High Order Discontinuous Galerkin Schemes for Coupled Physical-Biogeochemical Ocean Modeling

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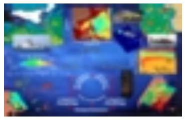
OUTLINE

- Introduction/Motivation
- Problem setup
- Meshing
- Flow Field, curved vs. straight mesh
- Quadrature-based vs. Quadrature-free
- High order vs. low order
- Filtering/Slope limiting
- Future work

IMUM 2010
International Workshop on
Multiscale (Un)-structured Mesh Numerical Modelling
for Coastal, Shelf, and Global Ocean Dynamics



Multi-Scale Biological-Physical Dynamics

❖ Biology Motivation

- What are fundamental biological-physical dynamics in Straits?
- Understand biological responses to multiple physical forcing (from rapid tidal overflows to slow water-mass driven overflows)
- Are there resonances between physics and biology in Straits leading to key nonlinear balances? (resonant intrinsic time and space scales)
- Start by investigating 2D dynamics (along-strait and depth)

❖ Physics Motivation

- Bathymetric features (straits/shelfbreaks) affecting flows in euphotic zone, hence biology
- Our complex regions of interest
  - Philippine Archipelago Straits, Middle Atlantic Bight shelfbreak, Monterey Bay shelfbreak, Taiwan region shelfbreak
- These regions involve multiscale dynamics (steep bathymetries, strong tides and mesoscales, shallow and deep areas)

Numerical Modeling Goals and Challenges

❖ Modeling Motivation

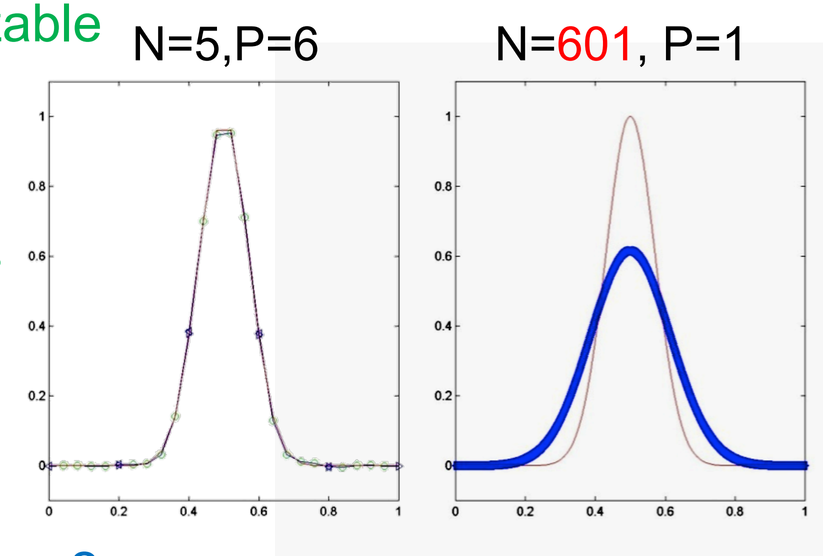
- Accurate numerics for biogeochemical ocean dynamics essential
  - Coastal ecosystems, environment, management, energy, and climate
- Providing computational requirements for such often highly nonlinear and multiscale dynamics critical, but very little (almost nothing) done so far
- Goal: define benchmarks and rules-of-thumb by comprehensive numerical analyses, comparing low to high order schemes, both in time and space

❖ Challenges

- Widely varying physics and biological scales
- Grid resolution has significant impact on simulated flows in these regions.
  - Likely have significant (even more?) impact on biology?
- Complex processes with chaotic dynamics
- Non-linear biological balances sensitive to numerics

Methodology

- High-Order Numerical Schemes – Why?
  - Less numerically dissipative than lower-order schemes
  - Levy et al. (2001): 5 different low-order finite volume advection schemes gave 30% difference in new production estimates for biology
- Various different possibilities:
  - Spectral, WENO/ENO, Finite Elements (Discontinuous Galerkin)
- DG Advantages
  - Localized memory access - parallelizable
  - Higher order accuracy
  - Well-suited to adaptive strategies
  - Can be used for complex geometries
- DG Challenges
  - How to create good mesh for HO?
  - Is HO DG too expensive?
  - Will numerical oscillations ruin accuracy?



Comprehensive Sensitivity Studies

- Focus on Nutrient-Phytoplankton-Zooplankton (NPZ) dynamics under advection and diffusion in idealized two-dimensional ocean strait geometry
- Complete large number of dynamics sensitivity studies:
  - Investigate 3 biological regimes, one stable and two unstable with limit cycles.
  - Examine interactions that are dominated by the biology, by the advection, or that are balanced.
- Employ standard and Hybrid Discontinuous Galerkin FE Methods
- Study the sensitivity to multiple numerical parameters including:
  - Quadrature-free and quadrature-based discretizations of the source terms.
  - Order of the spatial discretizations.
  - Order of the temporal discretization in explicit schemes.
  - Resolution of the spatial mesh.
  - The effect of using curved and straight elements.

Ueckermann, M.P. 2009, MIT SM Thesis.

Ueckermann, M.P. and P. F.J. Lermusiaux, 2010. Ocean Dynamics, (under review).

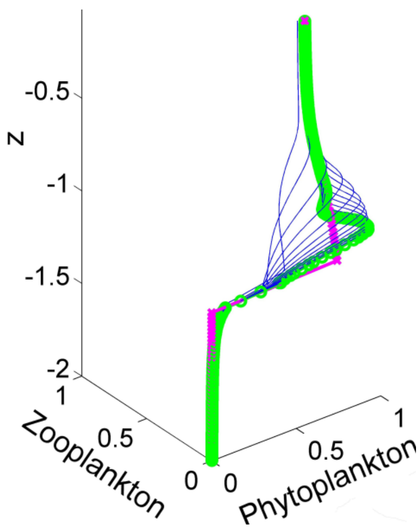
Idealized Setup

- Biological Dynamics in Straits
  - (N)utrient – (P)hytoplankton – (Z)ooplankton (NPZ) model
  - Various dynamical regimes: stable and unstable

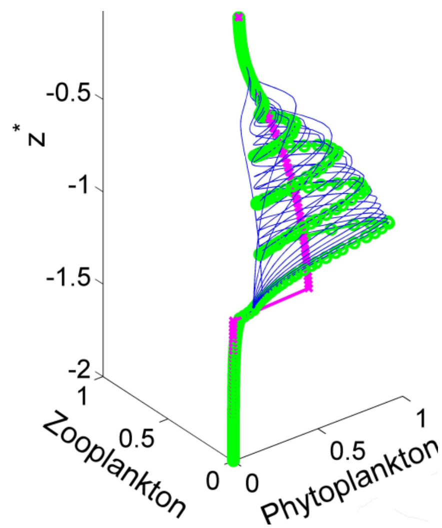
$$\frac{\partial \Phi}{\partial t} + \nabla \cdot (\mathbf{u}\Phi) - \kappa \nabla^2 \Phi = \mathbf{S}(\Phi, \mathbf{x}, t), \quad \text{in } \Omega$$
$$\Phi = \mathbf{g}_D, \quad \text{on } \Gamma_D$$
$$(\mathbf{u}\Phi - \kappa \nabla \Phi) \cdot \hat{\mathbf{n}} = \mathbf{g}_N, \quad \text{on } \Gamma_N$$

where $\Phi(\mathbf{x}, t) = [\phi^1(\mathbf{x}, t), \ldots, \phi^{N_c}(\mathbf{x}, t)]$ is the vector of N_c biological components

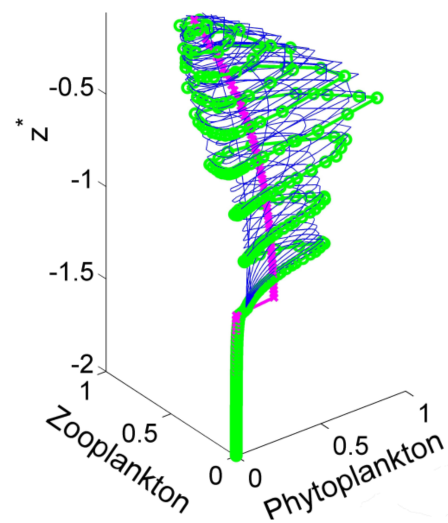
Stable



Unstable for z* in [0.4 0.9]



Unstable



Biology Equations and Parameters

- Non-dimensionalized equations

$$\frac{\partial \phi_N^*}{\partial t^*} + \nabla \cdot (\mathbf{u}^* \varphi_N^*) - \nabla \cdot \frac{1}{P_e} \nabla \varphi_N^* = -\mathcal{U}^* e^{z^*/h^*} \frac{\phi_P^* \phi_N^*}{\phi_N^* + k_s^*} + d_P^* \phi_P^* + d_Z^* \phi_Z^* + (1-a) g_\nu^* \phi_Z^* (1 - e^{-\nu^* \phi_P^*})$$

$$\frac{\partial \phi_P^*}{\partial t^*} + \nabla \cdot (\mathbf{u}^* \varphi_P^*) - \nabla \cdot \frac{1}{P_e} \nabla \varphi_P^* = \mathcal{U}^* e^{z^*/h^*} \frac{\phi_P^* \phi_N^*}{\phi_N^* + k_s^*} - d_P^* \phi_P^* - g_\nu^* \phi_Z^* (1 - e^{-\nu^* \phi_P^*})$$

$$\frac{\partial \phi_Z^*}{\partial t^*} + \nabla \cdot (\mathbf{u}^* \varphi_Z^*) - \nabla \cdot \frac{1}{P_e} \nabla \varphi_Z^* = -d_Z^* \phi_Z^* + a g_\nu^* \phi_Z^* (1 - e^{-\nu^* \phi_P^*})$$

