# High-resolution modeling of three-dimensional circulation in the Gulf of Mexico

Arash Fathi[1], Casey Dietrich[2], Clint Dawson[1], Kendra Dresback[3]

[1]Institute for Computational Engineering and Sciences, University of Texas at Austin
[2]Dept. of Civil, Construction, and Environmental Engineering, NC State University
[3]School of Civil Engineering and Environmental Science, University of Oklahoma

**February 12th, 2016**

# Outline

**3D Shallow Water Equations**

**Accurate computation of baroclinic pressure gradients and horizontal diffusion terms**

**Numerical experiments –toy problems**

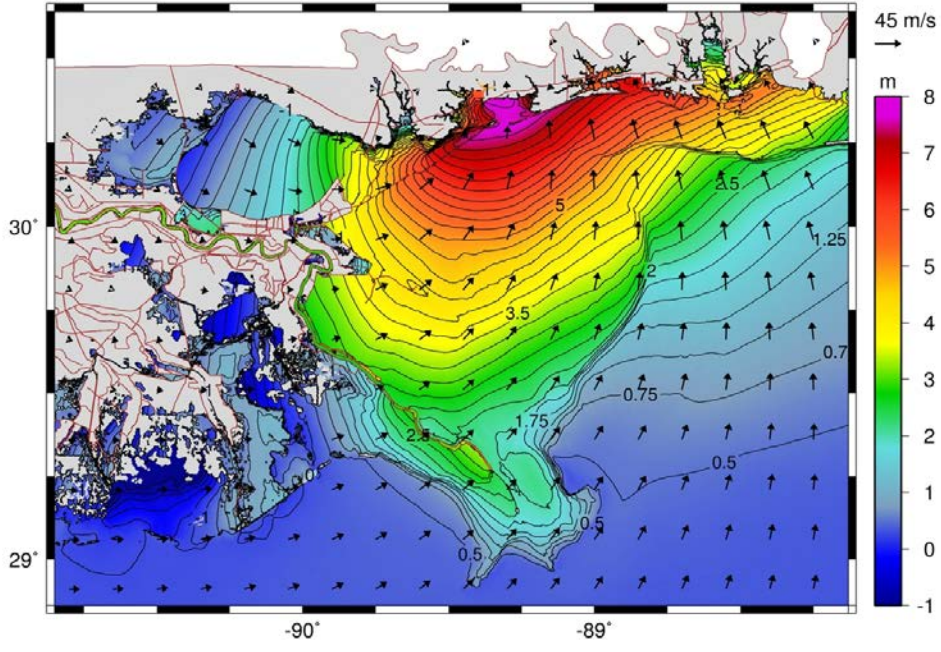
**Bathymetry smoothing**

**Gaussian filter for bathymetry/velocity**

**Biharmonic viscosity operator**

**Smagorinsky/Leith viscosity parameter**

**Simulation results of Gulf of Mexico**




Storm surge during Hurricane Katrina.

# 3D Shallow Water Equations (SWE)

**Spherical coordinate:**

- Continuity:

$$\frac{1}{R\cos\phi}\frac{\partial u}{\partial \lambda} + \frac{1}{R\cos\phi}\frac{\partial (v\cos\phi)}{\partial \phi} + \frac{\partial w}{\partial z} + \frac{2w}{R} = 0.$$

- Horizontal momentum:

$$\frac{\partial u}{\partial t} + \frac{u}{R\cos\phi}\frac{\partial u}{\partial \lambda} + \frac{v}{R}\frac{\partial u}{\partial \phi} + w\frac{\partial u}{\partial z} = fv - \frac{1}{R\cos\phi}\frac{\partial[g(\zeta-\alpha\eta)+p_s/\rho_0]}{\partial \lambda} + \frac{\partial}{\partial z}\left(\frac{\tau_{z\lambda}}{\rho_0}\right) - b_\lambda + m_\lambda,$$

$$\frac{\partial u}{\partial t} + \frac{u}{R\cos\phi}\frac{\partial u}{\partial \lambda} + \frac{v}{R}\frac{\partial u}{\partial \phi} + w\frac{\partial u}{\partial z} = -fu - \frac{1}{R}\frac{\partial[g(\zeta-\alpha\eta)+p_s/\rho_0]}{\partial \phi} + \frac{\partial}{\partial z}\left(\frac{\tau_{z\phi}}{\rho_0}\right) - b_\phi + m_\phi,$$

where: $b_\lambda = \frac{g}{\rho_0 R\cos\phi}\frac{\partial}{\partial \lambda}\int_z^\zeta \rho\, dz, \qquad b_\phi = \frac{g}{\rho_0 R}\frac{\partial}{\partial \phi}\int_z^\zeta \rho\, dz.$

ADCIRC does not solve the primitive continuity equation directly. It solves the generalized wave continuity equation, which is a combination of the primitive continuity equation, its temporal derivative, and spatial derivatives of the depth-integrated momentum equations.

# 3D Shallow Water Equations (SWE)

**Cartesian coordinate:**

$$S_p \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0,$$

$$\frac{\partial u}{\partial t} + u S_p \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} - f v = -S_p \frac{\partial [g(\zeta - \alpha\eta) + p_s/\rho_0]}{\partial x} + \frac{\partial}{\partial z}\left(\frac{\tau_{zx}}{\rho_0}\right) - b_x + m_x,$$

$$\frac{\partial v}{\partial t} + u S_p \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} + f u = -\frac{\partial [g(\zeta - \alpha\eta) + p_s/\rho_0]}{\partial y} + \frac{\partial}{\partial z}\left(\frac{\tau_{zy}}{\rho_0}\right) - b_y + m_y,$$

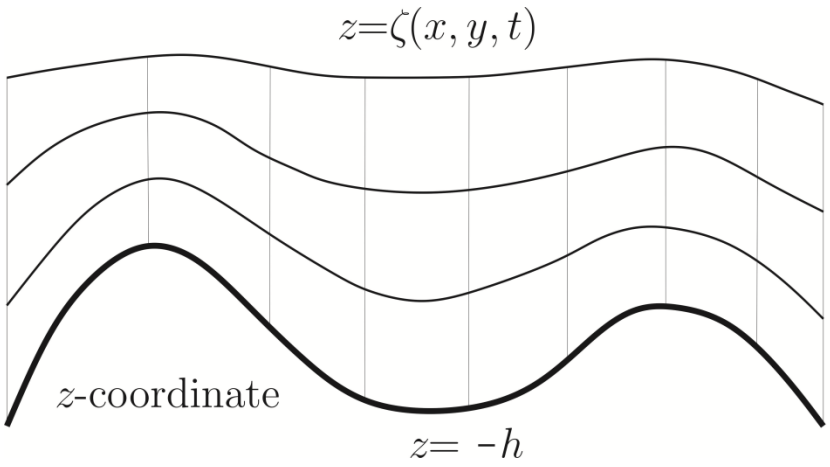
where $S_p = \frac{\cos\phi_0}{\cos\phi}$

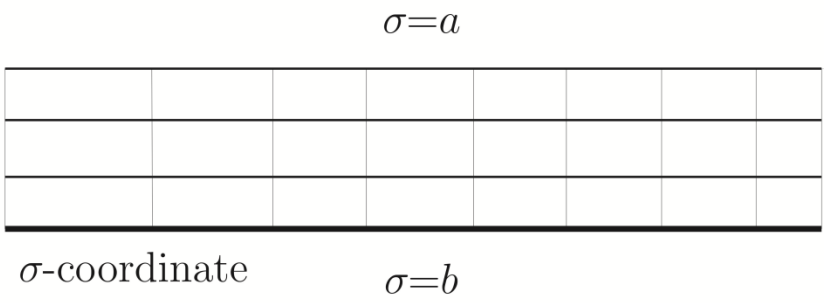
**Baroclinic pressure gradient:**

$$b_x = \frac{g}{\rho_0} S_p \frac{\partial}{\partial x} \int_z^\zeta \rho \, dz = \frac{g}{\rho_0} S_p \frac{\partial}{\partial x} \int_z^\zeta (\rho - \rho_o) \, dz,$$

$$b_y = \frac{g}{\rho_0} \frac{\partial}{\partial y} \int_z^\zeta \rho \, dz = \frac{g}{\rho_0} \frac{\partial}{\partial y} \int_z^\zeta (\rho - \rho_o) \, dz.$$

# Sigma coordinate




**Sigma coordinate:**

$$x_\sigma = x,$$

$$y_\sigma = y,$$

$$\sigma = a + \frac{a-b}{H}(z-\zeta), \quad a = +1, \quad b = -1,$$

$$t_\sigma = t.$$

# 3D Shallow Water Equations (SWE)

**Sigma coordinate:**

$$\frac{\partial u}{\partial t_\sigma} + uS_p\frac{\partial u}{\partial x_\sigma} + v\frac{\partial u}{\partial y_\sigma} + w_\sigma(\frac{a-b}{H})\frac{\partial u}{\partial \sigma} - fv =$$
$$- S_p\frac{\partial[g(\zeta-\alpha\eta)+p_s/\rho_0]}{\partial x} + (\frac{a-b}{H})\frac{\partial}{\partial\sigma}(\frac{\tau_{zx}}{\rho_0}) - b_x + m_x,$$
$$\frac{\partial v}{\partial t_\sigma} + uS_p\frac{\partial v}{\partial x_\sigma} + v\frac{\partial v}{\partial y_\sigma} + w_\sigma(\frac{a-b}{H})\frac{\partial v}{\partial \sigma} + fu =$$
$$- \frac{\partial[g(\zeta-\alpha\eta)+p_s/\rho_0]}{\partial y} + (\frac{a-b}{H})\frac{\partial}{\partial\sigma}(\frac{\tau_{zy}}{\rho_0}) - b_y + m_y,$$

$$w_\sigma = w - \Big(\frac{\sigma-b}{a-b}\Big)\frac{\partial\zeta}{\partial x} - u\Big[(\frac{\sigma-b}{a-b})\frac{\partial\zeta}{\partial x} + (\frac{\sigma-a}{a-b})\frac{\partial h}{\partial x}\Big] - v\Big[(\frac{\sigma-b}{a-b})\frac{\partial\zeta}{\partial y} + (\frac{\sigma-a}{a-b})\frac{\partial h}{\partial y}\Big].$$

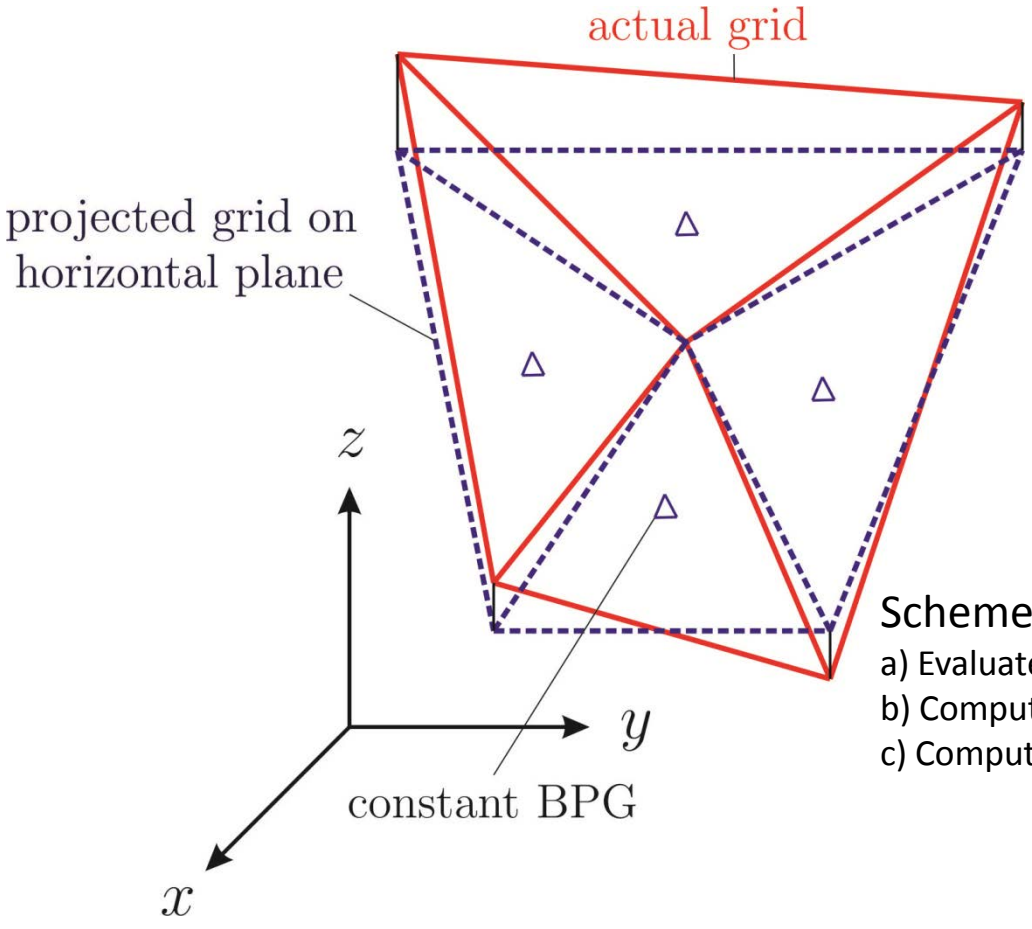
# Baroclinic pressure gradient (BPG)

