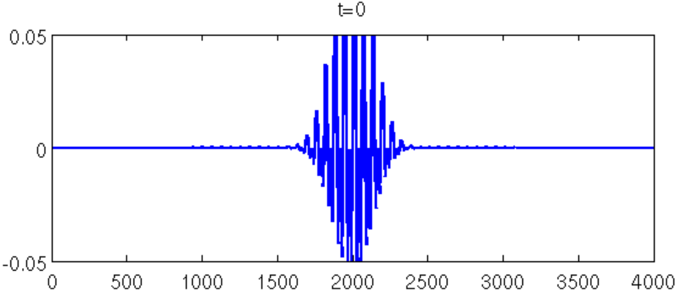
The "penalty term" is used to disallow large jumps in z at interfaces. If $\tau = 0$, the matrix representation of the Helmholtz operator possesses a singular eigenmode ($\lambda = 0$), and the problem is not invertible.

Elliptic Problems and Numerical Flux Choice

- There are various trade-offs to consider when choosing numerical flux functions for elliptic equations.
- The spatial-discretization of the elliptic operator can be represented as an $N_p K \times N_p K$ matrix $\mathcal{A}$.
- Different numerical fluxes result in different stencil-sizes and conditioning properties.

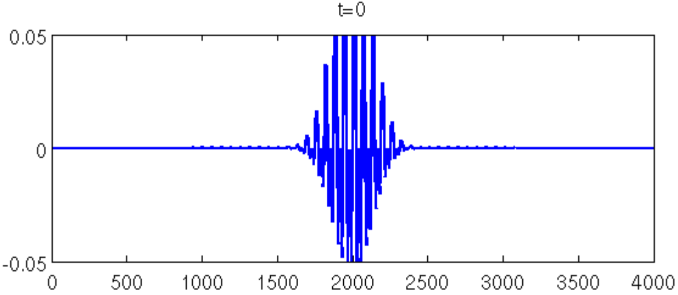
	u^*	q^*	Sparsity	Conditioning
Central	$\{\{u\}\}$	$\{\{q\}\} - \tau[\![u]\!]$	Worst	Best
LDG	$\{\{u\}\} + \hat{\mathbf{n}} \cdot [\![u]\!]$	$\{\{q\}\} - \hat{\mathbf{n}} \cdot [\![q]\!] - \tau[\![u]\!]$	Best	$\approx 2\kappa(\mathcal{A}_c)$
IP	$\{\{u\}\}$	$\{\{u_x\}\} - \tau[\![u]\!]$	Medium	$\approx \kappa(\mathcal{A}_c)$

Results: Dispersive Shortwaves, $N = 3$, $K = 630$, $DoF = 2520$



Time-stepped with 3rd order SSP RK method with adaptive Δt to $t = 200$. Total Run-Time = 14.8s.

Dispersive Shortwaves, $N = 20$, $K = 120$, $DoF = 2520$



Total Run-Time = 114s.

Extension to Two Dimensions: If I did it

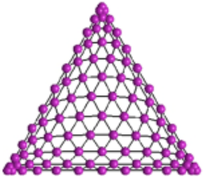


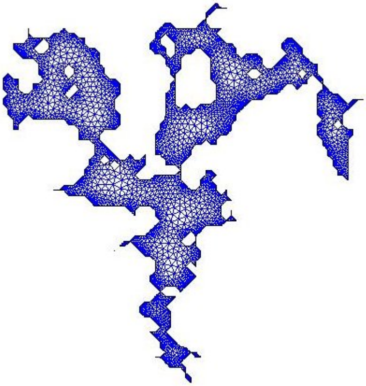
Image courtesy of Tim Warburton.

- Stay with the nodal approach. H & W (2008) have found a near optimal choice of 2D polynomial interpolation nodes on the triangle.
- 1D numerical experiments reveal that it is best to aim for high-order polynomials than for a large number of elements.
- Will this remain possible given the complex geometry of a lake?
- Use triangles, or do we need curvilinear elements?
- Less diffusive advective numerical fluxes than Lax-Friedrichs: HLL, HLLE, Roe?
- Choice of numerical flux for elliptic problems becomes important.
- Direct Solve (LU/Chol.) vs. Iterative Solve (GMRES/CG)?

Open Questions/Issues

- How to address lateral boundary-layer separation.
  - No-slip layer not resolved $\Rightarrow$ Use quadratic bottom drag law?
- Time-dependent BC's $\Rightarrow$ time-dependent operator.
  - Need linear harmonic lifting operator or change of variables work-around.
- Language? C or C++.
  - Nunn and Warburton have some 2D CFD (Euler, N-S) C++ code freely available under the GPL (project NUDG++).
- Parallel implementation:
  - Parallelize at what level?

Questions?



Opeongo Lake Triangular Mesh courtesy of Aidan Chatwin-Davies

Thank You!

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