Parameter	Description	[units]
$\mathcal{U}$	Phytoplankton uptake rate	[1/day]
k_s	Saturation concentration of phytoplankton	[μmol/L]
d_P	Mortality rate of Phytoplankton	[1/day]
d_Z	Mortality rate of Zooplankton	[1/day]
g	Grazing rate of Zooplankton	[L/(μmol$\cdot$day]
a	Assimilation (efficiency) rate	[]
h	e-folding depth for light (photosynthesis)	[m]
ν	Parameter for Ivlev form of grazing function	[L/μmol]
$\mathcal{N}_T$	Total biomass	[μmol/L]

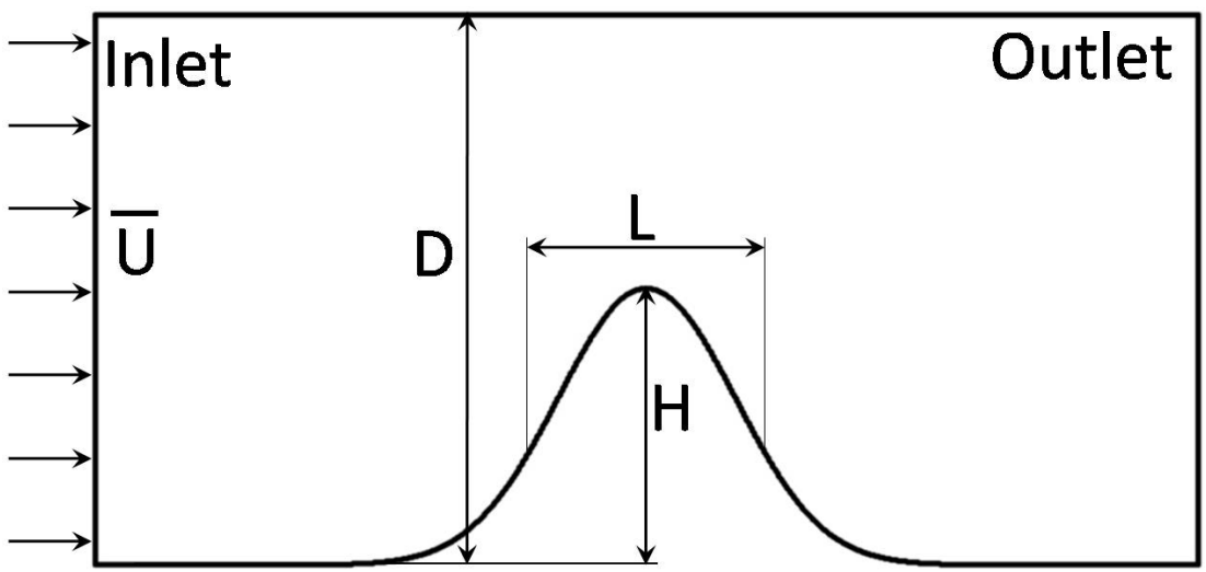
Parameter	Value
$\mathcal{U}^* = \mathcal{U}\bar{\tau}$	7.5
$k_s^* = \frac{k_s}{\mathcal{N}_T}$	$[\frac{1}{30}, \frac{1}{50}, \frac{1}{100}]$
$d_P^* = d_P \bar{\tau}$	0.2
$d_Z^* = d_Z \bar{\tau}$	1
$g_\nu^* = \frac{g\bar{\tau}}{\nu}$	12.5
$a^* = a$	0.4
$h^* = \frac{h}{H}$	0.34
$\nu^* = \mathcal{N}_T \nu$	[0.3, 0.5, 1]
$P_e = \frac{\bar{\mathbf{u}}L}{\kappa}$	∞
$D^* = \frac{D}{H}$	2

Idealized Setup

- Idealized Potential Flowfield
  - Strait width << Ro, Small Fr, Rigid lid, constant density

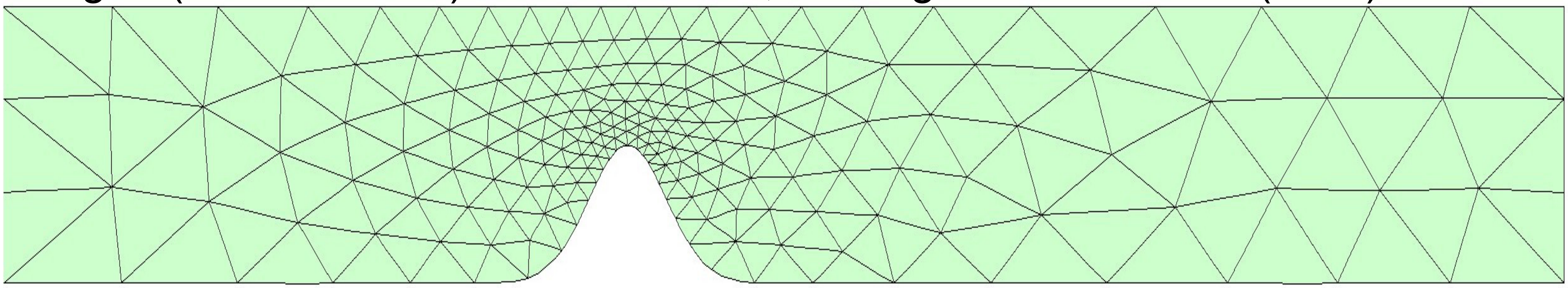
$$\nabla^2 \psi = 0, \quad \text{in } \Omega$$
$$\mathbf{u} = \nabla \times \psi$$

- Solved on straight and curved meshes with various order/ refinements

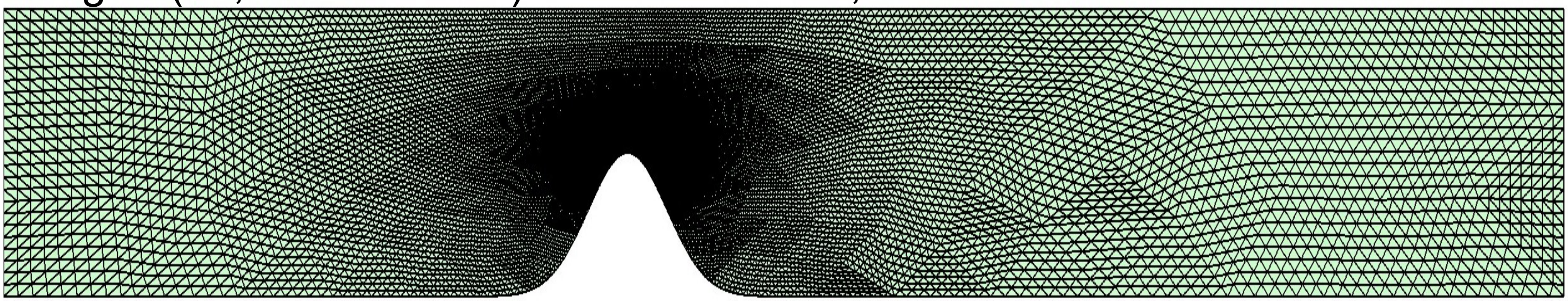


Triangular meshes

- g=1 (350 elements) for P=6 have 9,800 degrees of freedom (DOF)



- g=4 (22,400 elements) for P=1 have 67,200 DOF



- High order (g1,P6) less expensive than low order solution (g4,P1)
  - Factor of 2-3
- Five spatial mesh resolutions, with straight and curved boundary elements

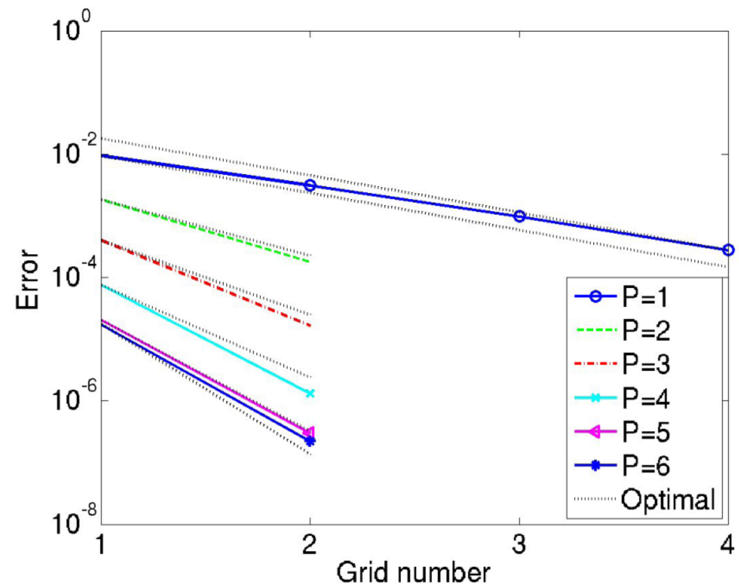
Reference solution calculated on g=5, P=1 (89,600 elements, 268,800 DOF)