**Sigma coordinate:**

$$P = \frac{g}{\rho_0} \int_z^{\zeta} \rho \, dz$$

$$b_x = \frac{\partial P}{\partial x} = \frac{\partial P}{\partial x_\sigma} + \frac{\partial P}{\partial \sigma} \frac{\partial \sigma}{\partial x}$$

# Baroclinic pressure gradient: z-coordinate



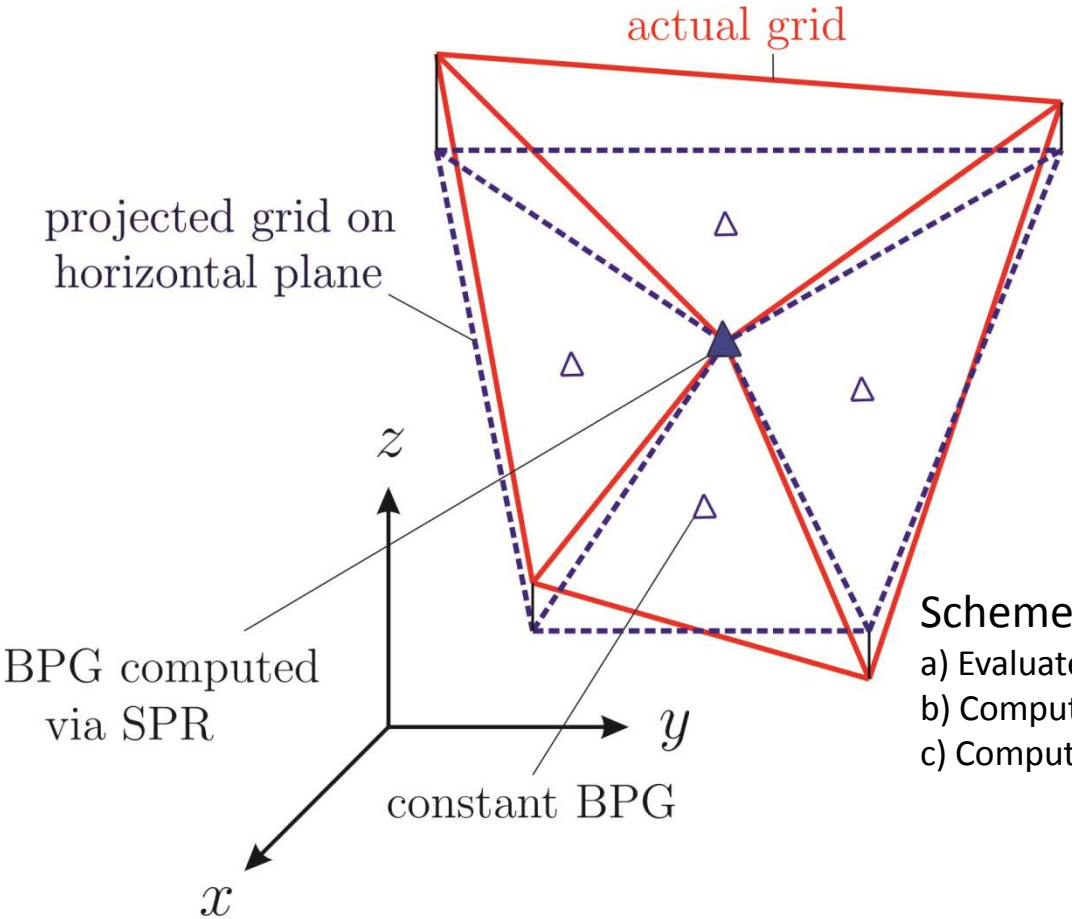

Scheme 1:

a) Evaluate pressure at the vertices of the projected elements.

b) Compute constant $BPG_{x/y}$ for each element.

c) Compute the weak form: ($BPG_{x/y}$ , test function).

# Baroclinic pressure gradient: z-coordinate

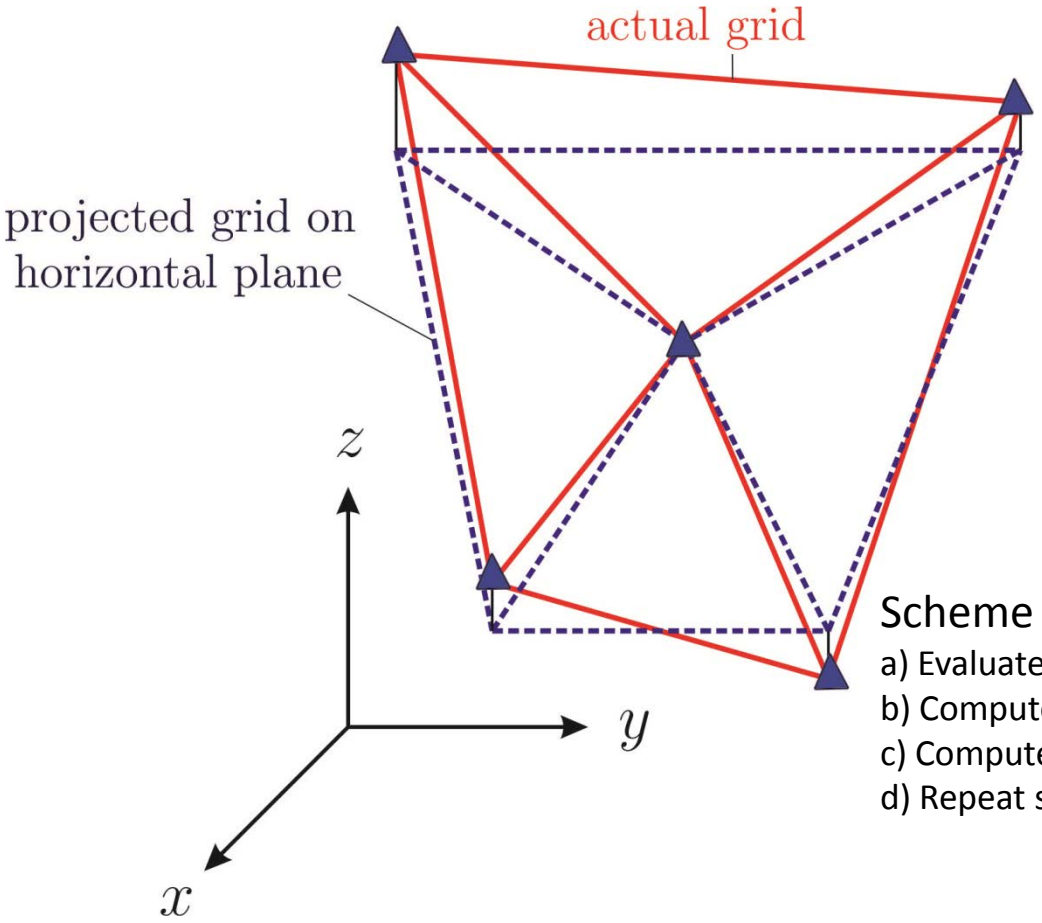



Scheme 2:

a) Evaluate pressure at the vertices of the projected elements.
b) Compute constant $BPG_{x/y}$ for each element.
c) Compute $BPG_{x/y}$ for the vertex of interest via SPR.

SPR: superconvergent patch recovery - OC Zienkiewicz and JZ Zhu (1992). The superconvergent patch recovery and a posteriori error estimates. Part 1: The recovery technique. *IJNME*, 33(7), 1331-1364.

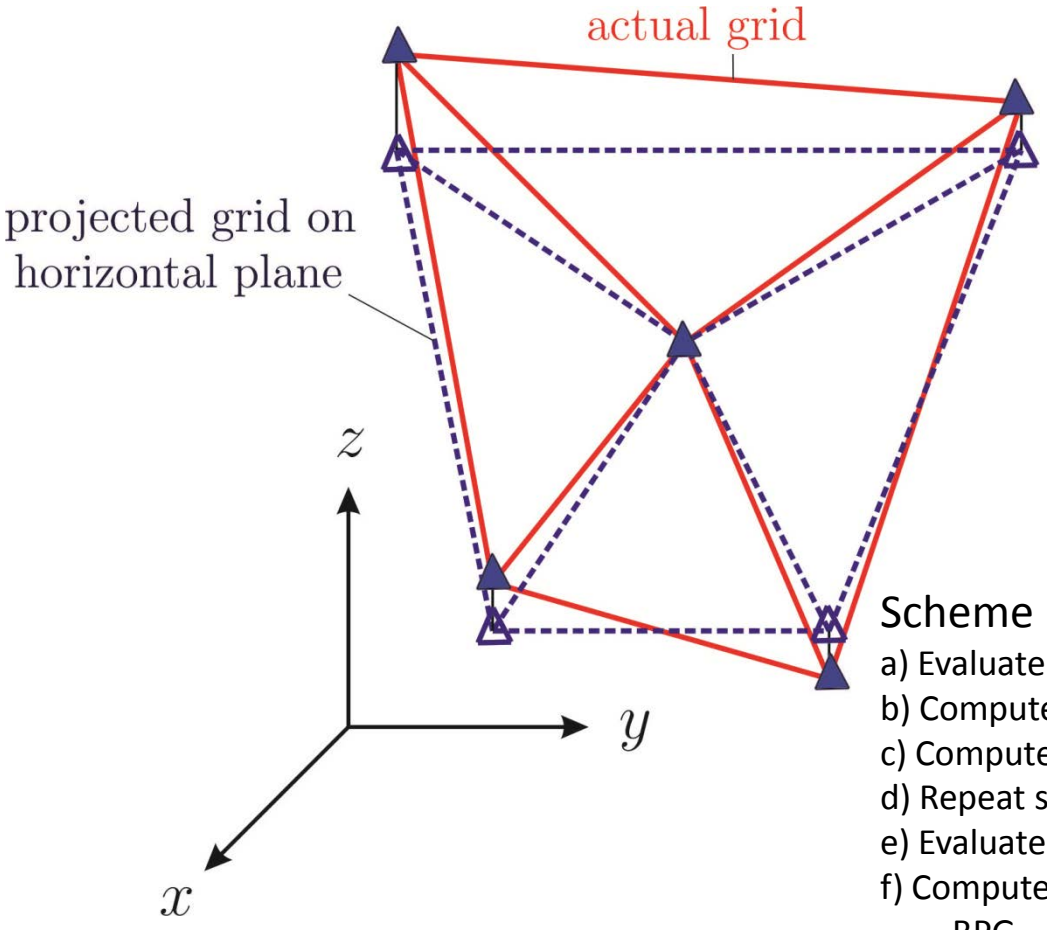
# Baroclinic pressure gradient: z-coordinate




Scheme 2:

a) Evaluate pressure at the vertices of the projected elements.
b) Compute constant $BPG_{x/y}$ for each element.
c) Compute $BPG_{x/y}$ for the vertex of interest via SPR.
d) Repeat steps a-c for all vertices.

