Simulation of stratified mixing in thin aspect ratio domain using a spectral element method: Handling small scale noise and improving the iterative Poisson solver

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Overview

Motivation

The Model
  Model Features

Estimating DG-induced mixing
  Estimating Implicit Mixing

Boutique solver
  Domain Decomposition Algorithm
  Remarks

Conclusion
Gravity Current Simulation

- Mixing and entrainment in gravity currents transform source waters into deep and intermediate waters.
- Carried by large scale ocean currents $O(10\text{-}100 \text{ km})$.
- Dynamical scales of mixing instabilities are small compared to oceanic scales: SGS needed to model mixing.
- Parameterization need to be validated against observation and DNS-type simulation.
- Increase modeled $Re$ or increase size of computational domain to follow evolution of gravity current.
- Process-oriented studies in idealized channels.
Gravity Current Simulation

\[
\frac{\partial \zeta}{\partial t} + \vec{\bar{u}} \cdot \nabla \zeta = \frac{1}{R_e} \nabla^2 \zeta - \frac{1}{F_r^2} \rho_x, \quad R_e = \frac{UL}{\nu}, \quad F_r = U \left( g \frac{\Delta \rho}{\rho_0} L \right)^{-\frac{1}{2}}
\]

\[
\nabla^2 \psi + \zeta = 0
\]

\[
\frac{\partial \rho}{\partial t} + \vec{\bar{u}} \cdot \nabla \rho = \frac{1}{P_r R_e} \nabla^2 \rho, \quad P_r = \frac{\nu}{\nu_{\rho}}
\]

- Currently a 2D model built on Boussinesq NS equations in a $\zeta - \psi$ formulation.
- A salt-like tracer evolves according to an advection diffusion equation, and provides buoyancy forcing.
Model Highlights

- $\zeta - \psi$ equations discretized using spectral elements.
  - Dual paths $h-p$ convergence rates for smooth solutions
  - Excellent scalability on parallel computers
  - Phase fidelity and no numerical dissipation.

- Poisson equation solved using substructuring and PCG on the Schur complement.

- Tracer equation discretized with spectral element DGM.
  - Discontinuous interpolation & local mass matrices.
  - Well-suited to advection-dominated flows.
  - Upwind flux bias controls Gibbs oscillations.
Gravity Current Simulation at $R_e = 50,000$

Impact of varying inlet current height

Grid: 300x50 elements of degree 8 with refinement near bottom

steady

varying
Transport in Density Classes $R_e = 50,000$

Impact of varying inlet current height

- Densest water mixed in both cases
- In steady case most transport is in 0.4-0.6 class
- In time-varying case transport is in 0.2-0.4 class
Questions

- Can DG deliver reliable estimate of mixing? Convergence analysis
- Can we increase domain size while keeping cost low and/or high scalability? Improve iterative solver
Estimating Implicit Mixing in DG solution

- How much of the mixing is spurious (numerical)
- Sequence of CG/DG solutions to verify convergence
  - $R_e = 2,000, \ P_r = 7$
  - $R_e = 10,000, \ P_r = 7$
- Metrics for judging solution
  - monotonicity of $\rho$:
    \[
    \min[\rho(\vec{x}, t = 0)] \leq \rho(\vec{x}, t) \leq \max[\rho(\vec{x}, t = 0)]
    \]
  - density classes
  - Energy budget
Energy Equation for Closed Insulated Domain

\[
\frac{d}{dt} \left( \int_A E \, dA \right) = - \int_A \left[ \frac{\zeta^2}{Re} + \frac{\nabla z \cdot \nabla \rho}{RePrFr^2} \right] \, dA
\]  

\[ E = E_k + E_p = \frac{\vec{u} \cdot \vec{u}}{2} + \frac{\rho z}{Fr^2} \]  

\[ E_p = E_a + E_b = \frac{\rho(z - z_*)}{Fr^2} + \frac{\rho z_*}{Fr^2} \]