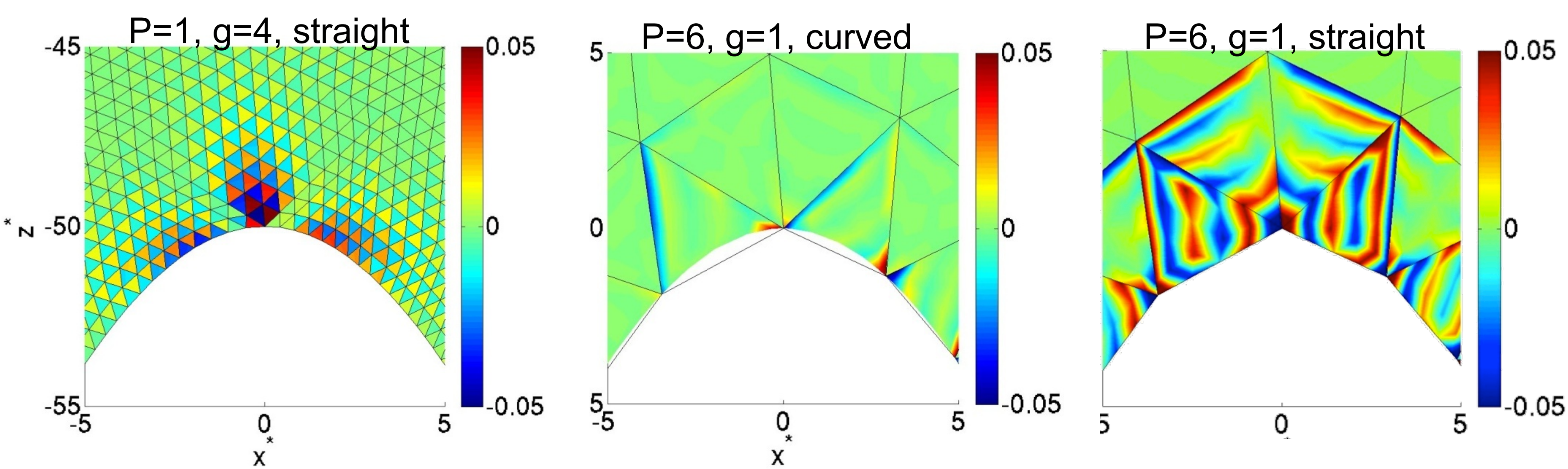
Flow field: Convergence and boundary treatment

- Hybrid Discontinuous Galerkin Method
  - Gradient converges at O(P+1)

$$\nabla^2 \psi = 0, \quad \text{in } \Omega \qquad \boxed{\mathbf{u} = \nabla \times \psi}$$

- Velocity Divergence
  - Low order: smaller amplitude error
  - High order: smaller L^2 error
  - Straight Mesh: O(1) error
- Curved boundary mesh is necessary for high-order schemes.





Source Term Implementation QB vs QF

- Quadrature-based (QB) integration
  - More accurate
  - More expensive (4 x #Components x #quadpoints x #bases) [$4N_cN_qN_p$]

$$\left(S^i(\Phi_h, \mathbf{x}_i, t), w_k\right)_K = \left(S^i(\Phi_j\theta_j, \mathbf{x}, t), w_k\right)_K$$
$$\boxed{\approx} S^i\left(\Phi_j\theta_j(\mathbf{x}_i), \mathbf{x}_i, t\right) w_k(\mathbf{x}_i)\omega_i$$
$$= \mathcal{W}_{ki}\left[S^i\left(\Phi_j\Theta_{ji}, \mathbf{x}_i, t\right)\omega_i J_i\right]$$

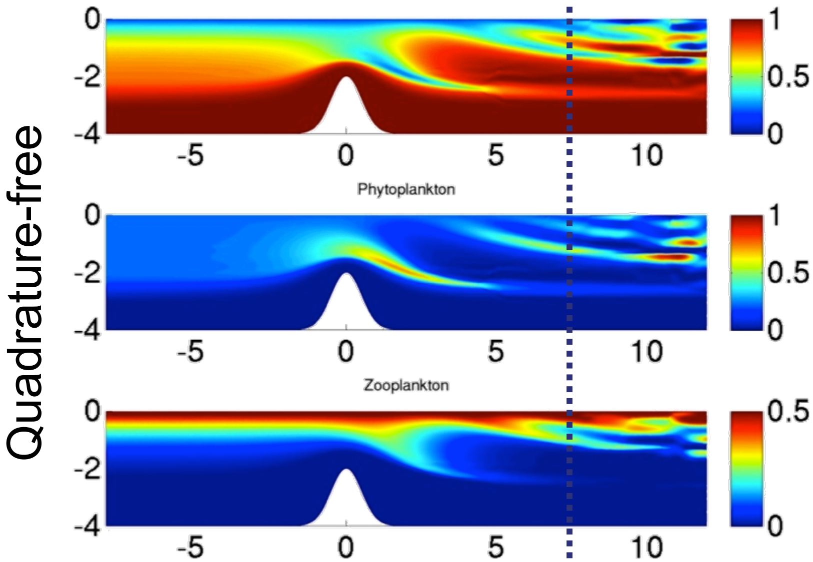
Approximate integral with quadrature rules

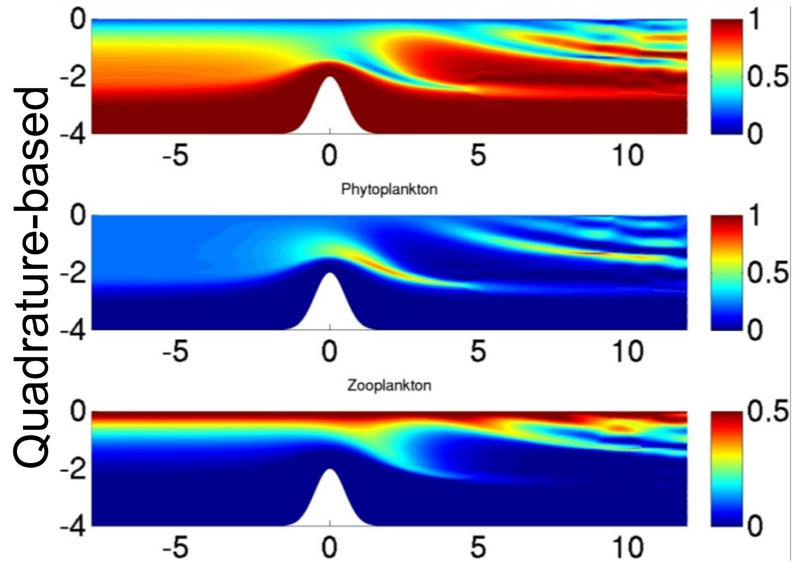
- Quadrature-free (QF) integration
  - Smaller cost (#bases x Cost to evaluate source terms) [C_sN_p]

$$\left(S^i(\Phi_h, \mathbf{x}, t), w_k\right)_K \boxed{\approx} \left(S^i\left(\Phi_j, \mathbf{x}_j, t\right)\theta_j, w_k\right)_K$$
$$= \left(\theta_j, w_k\right)_K S^i\left(\Phi_j, \mathbf{x}_j, t\right)$$
$$= \mathcal{M}_{kj} S^i\left(\Phi_j, \mathbf{x}_j, t\right)$$

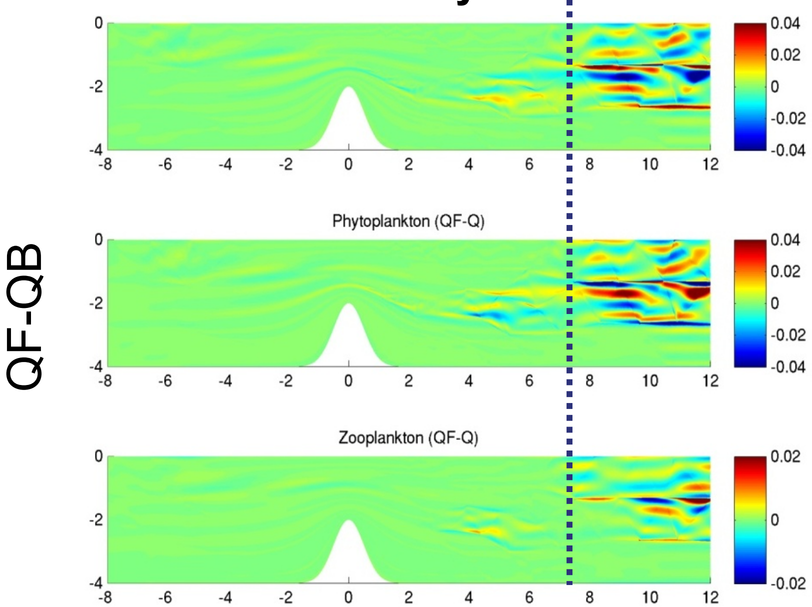
Approximate source function as polynomial of order P