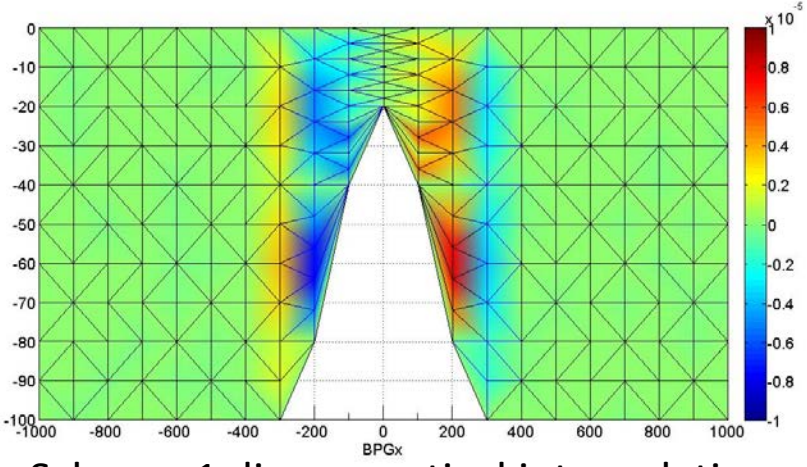
# Baroclinic pressure gradient: z-coordinate



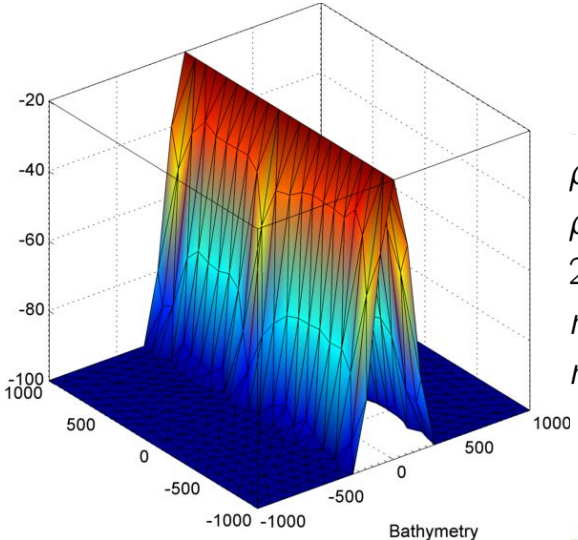

Scheme 2:

a) Evaluate pressure at the vertices of the projected elements.
b) Compute constant $BPG_{x/y}$ for each element.
c) Compute $BPG_{x/y}$ for the vertex of interest via SPR.
d) Repeat steps a-c for all vertices.
e) Evaluate $BPG_{x/y}$ at the vertices of the projected elements.
f) Compute the weak form: ($BPG_{x/y}$ , test function), where now $BPG_{x/y}$ varies linearly within an element, and is continuous across elements.

# Numerical experiment: BPG error for stratified fluid




Scheme 1: linear vertical interpolation



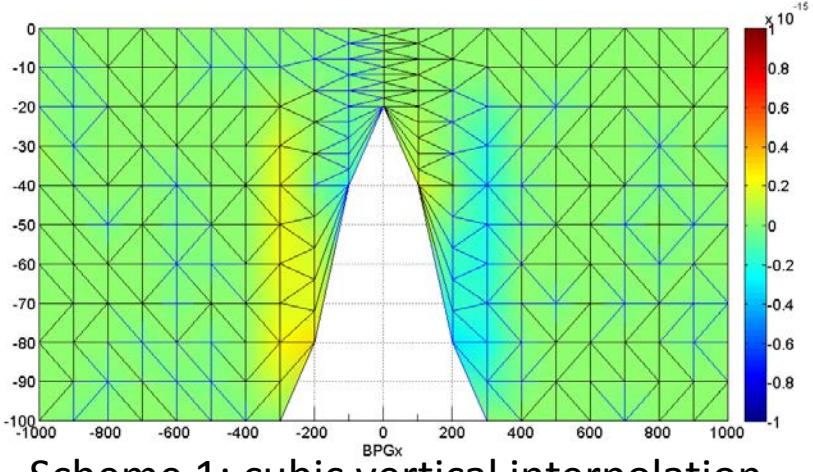
$\rho_{\text{top}} = 34$ psu

$\rho_{\text{bot}} = 35$ psu

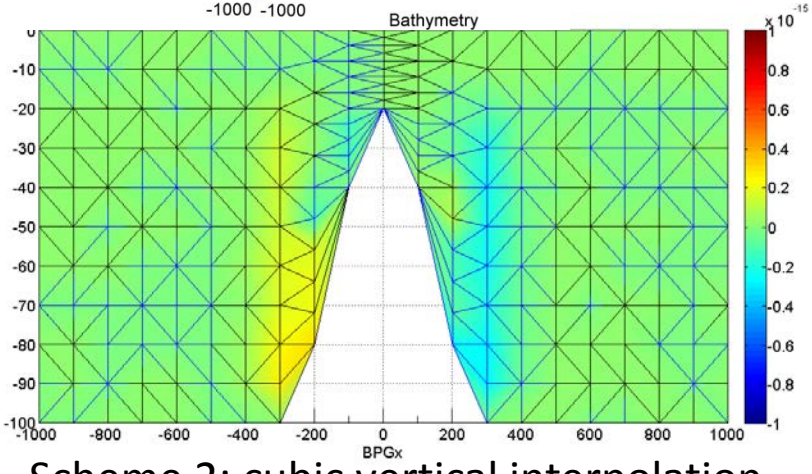
21 sigma layers

$rx_0 = 0.45$

$rx_1 = 17.6$

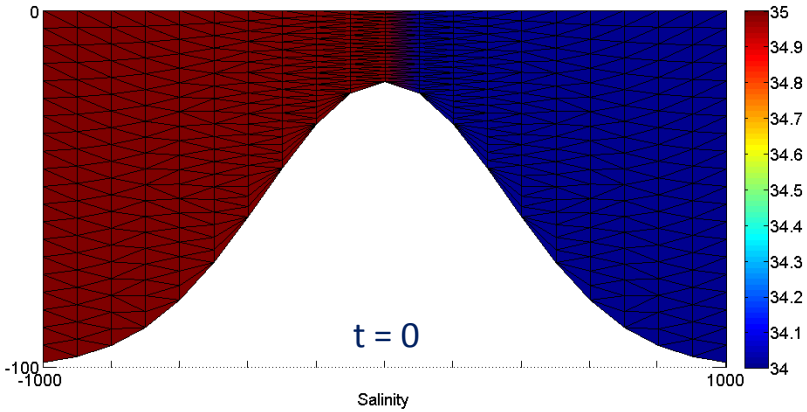



Scheme 1: cubic vertical interpolation




Scheme 2: cubic vertical interpolation

# Numerical experiment: lock-exchange problem



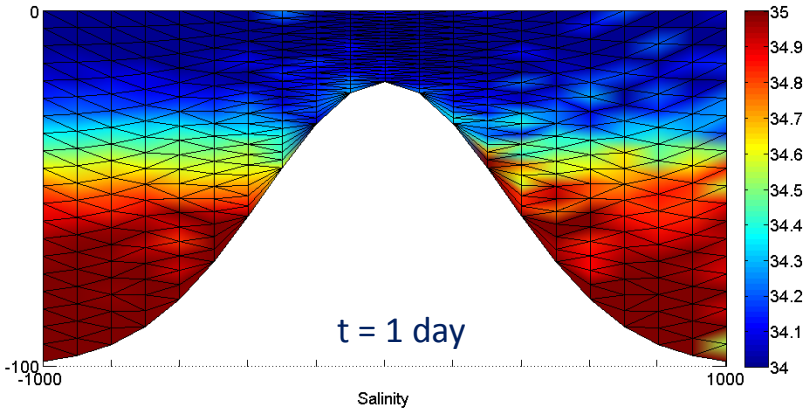

$\rho_{\text{left}} = 35$ psu

$\rho_{\text{right}} = 34$ psu

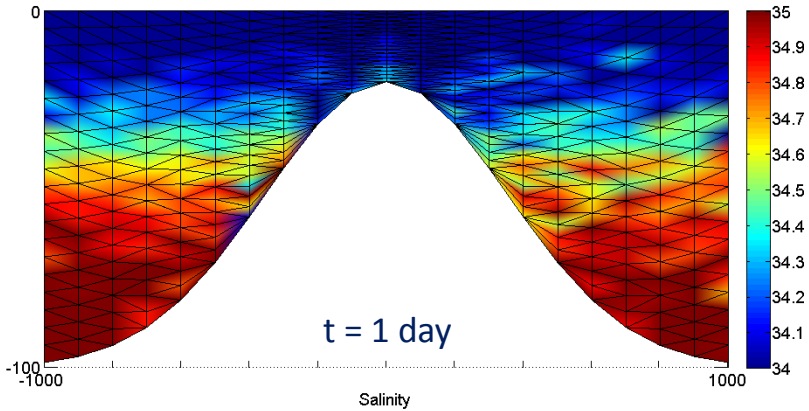
21 sigma layers

$rx_0 = 0.18$

$rx_1 = 7.1$




Scheme 1: cubic vertical interpolation




Scheme 2: cubic vertical interpolation

# Transport of salinity and temperature – horizontal diffusion

**Cartesian coordinate:**

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} + w\frac{\partial c}{\partial z} - \frac{\partial}{\partial x}\left(N_h\frac{\partial c}{\partial x}\right) - \frac{\partial}{\partial y}\left(N_h\frac{\partial c}{\partial y}\right) - \frac{\partial}{\partial z}\left(N_v\frac{\partial c}{\partial z}\right) = 0$$

**In sigma coordinate:**

$$\frac{\partial}{\partial x}\left(N_h\frac{\partial c}{\partial x}\right) = \frac{\partial}{\partial x_\sigma}\left(N_h\frac{\partial c}{\partial x_\sigma}\right) + \frac{\partial}{\partial x_\sigma}\left(N_h\frac{\partial c}{\partial \sigma}\frac{\partial \sigma}{\partial x}\right) + \frac{\partial}{\partial \sigma}\left(N_h\frac{\partial c}{\partial x_\sigma}\right)\frac{\partial \sigma}{\partial x} + \frac{\partial}{\partial \sigma}\left(N_h\frac{\partial c}{\partial \sigma}\frac{\partial \sigma}{\partial x}\right)\frac{\partial \sigma}{\partial x}.$$

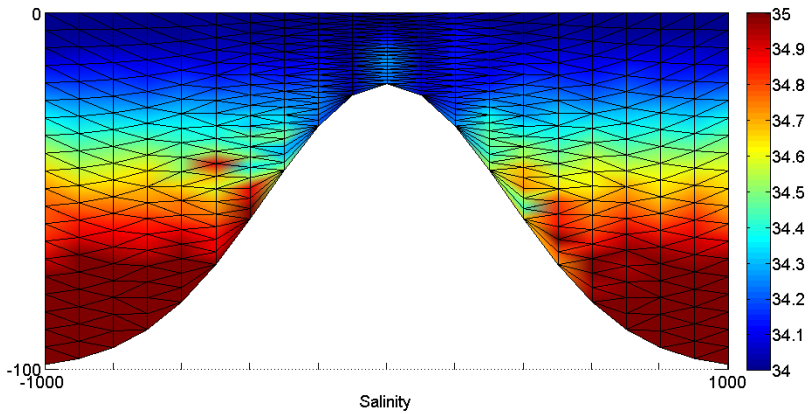
**Iso-sigma diffusion:**

$$\frac{\partial}{\partial x}\left(N_h\frac{\partial c}{\partial x}\right) \approx \frac{\partial}{\partial x_\sigma}\left(N_h\frac{\partial c}{\partial x_\sigma}\right).$$