- \text{\( z_* \): vertical position after adiabatic } \rho \text{-redistribution}
- \text{\( E_b \): Background potential energy responds only to diabatic processes}
- \text{\( E_a \): Available potential energy responds to reversible adiabatic processes only.}
<table>
<thead>
<tr>
<th>$R_e$</th>
<th>$K_x \times K_y \times N$</th>
<th>DG-Time</th>
<th>CG-Time</th>
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**Table**: table of experiments for $R_e = 10,000$
**Figure:** $h$-refinement DG density fields for Re=2,000
Figure: $h$-refinement DG density fields for $Re=10,000$
Out of range metric, $R_e = 2,000$

**Figure:** Out of range density fraction PDF for various CG and DG partitions at $N = 5$. The CG has a larger out of range fraction than DG for all cases except for the initial phase of the high resolution simulation with $320 \times 64$ partition.
Out of range metric, $R_e = 10,000$
Density Classes comparison at $t=80, \text{Re} = 2,000$

Figure: density PDF for the various runs for $N = 5$. 
Errors in water mass pdf at $t=20$, $R_e = 10,000$

**Figure:** Errors in pdf relative to CG reference
Energy history of reference simulation $R_e = 2,000$

**Figure:** Energy history for reference CG discretization at $N = 5$. 
Figure: Energy error histories for various DG discretization at $N = 5$. 
Figure: Energy error histories for various CG discretization at $N = 5$. 
Energy errors for $R_e = 10,000$

**Figure:** Energy errors normalized by TE of reference solution for a density DGM solution using $162 \times 34$ elements.
Conclusion for mixing

- Developed a model for gravity current mixing
- DGM discretization helps stabilize the model without excessive dissipation
- Water mass properties impacted more than energy
Iterative Solvers

1. currently substructuring (Schur complement)
2. Call standard libraries PETc
3. Tailored solver for current geometry
Domain Decomposition into $K$ rectangles

$$
\Omega_k = [x_{k-1} \ x_k] \times [-1 \ 0], \ k = 1, 2, \ldots, K
$$
Local Poisson problems

Equations 7 and 8 express the transmission conditions, namely the continuity of the function and its first derivative, across the $K - 1$ internal boundaries located at $x_k$. 

\[ \nabla^2 \psi^k = -\omega^k \text{ in } \Omega_k \]  
\[ \psi^k(x, 0) = \psi^k(x, -1) = 0 \]  
\[ \psi^1(x_0, z) = \psi^K(x_K, z) = 0 \]  
\[ \psi^k(x_k, 0) = \psi^{k+1}(x_k, z), \ k = 1, 2, \ldots, K - 1 \]  
\[ \psi^k_x(x_k, 0) = \psi^{k+1}_x(x_k, z), \ k = 1, 2, \ldots, K - 1 \]
Domain Decomposition: Split Solution $\psi^k = \hat{\psi}^k + \overline{\psi}^k$

1. Poisson problem

$$\nabla^2 \hat{\psi}^k = -\omega^k \text{ in } \Omega_k \tag{9}$$

$$\hat{\psi}^k(x, 0) = \hat{\psi}^k(x, -1) = 0 \tag{10}$$

$$\hat{\psi}^k(x_{k-1}, z) = \hat{\psi}^k(x_k, z) = 0 \tag{11}$$

2. Laplace problem

$$\nabla^2 \overline{\psi}^k = 0 \text{ in } \Omega_k \tag{12}$$

$$\overline{\psi}^k(x, 0) = \hat{\psi}^k(x, -1) = 0 \tag{13}$$

$$\overline{\psi}^k(x_{k-1}, z) = \alpha^{k-1}(z) \tag{14}$$

$$\overline{\psi}^k(x_k, z) = \alpha^k(z) \tag{15}$$
Analytical solution to Laplace problem

\[
\psi^k(x, z) = \sum_{n=1}^{\infty} \frac{\alpha_{n}^{k-1} \sinh \lambda_n (x_k - x) + \alpha_{n}^{k} \sinh \lambda_n (x - x_{k-1})}{\sinh \lambda_n l_k} \sin \lambda_n z
\]

\[
\alpha_{n}^{k} = \frac{\int_{-1}^{0} \alpha^{k}(z) \sin \lambda_n z \, dz}{\int_{-1}^{0} \sin^2 \lambda_n z \, dz}
\]

\[
\lambda_n = n\pi, \quad n = 1, 2, \ldots
\]