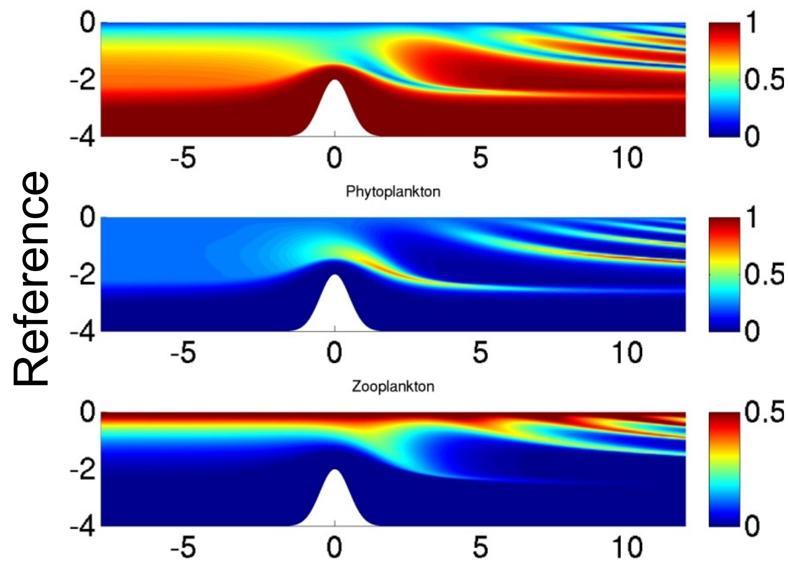
Source Term Implementation QB vs QF





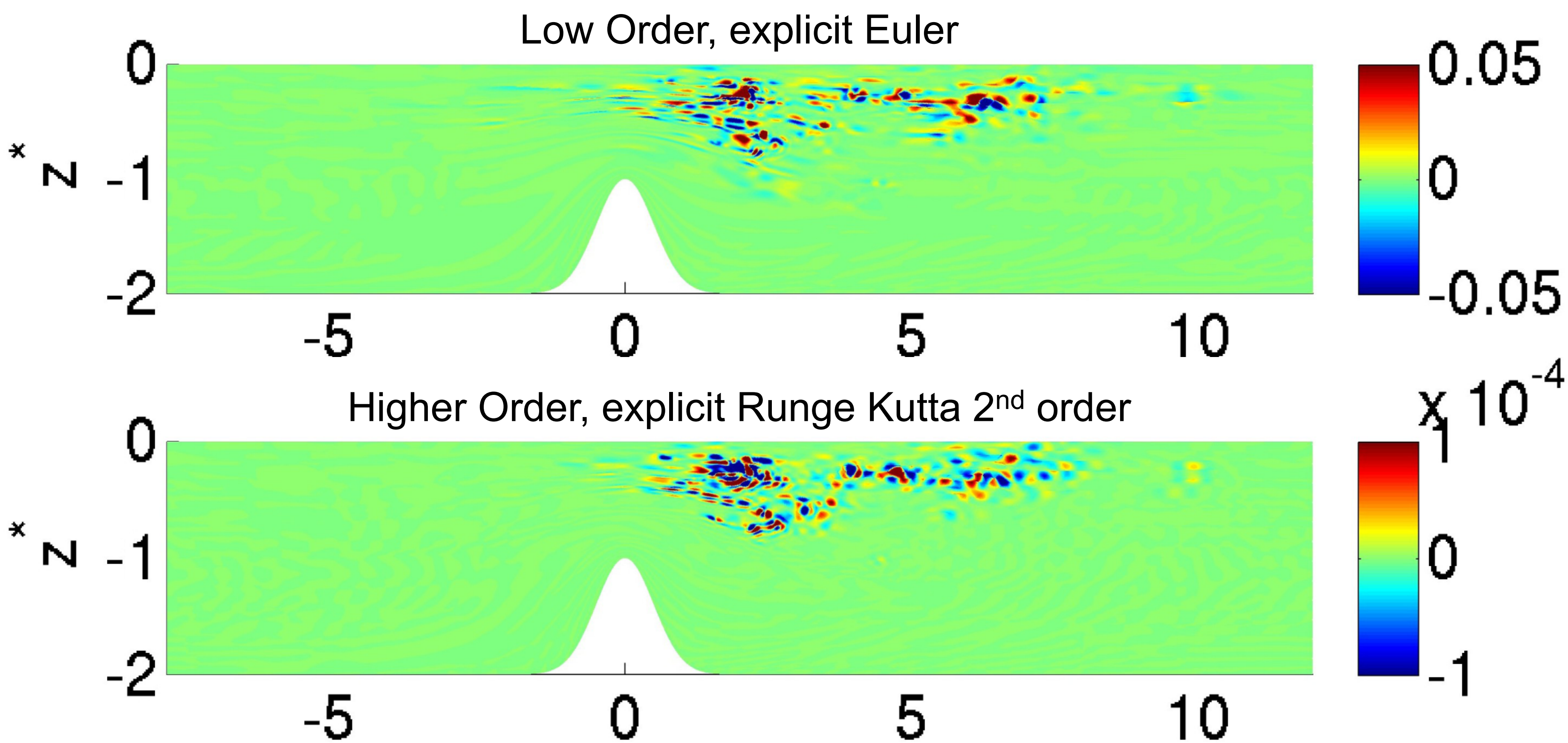
QB/QF similar accuracy ←



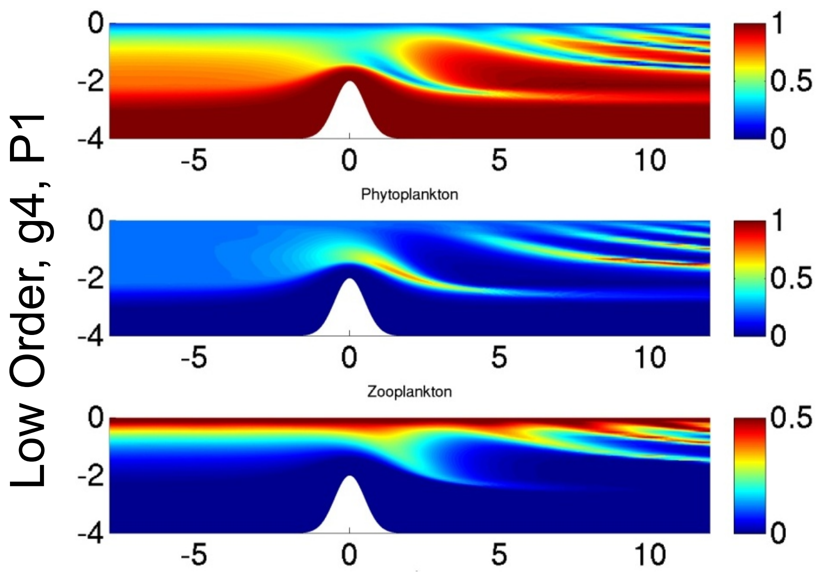


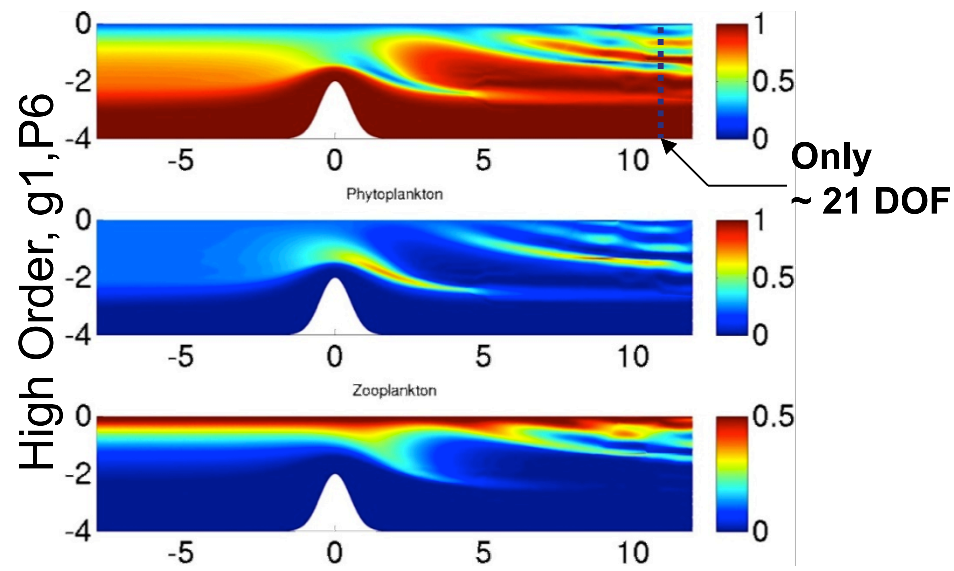
- Both quadrature-based and quadrature-free discretizations give accurate, convergent where well-resolved

- Low order time integration scheme loses accuracy much faster than higher-order scheme