# Transport of salinity and temperature – horizontal diffusion

**Sigma+Cartesian coordinate:**

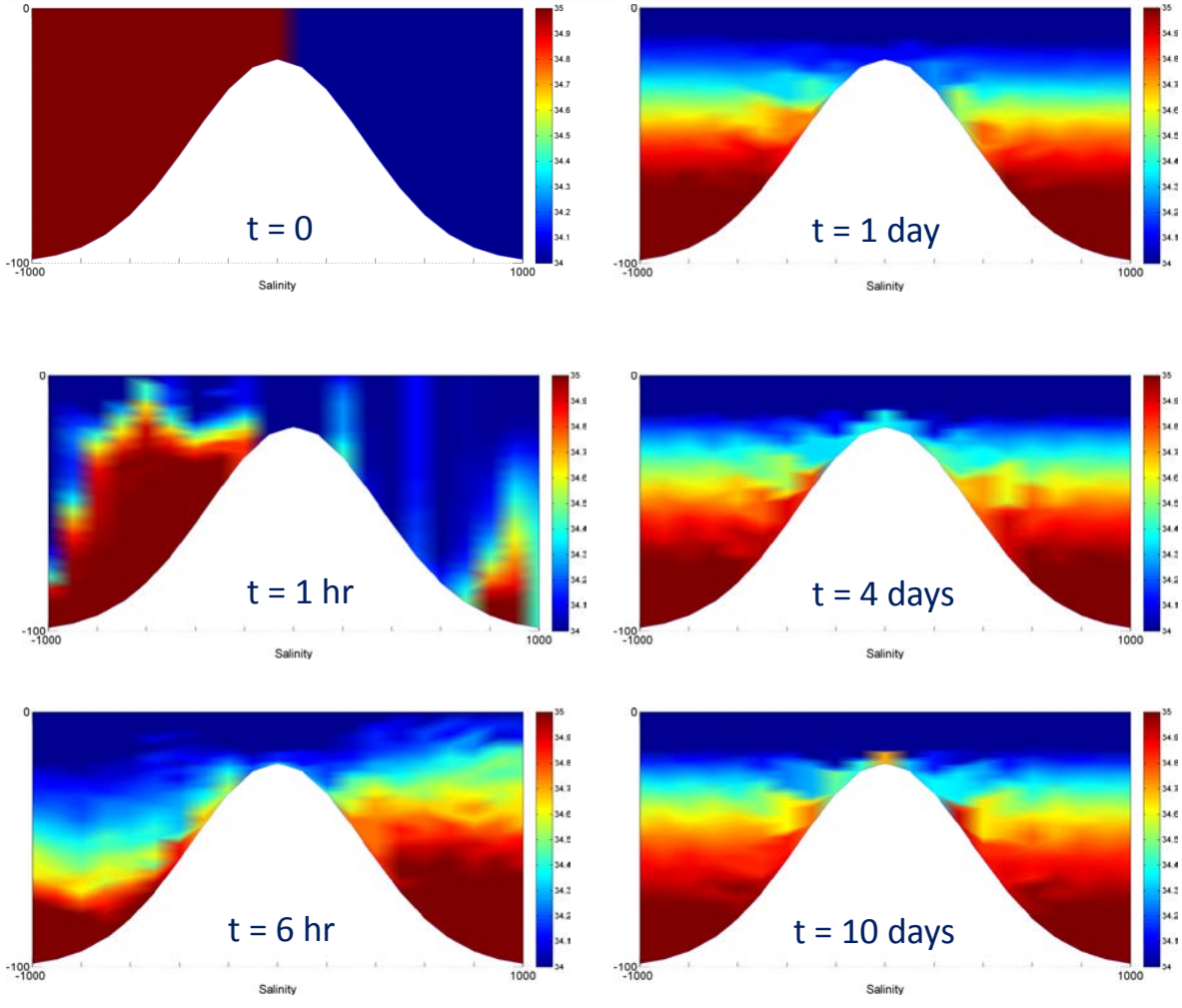
$$\overbrace{\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x_\sigma} + v\frac{\partial c}{\partial y_\sigma} + w_\sigma\left(\frac{a-b}{H}\right)\frac{\partial c}{\partial \sigma}}^{\sigma\text{-coordinate}} - \overbrace{\frac{\partial}{\partial x}\left(N_h\frac{\partial c}{\partial x}\right) - \frac{\partial}{\partial y}\left(N_h\frac{\partial c}{\partial y}\right)}^{z\text{-coordinate}} - \overbrace{\left(\frac{a-b}{H}\right)^2\frac{\partial}{\partial \sigma}\left(N_v\frac{\partial c}{\partial \sigma}\right)}^{\sigma\text{-coordinate}} = 0.$$

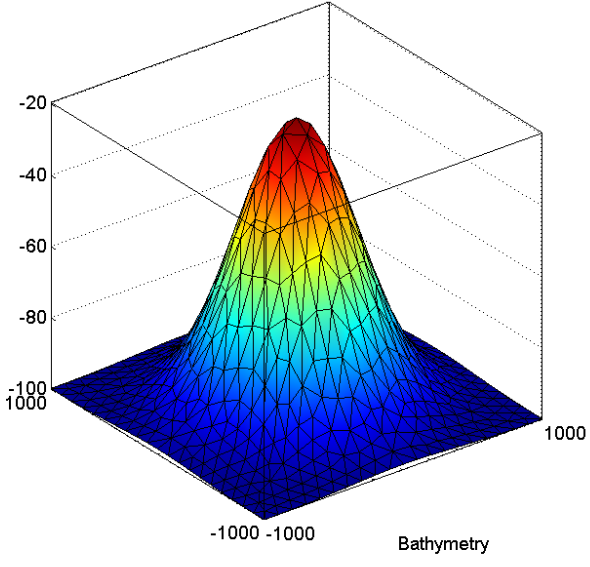



Iso-sigma diffusion (lock-exchange after 40 days).

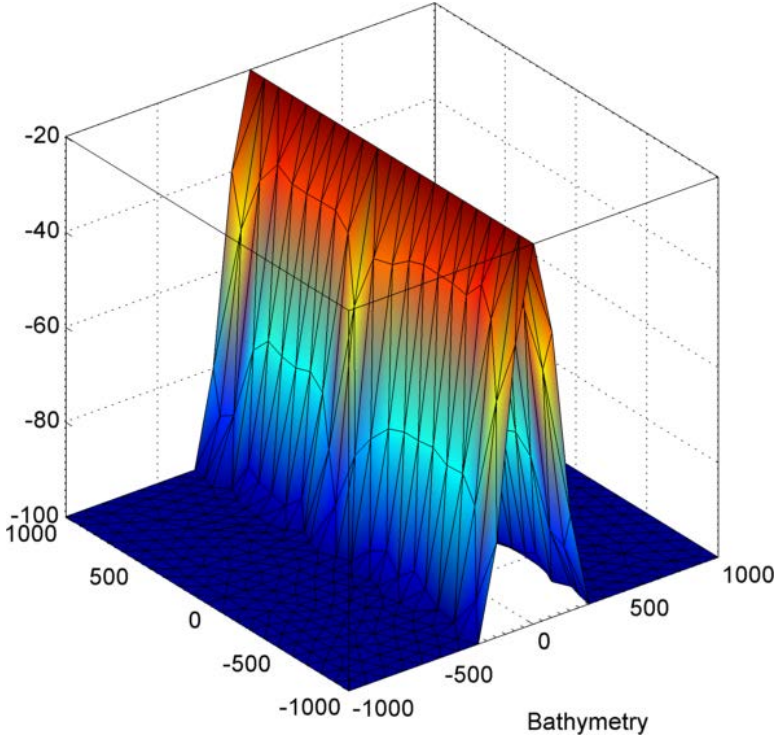
Correct treatment of horizontal diffusion (lock-exchange after 40 days).

# Numerical experiment: lock-exchange problem

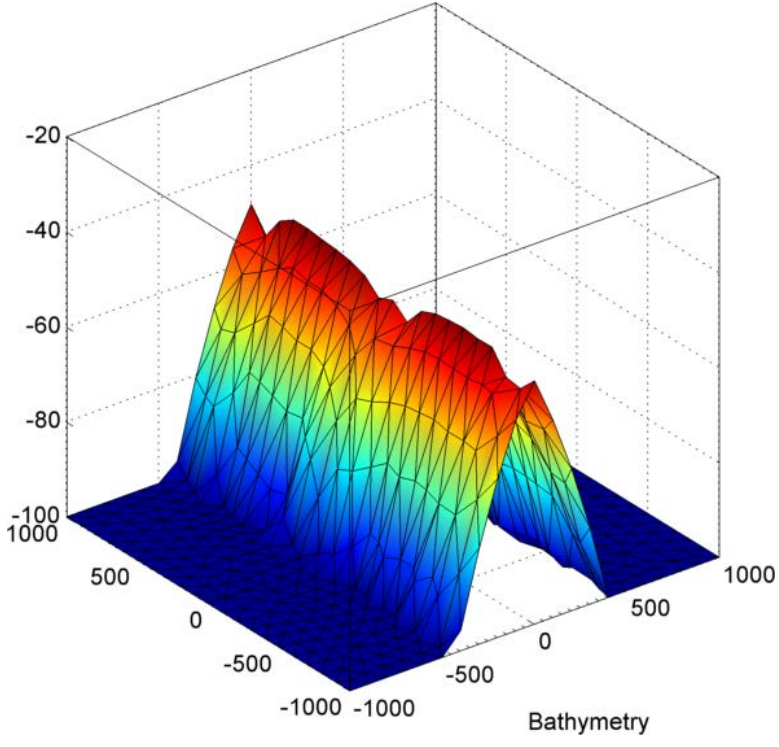


# Steep bathymetry - smoothing




$rx_0$=0.45, $rx_1$=17.6, maximum element slope=0.31
Unstable (<1 day)




$rx_0$=0.09, $rx_1$=3.6, maximum element slope=0.20
Stable (180 days)

# Steep bathymetry - smoothing for rx0

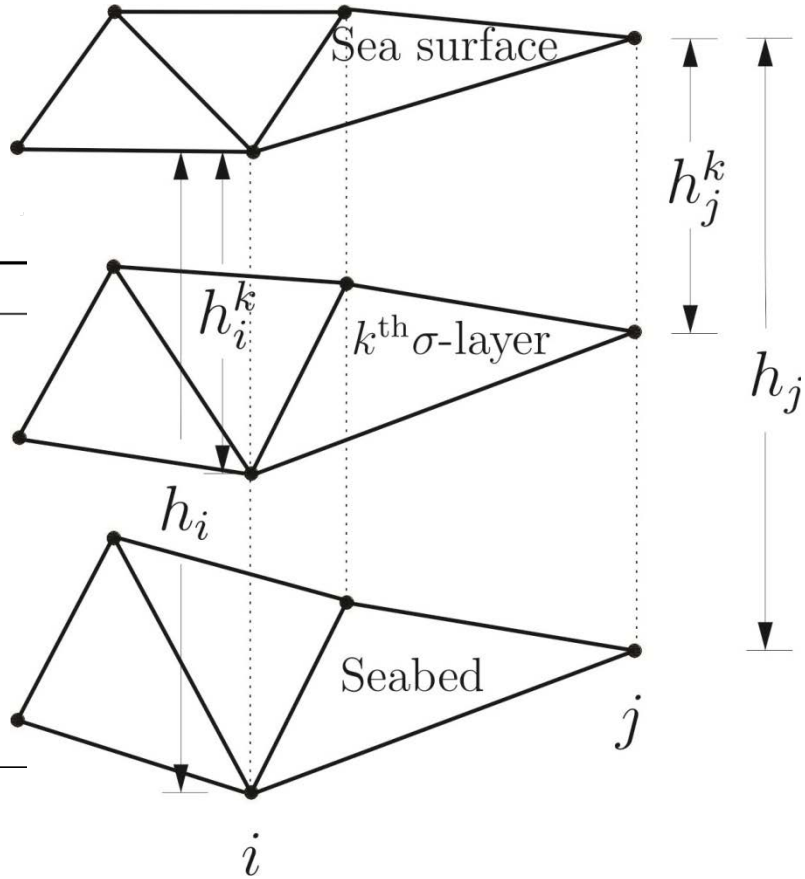
**Bathymetry roughness indicators:**

$$rx_0 = \frac{|h_i - h_j|}{h_i + h_j}, \quad (\text{range} : 0.15 - 0.2)$$

$$rx_1 = \frac{|h_i^k - h_j^k + h_i^{k-1} - h_j^{k-1}|}{h_i^k + h_j^k - h_i^{k-1} - h_j^{k-1}}, \quad (\text{range} : 3 - 8)$$

**Algorithm 1** Smoothing bathymetry for $rx_0$.

```
for iter = 1 : iter_max do
    loop over all elements
        loop over all edges of an element
            if |h_i − h_j| / (h_i + h_j) > r_desired then
                h_i = h_i − δ and h_j = h_j + δ s.t. |h_i − h_j| / (h_i + h_j) = r_desired
            end if
        end loop
    end loop
end for
```

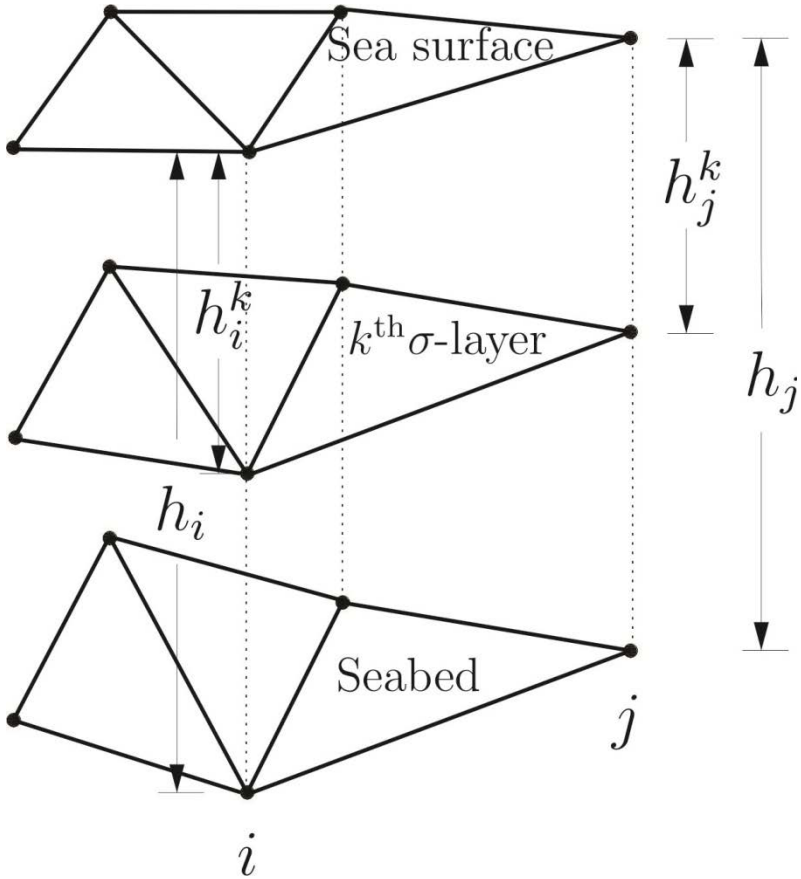



MD Sikiric, *et al.* (2009). A new approach to bathymetry smoothing in sigma-coordinate ocean models. *Ocean Modelling*, 29, 128-136.