\[l_k = x_k - x_{k-1}.\]
Constraints on $\alpha^k$

$$\partial \psi^{k+1} \bigg|_{x_k} - \partial \psi^k \bigg|_{x_k} = - \left( \partial \hat{\psi}^{k+1} \bigg|_{x_k} - \partial \hat{\psi}^k \bigg|_{x_k} \right)$$  \hspace{1cm} (16)

$$\frac{\alpha^{k-1}}{\sinh \lambda_n l_k} - \left[ \frac{\cosh \lambda_n l_k}{\sinh \lambda_n l_k} + \frac{\cosh \lambda_n l_{k+1}}{\sinh \lambda_n l_{k+1}} \right] \alpha^n + \frac{\alpha^{k+1}}{\sinh \lambda_n l_{k+1}} = - \frac{\beta^n}{\lambda_n}$$

$$\beta^n = \frac{\int_{-1}^{0} \left[ \hat{\psi}^{k+1}_x(x_k, z) - \hat{\psi}^k_x(x_k, z) \right] \sin \lambda_n z \, dz}{\int_{-1}^{0} \sin^2 \lambda_n z \, dz}.$$  

External interfaces require that $\alpha^0 = \alpha^K = 0$. Symmetric tridiagonal system for each vertical mode $n$; Redundant parallel solution. Cut-off $n$? depends on $\beta^n_k$. For large $\lambda_n l_k >> 1$ the off-diagonal terms asymptote to zero. Diagonal term asymptotes to 2.
Domain Decomposition Algorithm

1. Solve inhomogeneous Poisson problem for $\hat{\psi}^k$.
2. Compute normal flux jump at internal interfaces $[\hat{\psi}_x^k]$.
3. Compute Fourier-sine coefficients: $\beta_n^k = S[\hat{\psi}_x^k]$.
4. Broadcast $\beta_n^k$ to all processors.
5. Solve tridiagonal systems on all processors $\alpha_n^k = T^{-1}\beta_n^k$.
6. Compute interfacial solution $\alpha^k = S^T\alpha_n^k$.
7. Solve local Laplace problems.
Domain Decomposition Algorithm

1. Schur complement problem: $\alpha^k = S^T T^{-1} S \left[ \hat{\psi}^k_x \right]$

2. When geometry is not rectangular the above provide for symmetric preconditioner for the Schur complement problem.
Weak scalability analysis

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<th>$K_y$</th>
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<tr>
<td>288</td>
<td>8</td>
<td>18</td>
<td>0.1583</td>
</tr>
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</table>

Table: Scalability for 128 elements/processor
Analytical solution of tridiagonal system for $l_k = l$

Define Fourier-sine transform along the partition index:

$$
\begin{pmatrix}
\alpha^k_n \\
\beta^k_n
\end{pmatrix} = \frac{2}{K} \sum_{m=1}^{K-1} \begin{pmatrix}
\hat{\alpha}^m_n \\
\hat{\beta}^m_n
\end{pmatrix} \sin \frac{\pi km}{K}
$$

(17)

Orthogonality of the functions $\sin \frac{\pi km}{K}$:

$$
\hat{\alpha}^m_n = \frac{\hat{\beta}^m_n}{2\lambda_n} \left[ \coth \lambda_n l - \sinh^{-1} \lambda_n l \cos \frac{m\pi}{K} \right].
$$

(18)
Analytical solution of tridiagonal system for $l_k = l$

\[
\alpha_n^k = \frac{2}{K} \sum_{m=1}^{K-1} \frac{\hat{\beta}_m^j}{2\lambda_n} \left[ \coth \lambda_n l - \sinh^{-1} \lambda_n l \cos \frac{m\pi}{K} \right] \sin \frac{\pi km}{K}
\]

\[
= \sum_{j=1}^{K-1} \frac{1}{\lambda_n K} \sum_{m=1}^{K-1} \frac{\sin \frac{\pi km}{K} \sin \frac{\pi jm}{K}}{\coth \lambda_n l - \sinh^{-1} \lambda_n l \cos \frac{m\pi}{K}} \beta_n^j
\]

where the matrix $B_{jk}^n$ is the inverse of the tridiagonal matrix.
Analytical solution of tridiagonal system for $l_k = l$