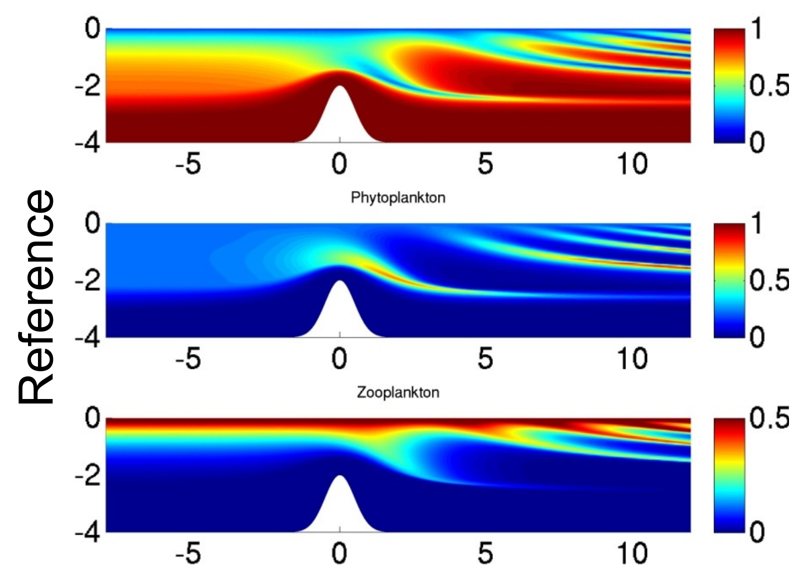


High Order vs. Low Order in Space

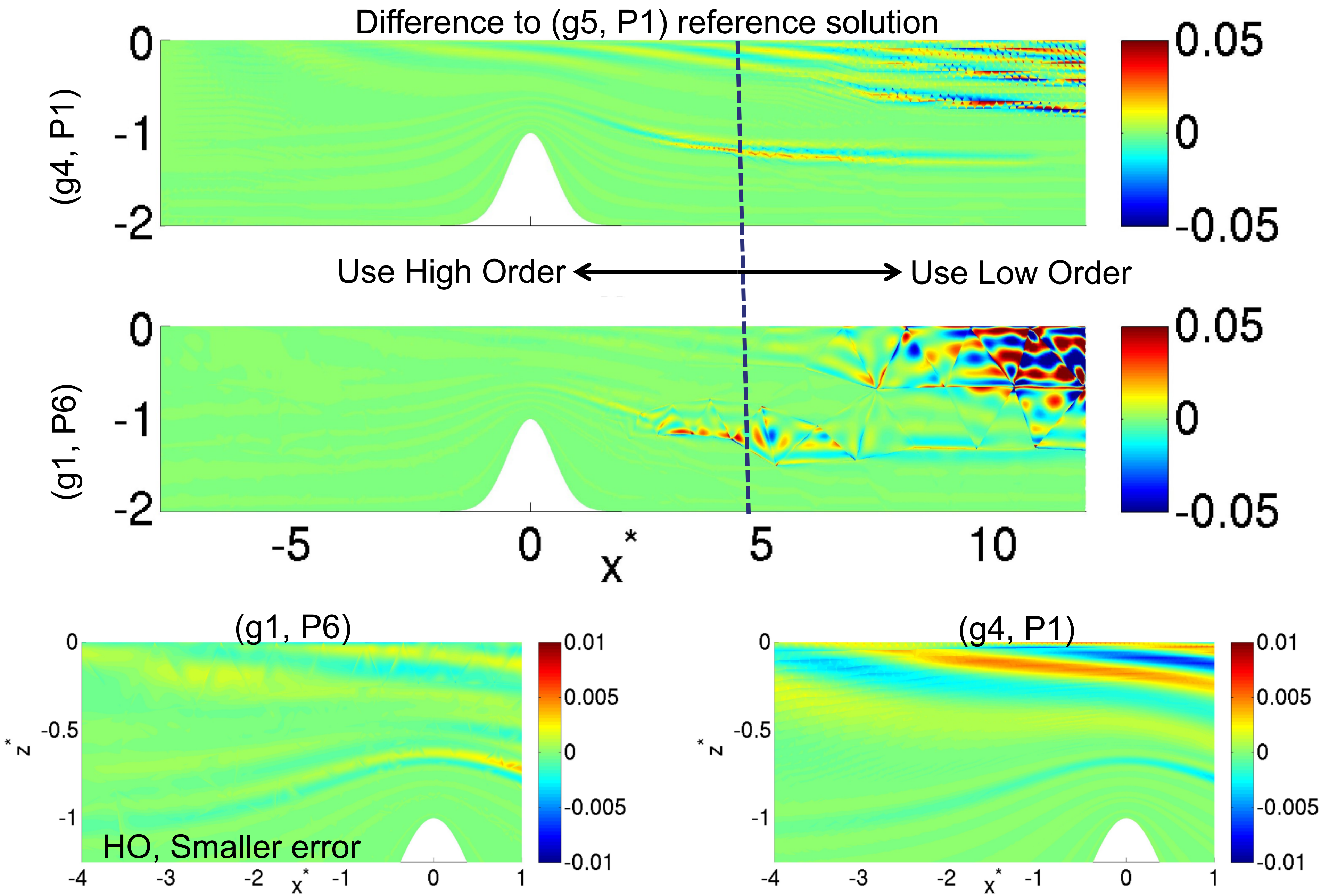




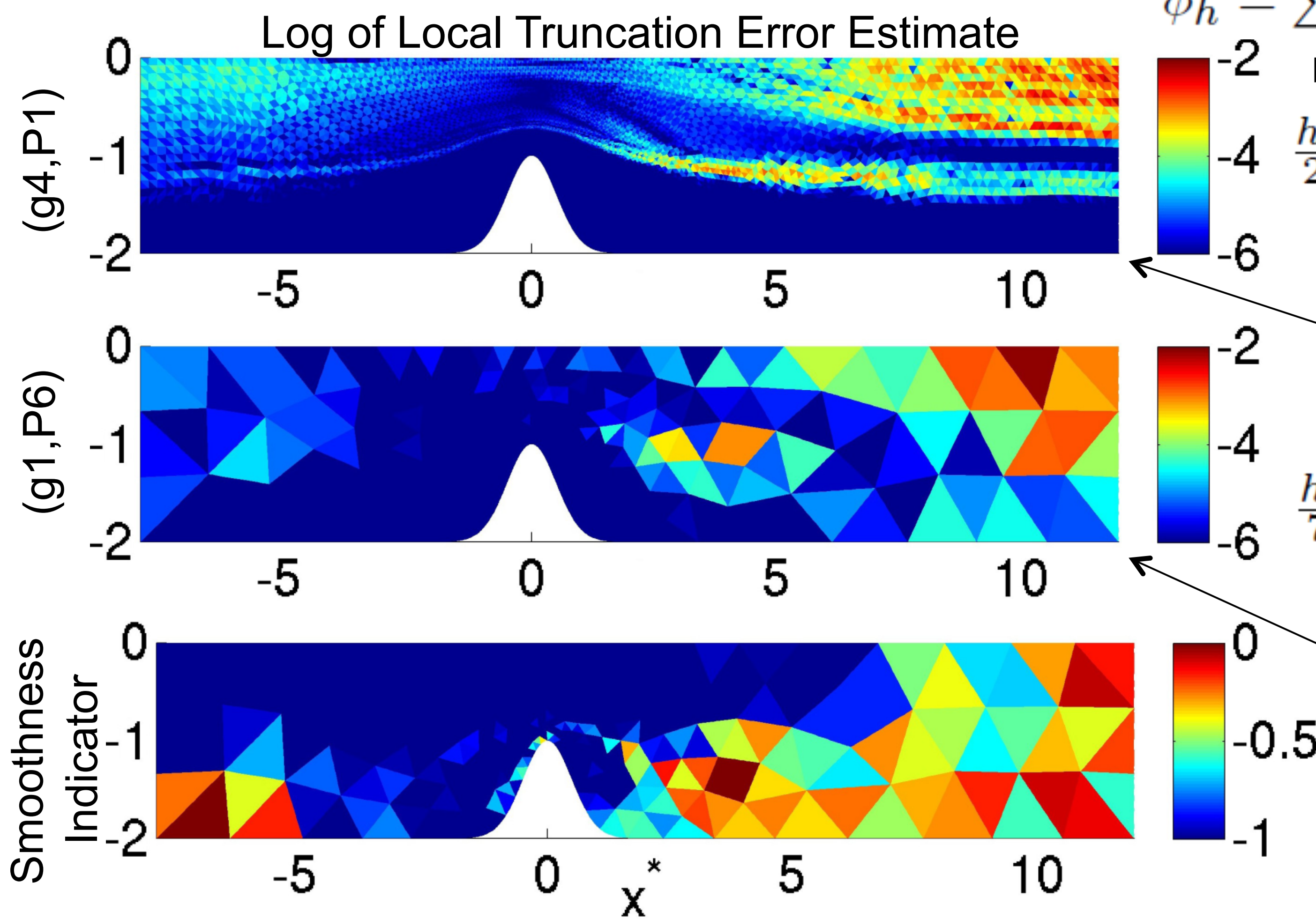
- Unstable biology throughout water column
- Qualitative comparison
  - Low order (LO) scheme seems better for x* > 5
  - High order (HO) and LO scheme similar for x*<5



High Order vs. Low Order: Difference plots



Smoothness Determines HO/LO



$$\phi_h = \sum_i \phi_i \theta_i = \sum_{ij} a_{ij} P_{ij}$$

Leading order truncation

$$\frac{h^2}{2!}\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right)^2 \phi(\mathbf{x}_\eta)$$

Approximate log (calculated on P=2 mesh)

$$log_{10}(\textstyle\sum_{i+j=2} a_{ij})$$

Leading order truncation

$$\frac{h^7}{7!}\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\right)^7 \phi(\mathbf{x}_\xi)$$

Approximate log (calculated on P=7 mesh)

$$log_{10}(\textstyle\sum_{i+j=7} a_{ij})$$

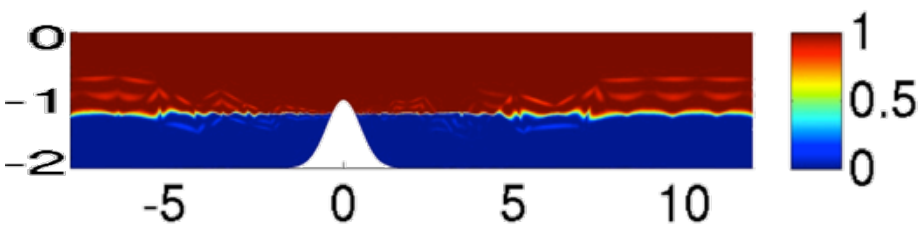
"Smoothness": linear fit to $\log_{10}$ of a_{ij} coefficients [Mavriplis, 1989]

- Higher-order spatial discretizations more accurate for the smaller cost where the solution was "smooth"
  - "Smooth" functions have exponentially decreasing polynomial expansion coefficients

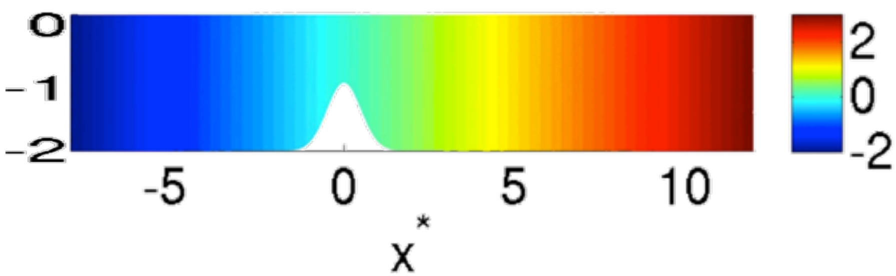
Advection on Periodic Domain

- Need to address numerical oscillations (Gibbs phenomena) issue
  - Occur for both LO and HO scheme
  - Can we damp oscillations and retain high-order accuracy?