# Steep bathymetry - smoothing for rx1

**Algorithm 1** Smoothing bathymetry for $rx_1$.

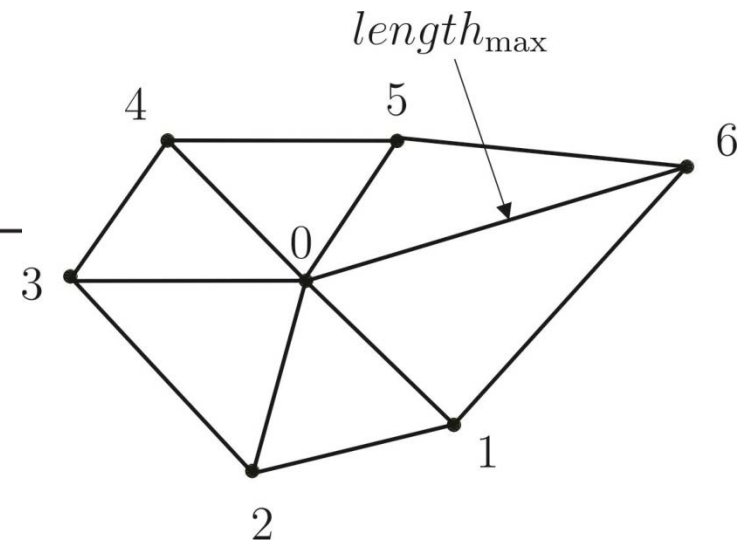
**for** iter $= 1 :$ iter$_{\max}$ **do**
  **loop** over all elements
    **loop** over all edges of an element
      **loop** over all vertical layers
        **if** $\frac{|h_i^k - h_j^k + h_i^{k-1} - h_j^{k-1}|}{h_i^k + h_j^k - h_i^{k-1} - h_j^{k-1}} > r_{\text{desired}}$ **then**
          $h_i = h_i - \delta$ and $h_j = h_j + \delta$
          s.t. $\frac{|h_i^k - h_j^k + h_i^{k-1} - h_j^{k-1}|}{h_i^k + h_j^k - h_i^{k-1} - h_j^{k-1}} > r_{\text{desired}}$
        **end if**
      **end loop**
    **end loop**
  **end loop**
**end for**



# Gaussian filter (smoother)

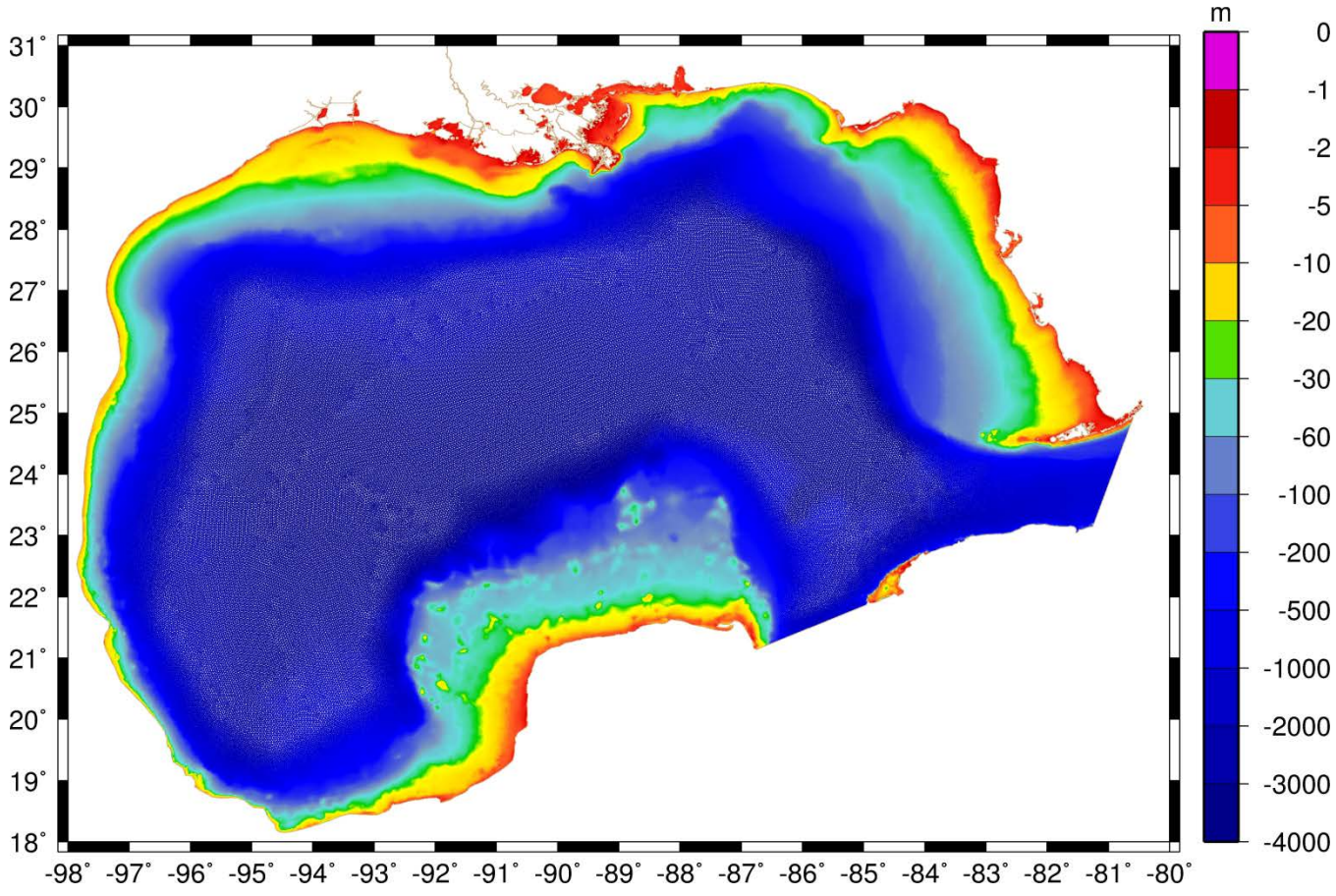
**Algorithm 3** Gaussian smoother: $q \rightarrow q_{\text{smooth}}$

```
loop over all nodes
    loop over all neighbor nodes of the above node          ▷ Number of neighbors = N
        find l_max: maximum distance from the center node to its neighbors
        σ = l_max × α                                       ▷ e.g. α = 0.7
    end loop
    loop over the center node and all of its neighbors
        find the distance l_i from the central node to the neighbor node
        compute node's weight: w_i = exp(−l_i^2 / (2σ^2))
        normalize weights, such that: Σ_0^N w_i = 1
        q_smooth(0) = Σ_0^N q_i w_i
    end loop
end loop
```



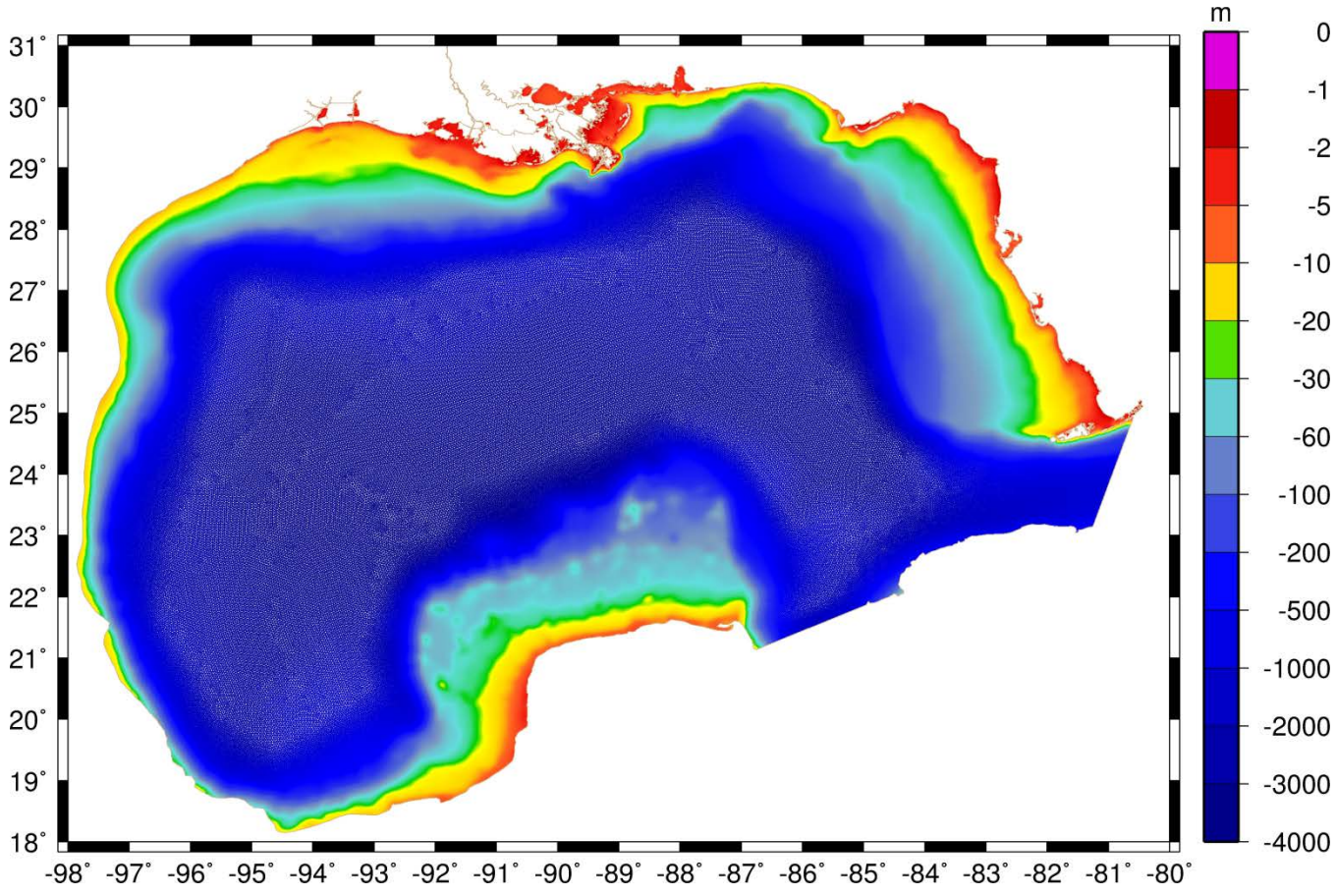

Another bathymetry smoothing technique: diffusion (MITgcm)

