Scalar Conservation Mapping in Dynamics to Physics Coupling

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Outline

- Motivation

- Mapping challenges

- Positivity-preserving mapping

- Application results with 1D BOMEX

- Discussion and closing remarks

Motivation

- Dynamics uses spectral method (SM) with non-uniform mesh.
- Dynamics' results are evaluated at uniform mesh points and passed to physics.
- Physics results are then evaluated at non-uniform mesh points to pass back to dynamics.
- SM enables a high-order accuracy and a better usage of compute resources.
- The mapping between physics and dynamics in NEPTUNE does not preserve positivity.
- **Preserving positivity may be critical for a more accurate forecast.**

non-uniform mesh

uniform mesh

Dynamics
(non-uniform mesh)

Physics
(uniform mesh)
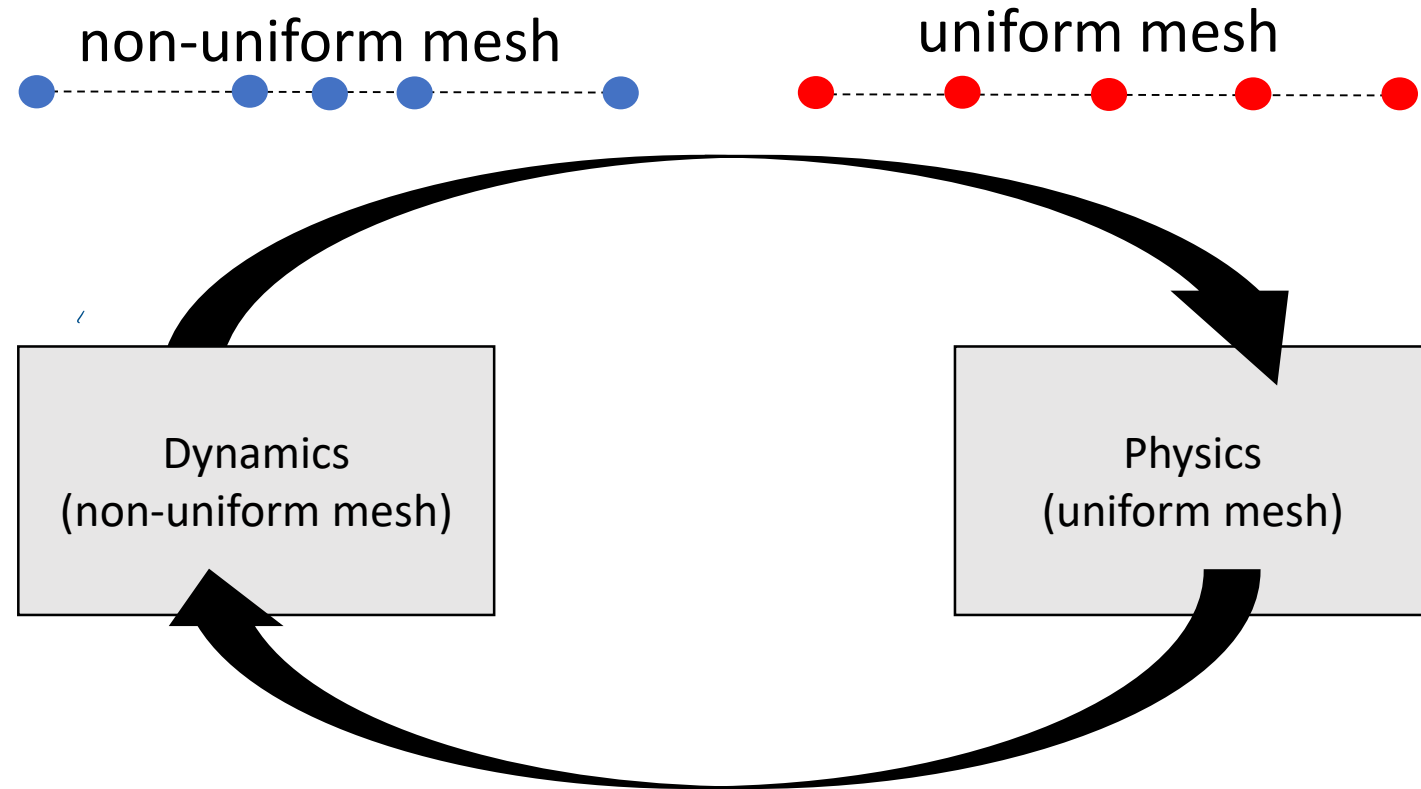
Example of Case Studies From Skamrock et al.

- The top two figures are not positivity preserving and the bottom two are.

- Non positivity-preserving in advection scheme contributes to the large positive bias found in the precipitation forecast.

- The 24-h accumulated precipitation valid at (left) 1200 UTC 5 Jun 2005 and (right) 1200 UTC 14 Apr 2007: (top) 12–36-h ARW non-PD forecasts, and (bottom) 12–36-h ARW PD forecasts.