1. Constant tracer

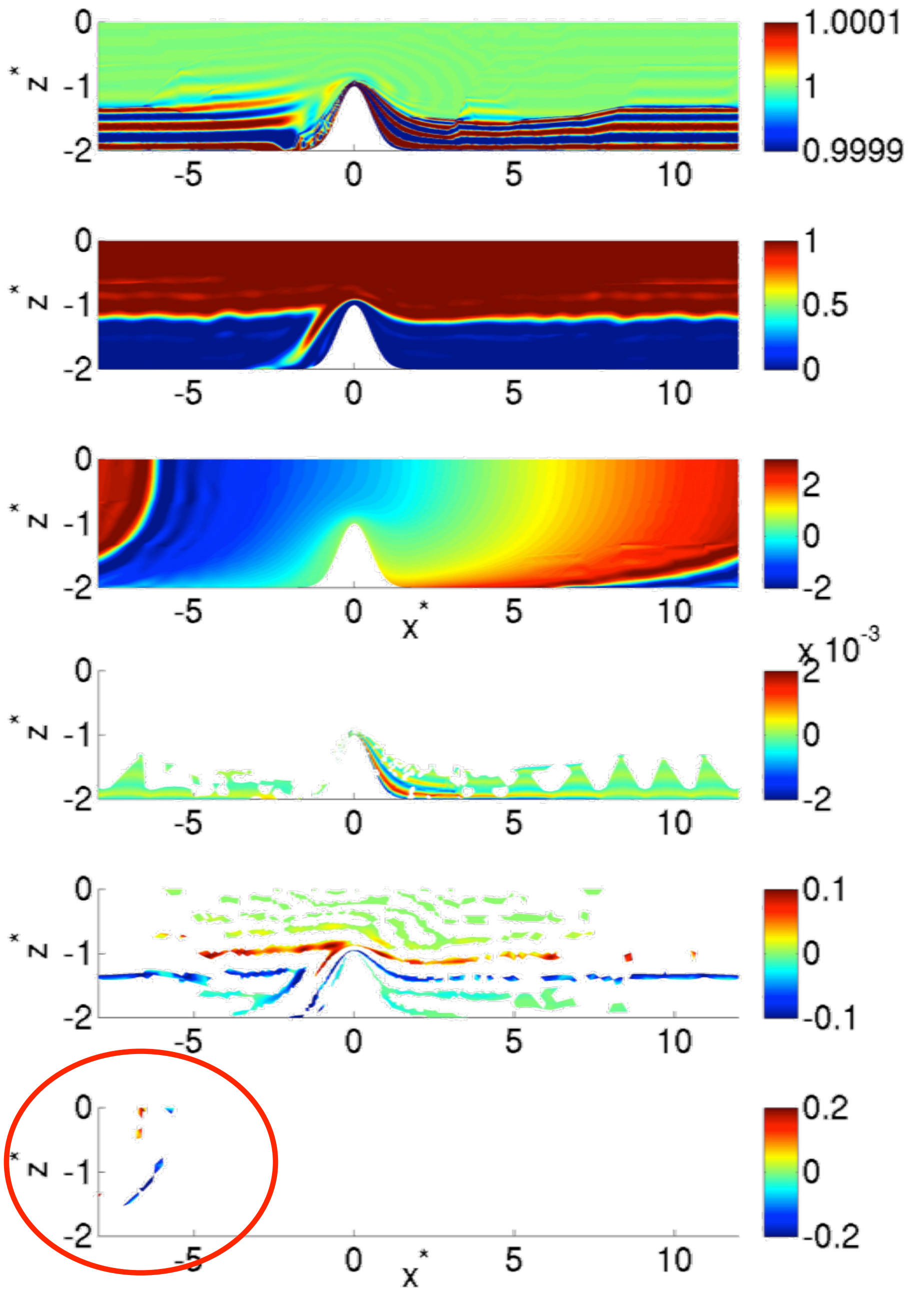


2. Vertical jump
   - initial condition oscillatory

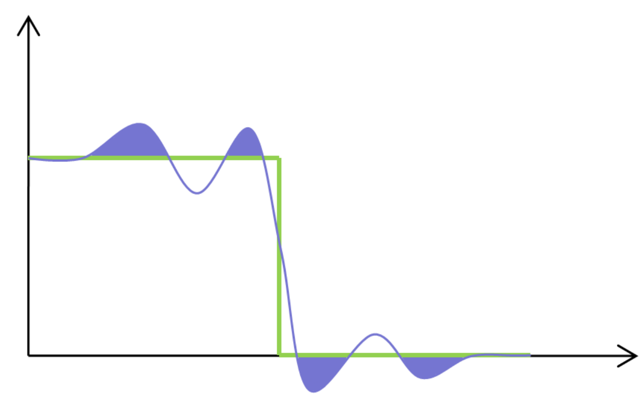


5. Horizontal jump
   - initial condition non-oscillatory (jump is over elements)

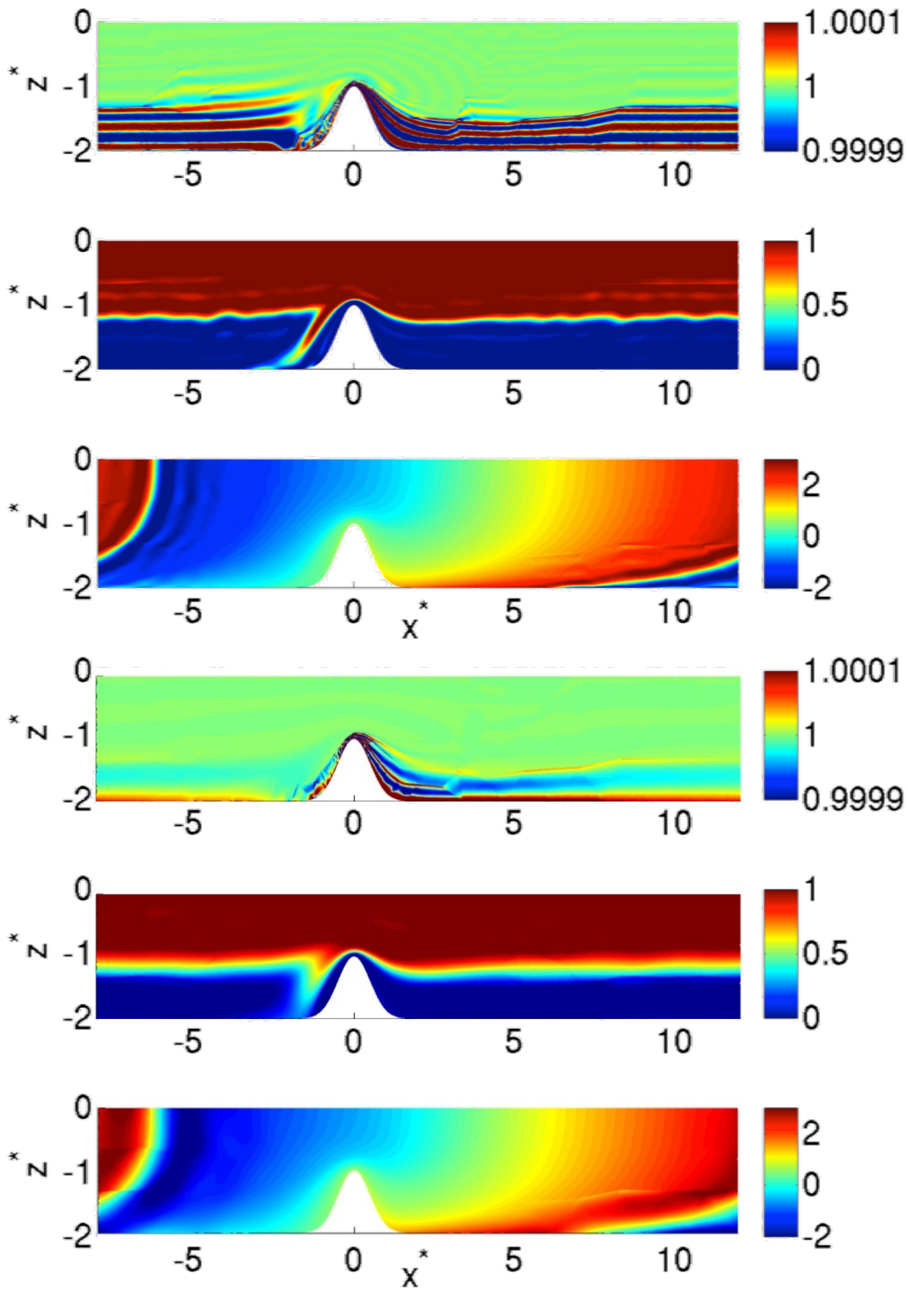
Advection on Periodic Domain



- Error plots show solution outside total variation of solution
  - Large oscillations can have significant effect on biological dynamics