# SL-16 finite element mesh for Southeastern Louisiana

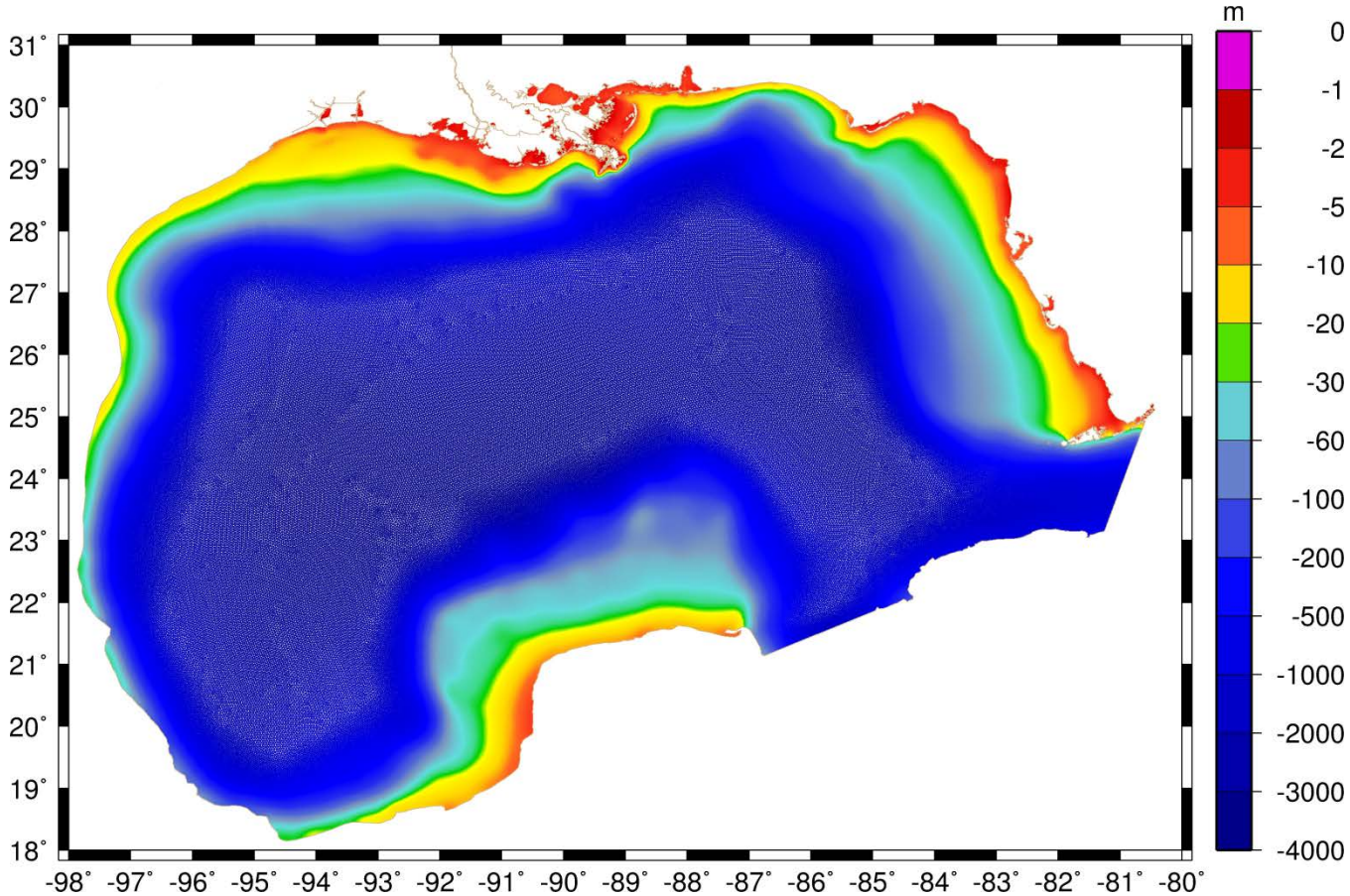



4’751’299 elements
2’437’172 nodes

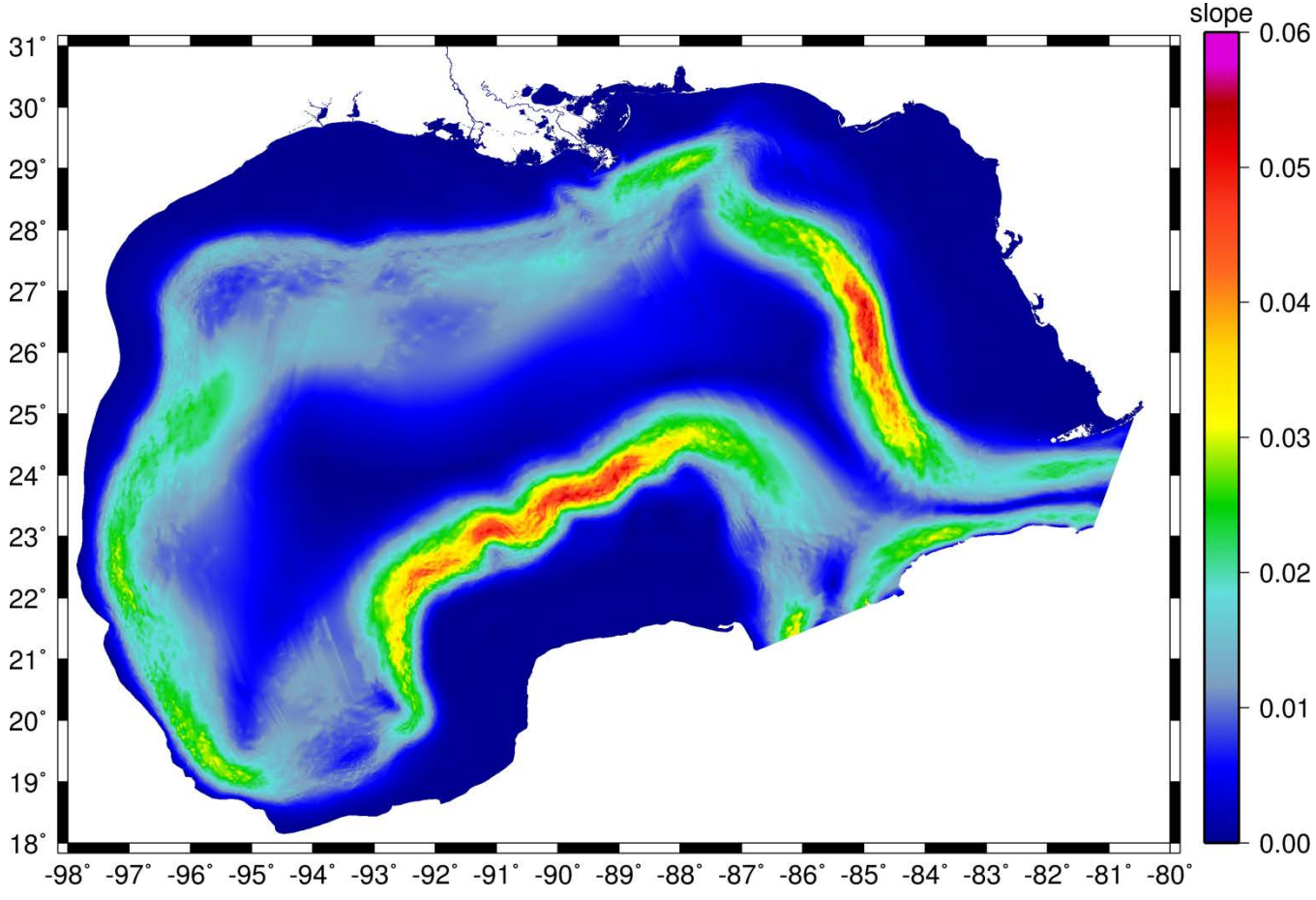
# SL-16 after smoothing for rx0 and rx1



# SL-16: rx0, rx1 + repeated application of the Gaussian filter



# Slope parameter



# Bhharmonic viscosity operator

- Laplacian viscosity operator:

$$m_x = k_L \nabla^2 u$$

- Biharmonic viscosity operator (enhanced scale-selectivity):

$$m_x = -k_B \nabla^2 \nabla^2 u$$

Show weak form.

- One-dimensional example:

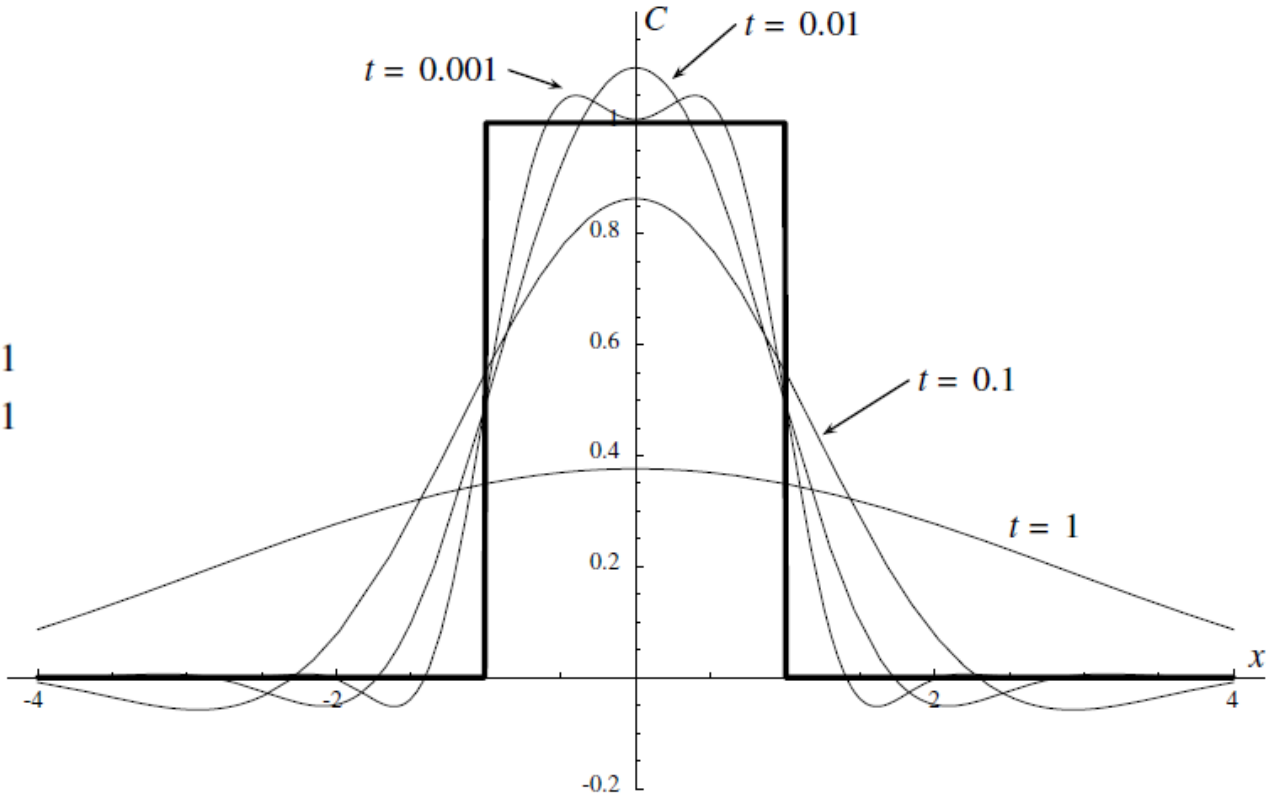
$$u_t = k_L u_{xx}$$

$$u_t = -k_B u_{xxxx}$$

# Bhharmonic viscosity operator – overshoot/undershoot

$$\begin{cases} \dfrac{\partial C}{\partial t} = -\dfrac{\partial^4 C}{\partial x^4} \\ C(0,x) = C_0(x) \end{cases}$$

$$C_0(x) = \begin{cases} 0 & \text{for } |x| > 1 \\ 1 & \text{for } |x| < 1 \end{cases}$$




Eric J M Delhez, *et al.* (2007). Overshootings and spurious oscillations caused by biharmonic mixing. *Ocean Modelling*, 17, 183-198.