Left: $\left| \frac{\sinh \lambda_n l}{\cosh \lambda_n l - 1} - 1 \right|$ versus $n$

Right: $\frac{1}{2\lambda_n} \max_{1 \leq i \leq N} (|C_{i,n}^{e,k}|, |S_{i,n}^{e,k}|)$ versus $n$. 
Computation of Fourier-sine coefficients

\[
\beta_{kn} = 2 \int_{-1}^{0} \left[ \hat{\psi}_x^k(x_k, z) \right] \sin \lambda_n z \, dz \\
= \sum_{e=1}^{E} \Delta z_e \int_{-1}^{1} \left[ \hat{\psi}_x^k(x_k, \sigma) \right] \sin \lambda_n \left( \Delta z_e \frac{\sigma + 1}{2} + z_{e-1} \right) \, d\sigma \beta_{kn} \\
= \sum_{e=1}^{E} \sum_{i=1}^{N} \left( C_{i,n}^{e,k} \cos \lambda_n z_e + S_{i,n}^{e,k} \sin \lambda_n z_e \right) \left[ \hat{\psi}_x^k(x_k, z_i^e) \right]
\]

\[
C_{i,n}^{e,k} = \Delta z_e \int_{-1}^{1} h_i(\sigma) \sin \frac{\lambda_n \Delta z_e \sigma}{2} \, d\sigma \\
S_{i,n}^{e,k} = \Delta z_e \int_{-1}^{1} h_i(\sigma) \cos \frac{\lambda_n \Delta z_e \sigma}{2} \, d\sigma
\]
Computation of Fourier-sine coefficients

\[ h_i(\sigma) = \sum_{m=0}^{N-1} h_{i,m} P_m(\sigma) \] (19)

\[ C_{i,n}^{e,k} = \Delta z_e \sum_{m=0}^{N-1} h_{im} \int_{-1}^{1} P_m(\sigma) \sin \frac{\lambda_n \Delta z_e \sigma}{2} \, d\sigma \] (20)

\[ S_{i,n}^{e,k} = \Delta z_e \sum_{m=0}^{N-1} h_{im} \int_{-1}^{1} P_m(\sigma) \cos \frac{\lambda_n \Delta z_e \sigma}{2} \, d\sigma \] (21)

\( P_m \): Legendre polynomial of degree \( m \).
\( h_{im} \): \( m \)-th Legendre spectral coefficient of \( h_i(\sigma) \)
Computation of Fourier-sine coefficients

\[ C_{i,n}^{e,k} = 2 \Delta z_e \sum_{m=1,3,5}^{N-1} (-1)^{\frac{m-1}{2}} \ h_{im} j_m \left( \frac{\lambda_n \Delta z_e}{2} \right) \]  \hspace{1cm} (22)

\[ S_{i,n}^{e,k} = 2 \Delta z_e \sum_{m=0,2,4}^{N-1} (-1)^{\frac{m}{2}} \ h_{im} j_m \left( \frac{\lambda_n \Delta z_e}{2} \right) \]  \hspace{1cm} (23)
Inverse Projection: Fourier-sine to Spectral element space

\[ u(z) = \sum_{n} \hat{u}_n \sin \lambda_n z = \sum_{i=1}^{N} u_i h_i(z) \quad z_{e-1} \leq z \leq z_e \]

The matrix equations for the Fourier coefficients become

\[ Mu = b \quad (24) \]

\[ b_j = \sum_{n} \hat{u}_n \int_{z_0}^{z_E} h_j(z) \sin \lambda_n z \, dz \quad (25) \]

\[ = \sum_{n} \hat{u}_n \sum_{e} \frac{1}{2} \left[ C_{j,n}^e \cos \lambda_n z_e + S_{j,n}^e \sin \lambda_n z_e \right] \quad (26) \]

\( M \) is 1D mass

\( C_{j,n}^e \) and \( S_{j,n}^e \) are as before
Solver Development Conclusion

- Validated transformation between SE and sine-spaces
- Developed and tested solver
- Initial scalability tests promising
- Room for improvement
- Compare specialized solver performance to other methods