Advection on Periodic Domain: Filtering



- Apply exponential filter

$$u_h = \sum_{|\mathbf{i}|\le P} u^{\mathbf{i}} \theta^{\mathbf{i}}$$

[Hesthaven and Kirby, Math. Comput. 2008]

$$u_{h,f} = \sum_{|\mathbf{i}|\le P} \sigma(\eta) u^{\mathbf{i}} \theta^{\mathbf{i}}$$

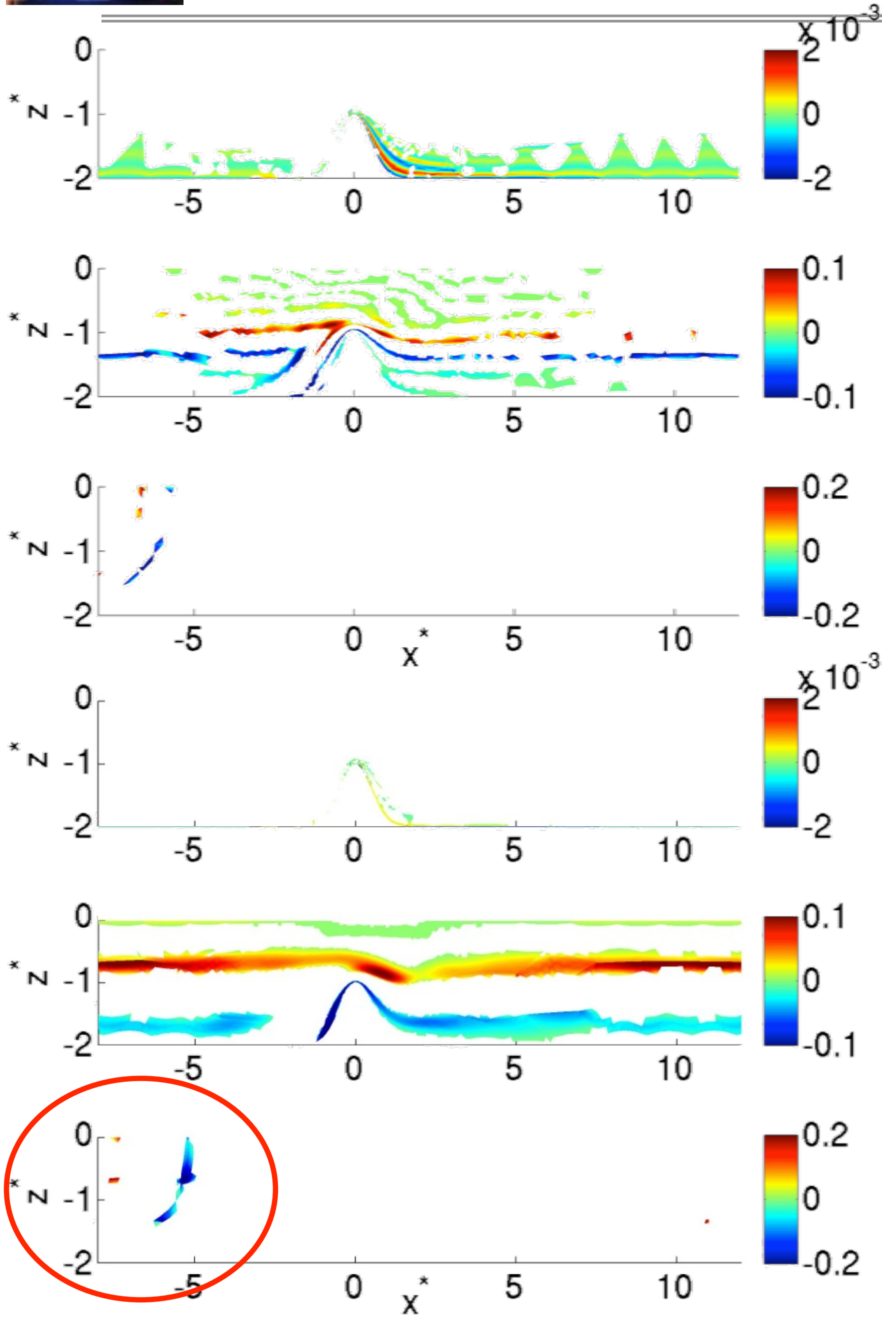
$$\sigma(\eta) = \exp(-\alpha \eta^s)$$

i – multi-index
s – order of filter

$$\eta = \frac{|\mathbf{i}|}{P}, \alpha = -\log(\varepsilon_{machine}) \rightarrow \sigma(1) = 0$$

- “Diffusive effect, greater in center of element, less at edges”
- “If filter less-smooth than solution: convergence not negatively impacted”
- Using Filter: Interface very diffused (s=10)

Advection on Periodic Domain: Filtering

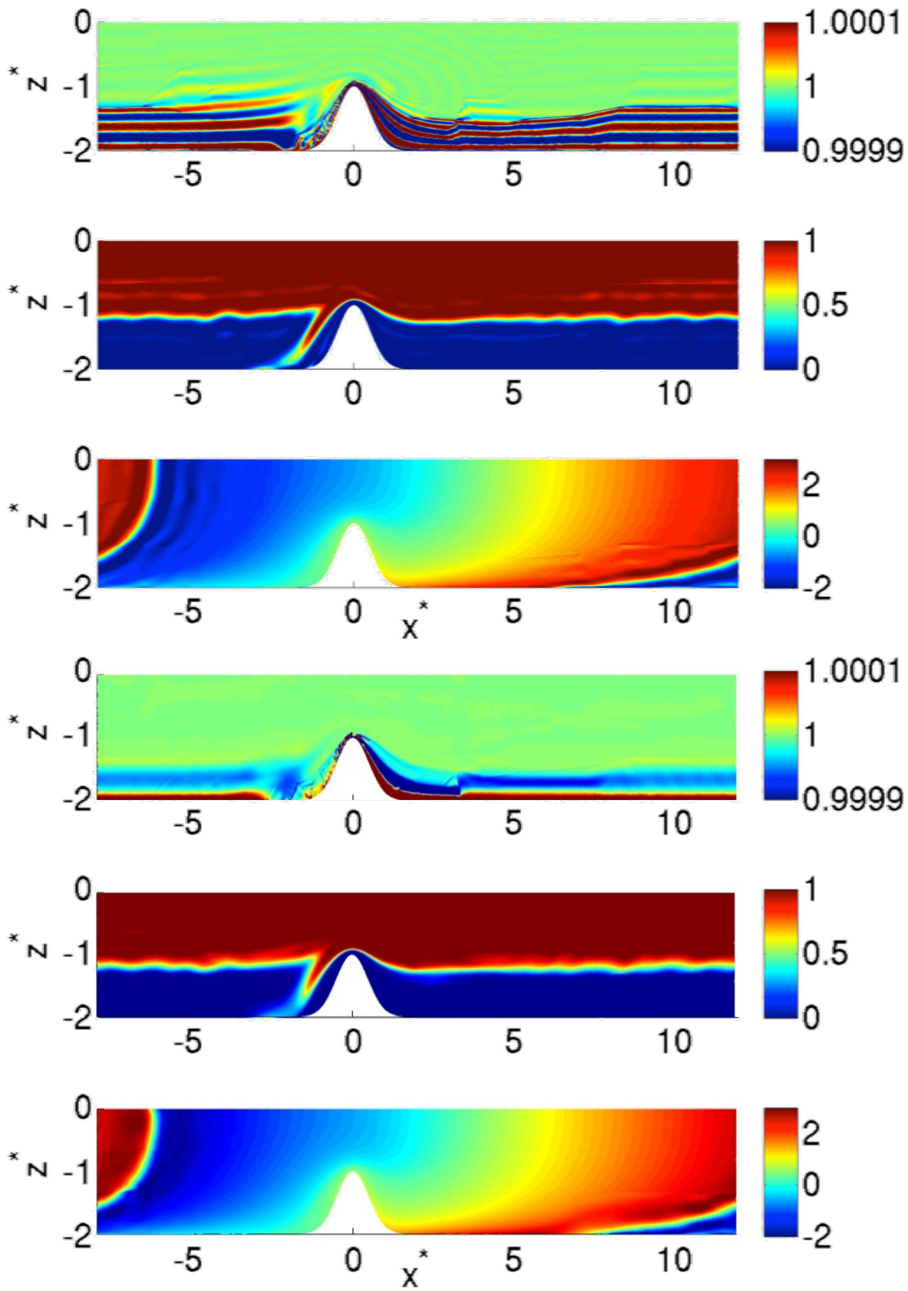


- Application of high, s=10, filter does not remove oscillations and diffuses solution everywhere.
- Also, with *α*, *η* definitions, highest modes are truncated.