# Smagorinsky viscosity

**3D turbulence theory - harmonic operator:**

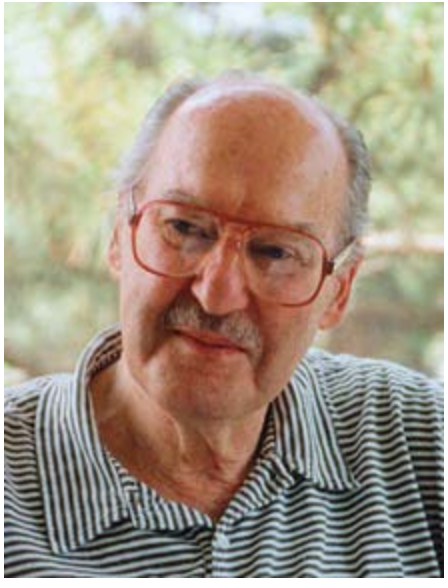
$$A_{Smag} = (\frac{\Lambda}{\pi})^2 \; L^2 \; |D|,$$

$$|D| = \sqrt{\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2},$$

**3D turbulence theory - biharmonic operator:**

$$A_{Smag} = (\frac{\Lambda}{\pi})^2 \; \frac{L^4}{8} \; |D|,$$

$$|D| = \sqrt{\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2},$$



**Joseph Smagorinsky**
(29 January 1924 – 21 September 2005)

# Leith viscosity

**2D turbulence theory - harmonic operator:**

$$A_{Leith} = (\frac{\Lambda}{\pi})^3 \; L^3 \; |\nabla\omega|$$

$$|\nabla\omega| = \sqrt{\left[\frac{\partial}{\partial x}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\right]^2 + \left[\frac{\partial}{\partial y}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\right]^2}$$

**2D turbulence theory - biharmonic operator:**

$$A_{Leith} = (\frac{\Lambda}{\pi})^3 \; \frac{L^5}{8} \; |\nabla\omega|$$

$$|\nabla\omega| = \sqrt{\left[\frac{\partial}{\partial x}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\right]^2 + \left[\frac{\partial}{\partial y}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\right]^2}$$

CFL condition:

$$A_{Laplacian} < \frac{L^2}{4 \; \Delta t}$$

$$A_{Biharmonic} < \frac{L^4}{32 \; \Delta t}$$

# Modified Leith viscosity

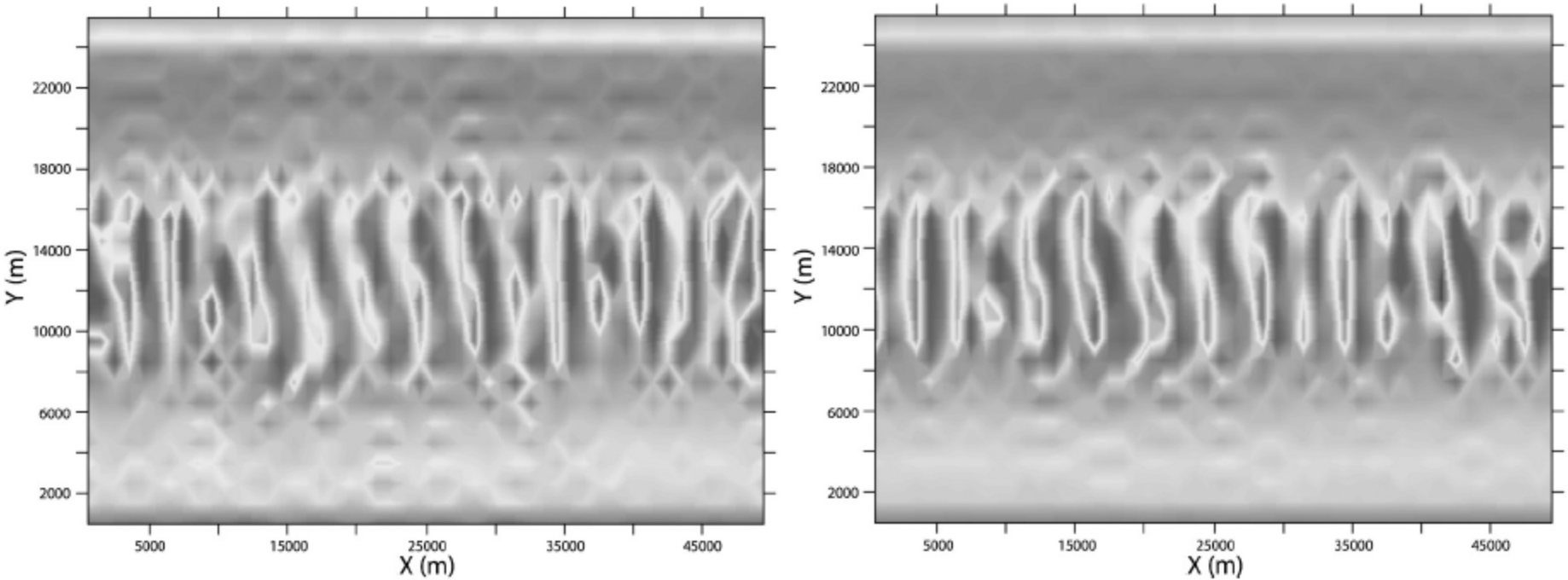
**2D turbulence theory - biharmonic operator:**

$$A_{Leith} = (\frac{1}{\pi})^3 \, \frac{L^5}{8} \, \sqrt{\Lambda^6 |\nabla\omega|^2 + \Lambda_d^6 |\nabla\nabla \cdot u_h|^2}$$

$$|\nabla\omega| = \sqrt{\left[\frac{\partial}{\partial x}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\right]^2 + \left[\frac{\partial}{\partial y}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\right]^2}$$

$$|\nabla\nabla \cdot u_h| = \sqrt{\left[\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)\right]^2 + \left[\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)\right]^2}$$

# Modified Leith viscosity – consequences: less noise

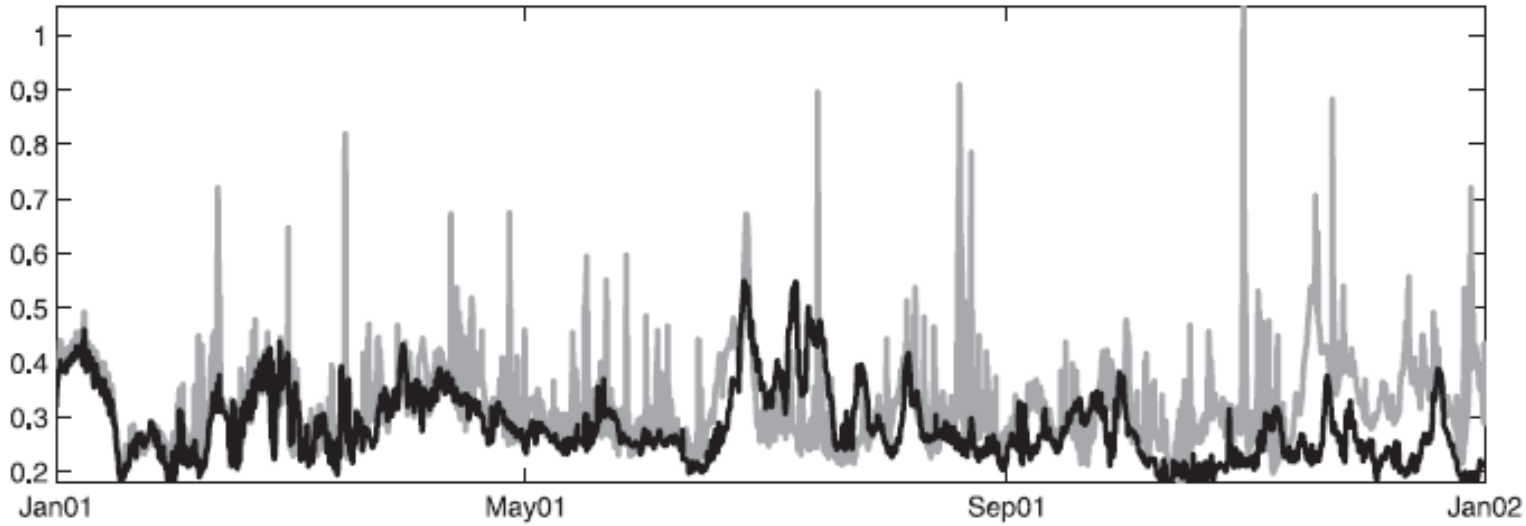



Vertical velocity from a simulation of spindown and instability of a temperature front in a reentrant channel. A simulation with the Leith viscosity applied to the horizontal velocities (left) and a simulation with the modified Leith viscosity (right) are shown. *Light colors are near zero; colors represent upward or downward motion.*

B Fox-Kemper, *et al.* (2008). Can large eddy simulation techniques improve mesoscale rich ocean models? *Ocean Modelling*, 117, 319-337.

# Modified Leith viscosity – consequences: better stability

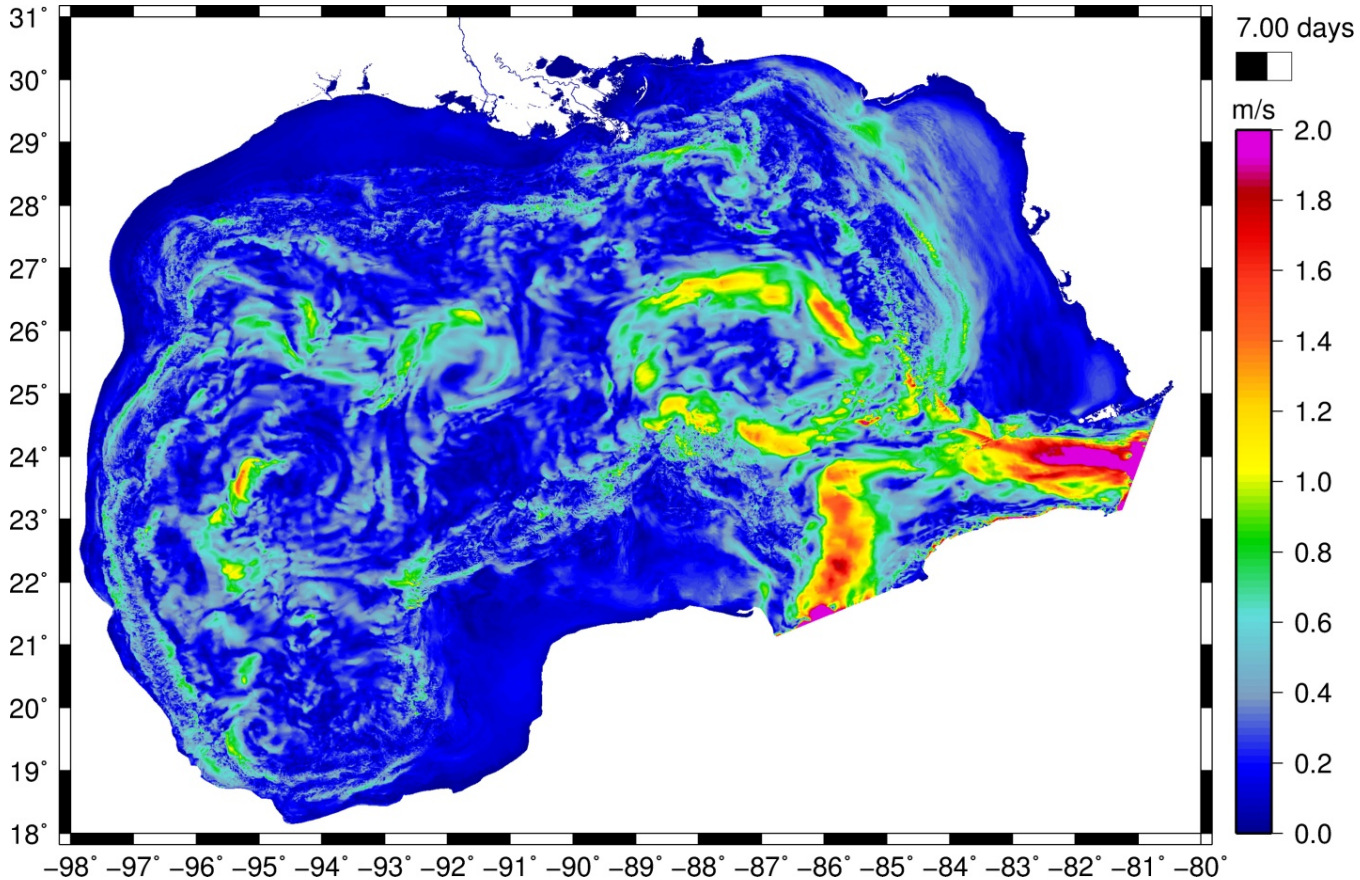
A Global Ocean Simulation with MITgcm:




Maximum Courant number. *Gray line is from the Leith integration, and black line is* from the modified *Leith integration.*

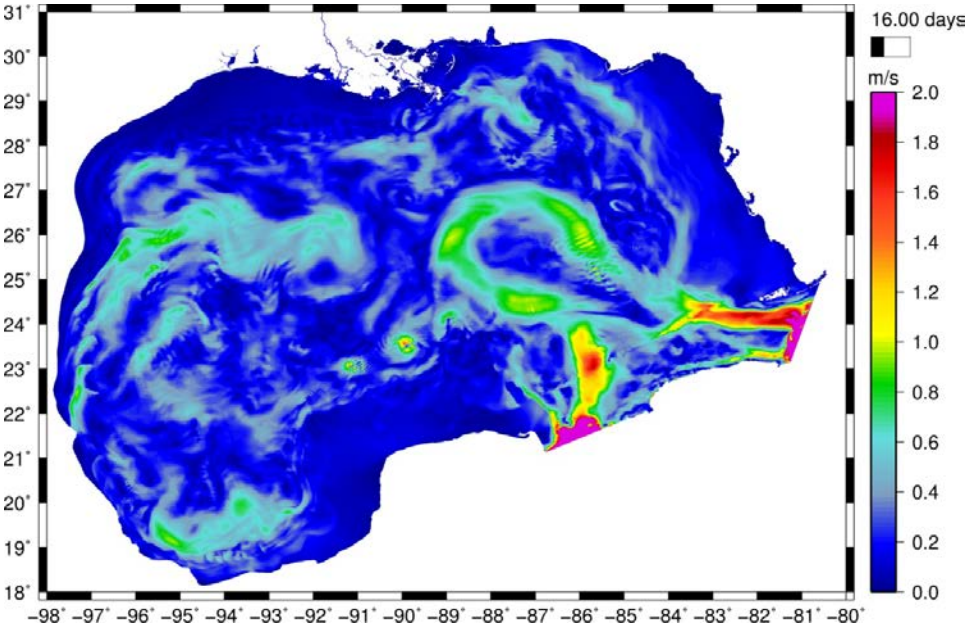
B Fox-Kemper, *et al.* (2008). Can large eddy simulation techniques improve mesoscale rich ocean models? *Ocean Modelling*, 117, 319-337.

# Gulf of Mexico simulation results: spinup

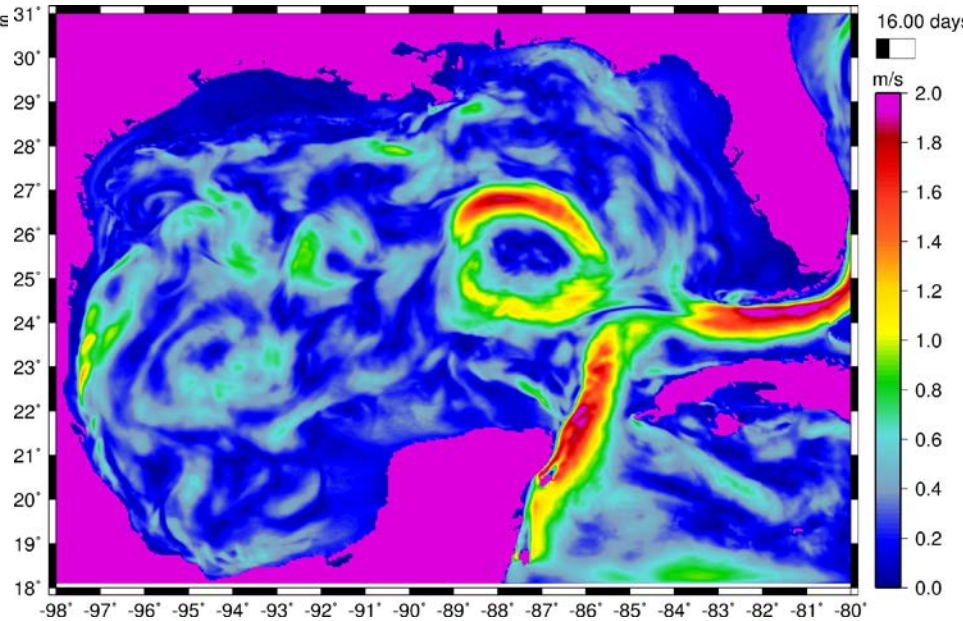



Velocity field during a spin-up simulation on the SL16 mesh with wind and baroclinic forcings (June 2010). The Loop Current and other eddies can be seen in the figure.

# Gulf of Mexico simulation results: full-run



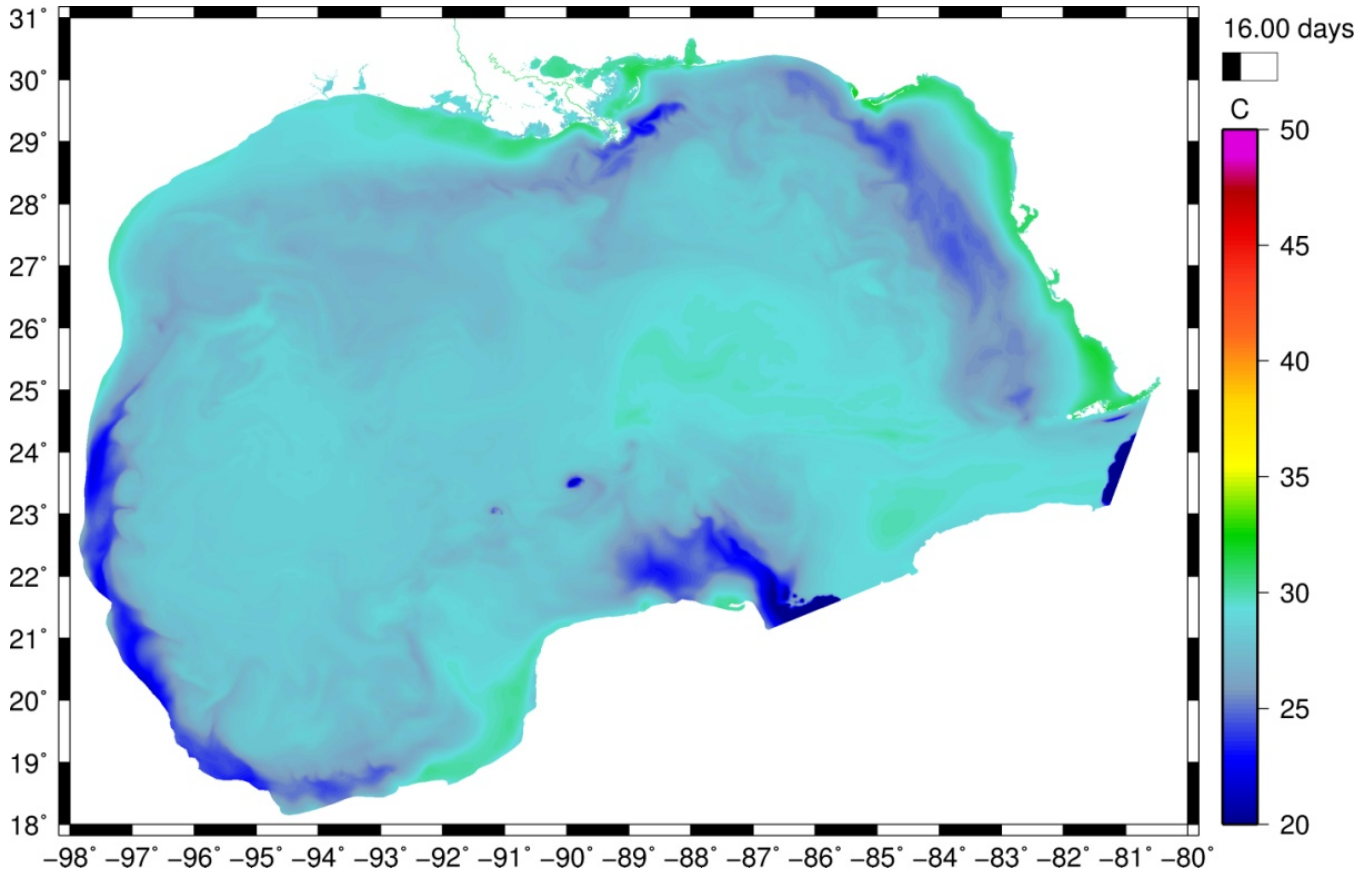

ADCIRC 3D




HYCOM

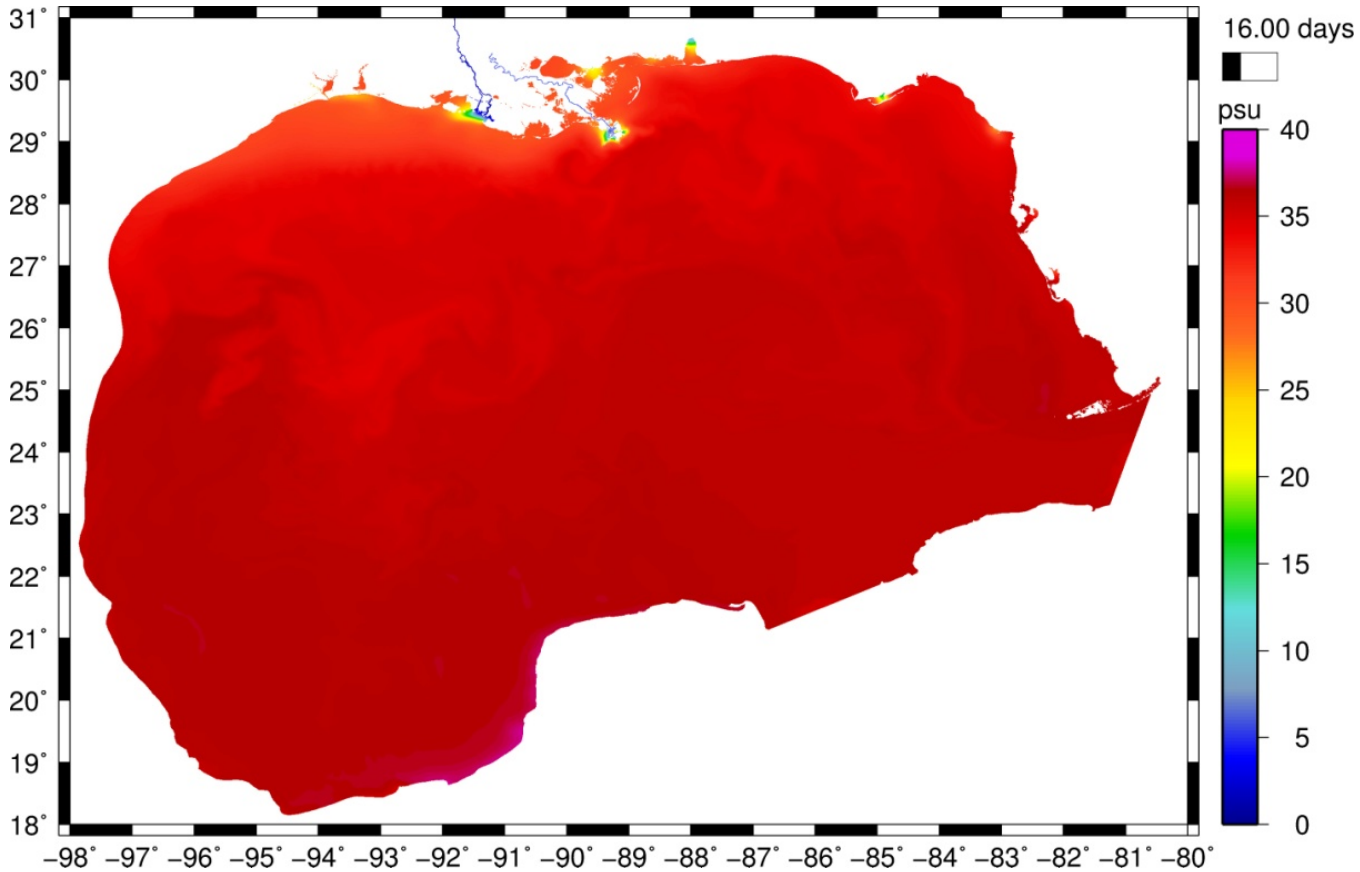
Velocity field during a prognostic simulation on the SL16 mesh (June 16th 2010). The Loop Current and other eddies can be seen in the figure.

# Gulf of Mexico simulation results: temperature




Temperature field during a prognostic simulation on the SL16 mesh (June 16th 2010).

# Gulf of Mexico simulation results: salinity




Salinity field during a prognostic simulation on the SL16 mesh (June 16th 2010).

movies

# Concluding Remarks

- Algorithmic improvements, leading to the accurate computation of the baroclinic pressure gradients and horizontal diffusion terms of the transport equations, by evaluating these terms directly in the $z$-coordinate, and using higher-order vertical interpolation.
- Systematic schemes for smoothing bathymetry.
- Better accounting for horizontal viscosity by using a biharmonic operator, which is more scale-selective, and also computing the viscosity parameter at every grid point, dynamically, according to a modified version of Leith.
- Stable simulation of the entire Gulf of Mexico on a high-resolution mesh during 2010/06/13 - 2010/06/25.

**Acknowledgments**

Funding for this work has been provided by BP and the Gulf of Mexico Research Initiative, under Consortium for Advanced Research on Transport of Hydrocarbon in the Environment- (CARTHE) II. Simulations were performed on Stampede and Lonestar HPC systems of Texas Advanced Computing Center (TACC) at The University of Texas at Austin.