Improvements

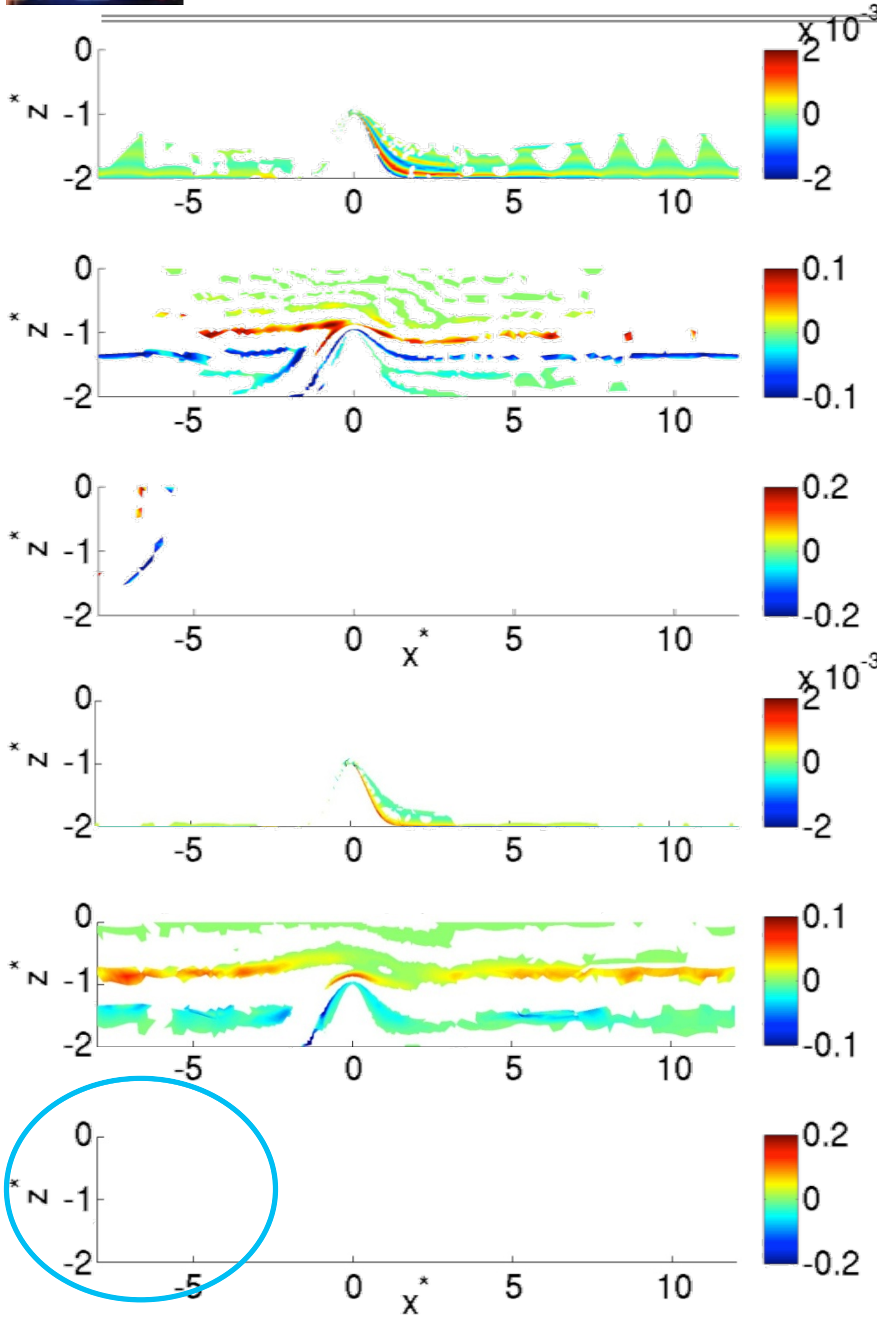
- Don't solve for truncated mode: $\eta = \frac{|\mathbf{i}|}{P+1}, \; \alpha = -\log(0.01)$
- Only filter when not "smooth": "selective filter"
  - Use "smoothness" criterion

Advection on Periodic Domain: Filtering



- More aggressive (s=5) "selective filter," only filters when not smooth:
- Does smooth interface, but much sharper than before.
- Constant case also with less noise.
- Appears as though oscillations reduced, eliminated?

Advection on Periodic Domain: Filtering

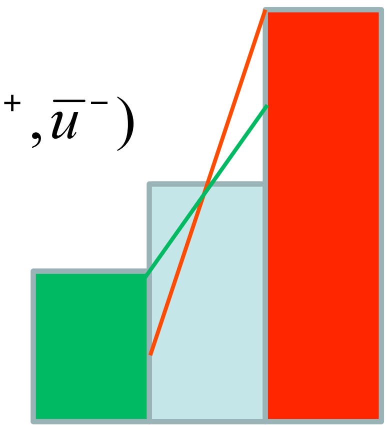


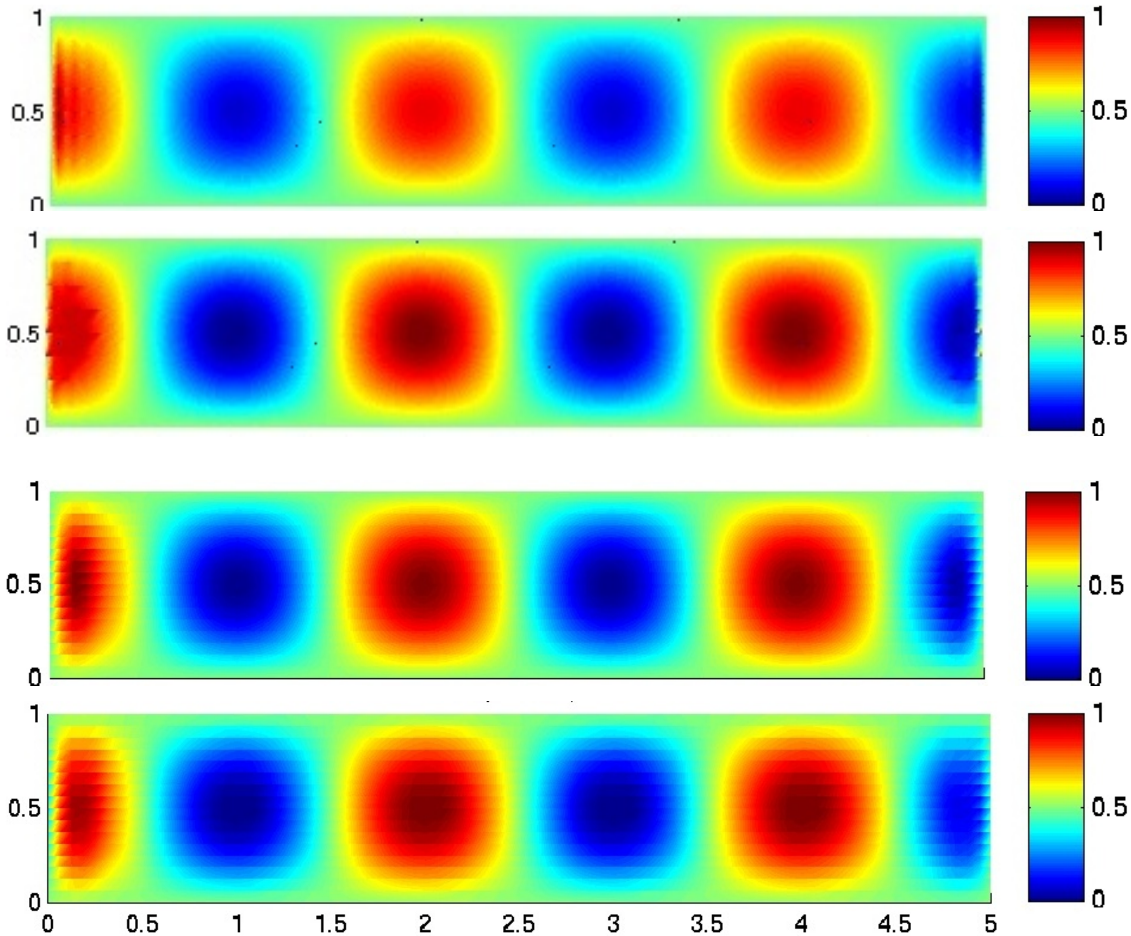
- Smoother solution for case 2, oscillations not eliminated.
  - Reasonable since initialized with oscillatory field.
- Oscillations eliminated for case 3
- Cost of filtering
  - For modal basis: essentially free.
  - For nodal basis: need to transform to modal set, filter, transform back ~ 2 matrix-vector multiplications.

Preliminary Slope Limiting vs. Filtering

- HO slope limiting on triangles open problem – generally limited to first-to-second order [Hoteit et. al. *Int. J. Numer. Meth. Engng 2004]*
- Solution should be Total Variation Diminishing

$$(1-\alpha)\overline{u}^{+} + \alpha \min(\overline{u}^{+}, \overline{u}^{-}) \le u_{mid}^{\pm} \le (1-\alpha)\overline{u}^{+} + \alpha \max(\overline{u}^{+}, \overline{u}^{-})$$





Unfiltered (g3,P6)

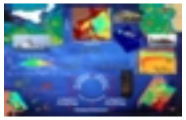
Filtered (s=3) (g3,P6)

Solution affected only on "non-smooth" regions

(g4,P1)

Slope Limited (g4,P1) [TVD]

Solution affected globally



Summary and Conclusions

- By quantitatively evaluating truncation error and "smoothness" of solutions, found that higher-order spatial discretizations more accurate for the same cost where "smooth."
- High resolution needed in biologically active regions.
- Smoothness criterion can be used to indicate adequacy of order/resolution for biology.
- Filtering is a viable solution to damp high-order oscillations
- Both quadrature-based and quadrature-free discretizations give accurate, convergent where well-resolved
  - Quadrature-based scheme has significantly smaller error where the solution is under-resolved.
- Curved boundary mesh is necessary for accurate advection using high-order schemes.
- Low-order temporal discretizations allow rapidly growing numerical errors.

Current and Future Work

- 3D Hybrid Discontinuous Galerkin code
  - Implement novel high-order-accurate formulation
  - Demonstrate on idealized problems
- Additional (potential) directions on slope limiting/ filtering
  - Develop filter tuning guidelines
  - Explore limits of “smoothness” definition/indicator
  - Combine filtering/slope-limiting approach
  - Explore “directional filtering”

- http://mseas.mit.edu
- Thanks!