- Positivity-preserving scheme reduces the moisture.

Non-PD ARW forecast

Non-PD ARW forecast

PD ARW forecast

PD ARW forecast

Skamrock et al. [1]
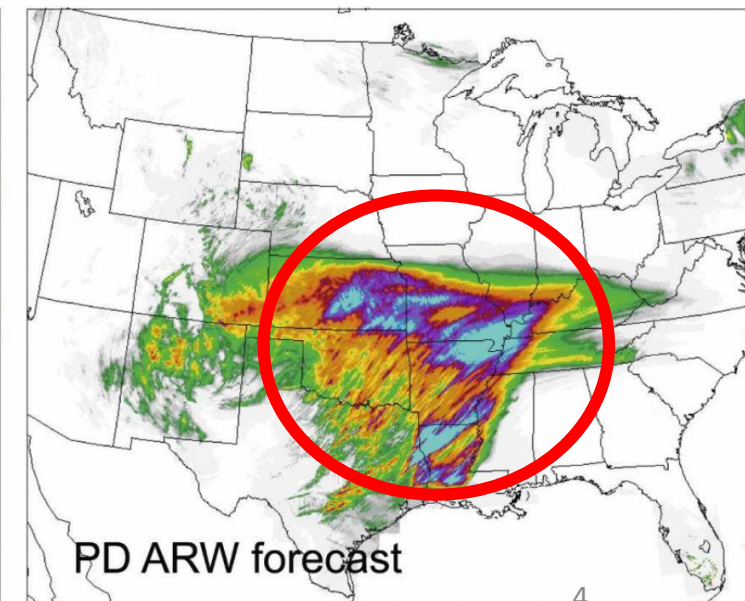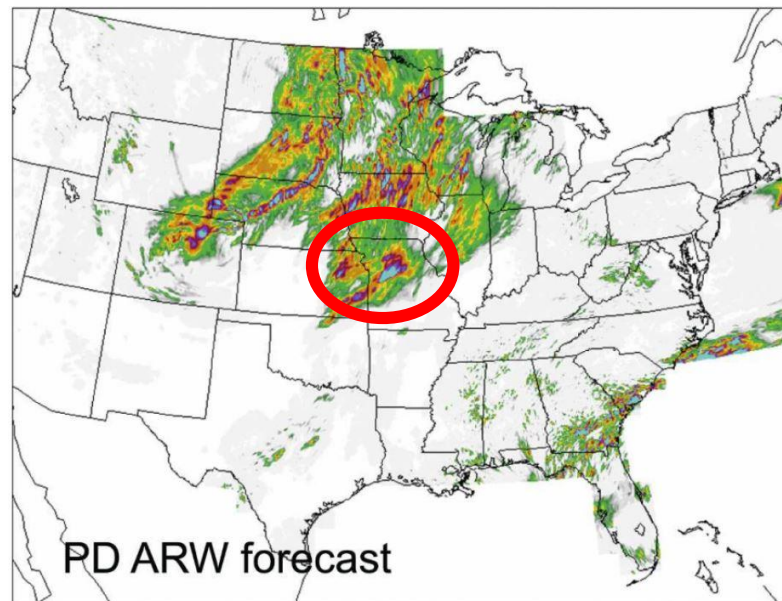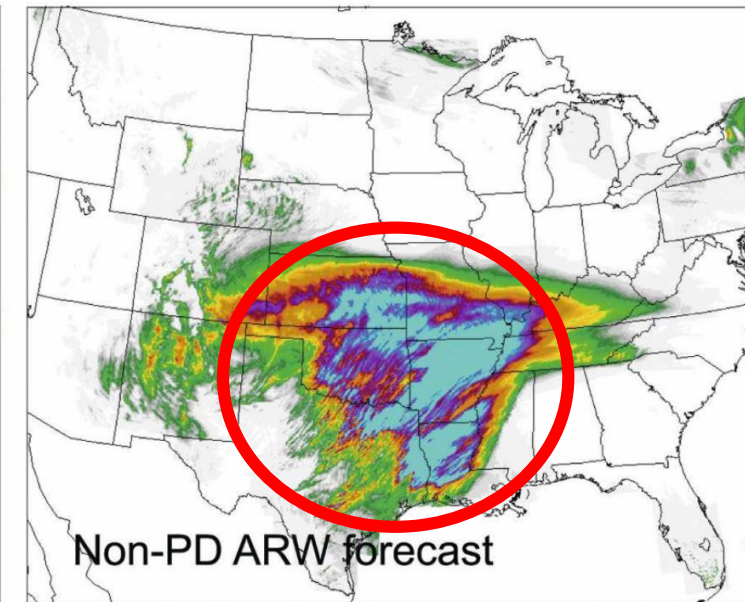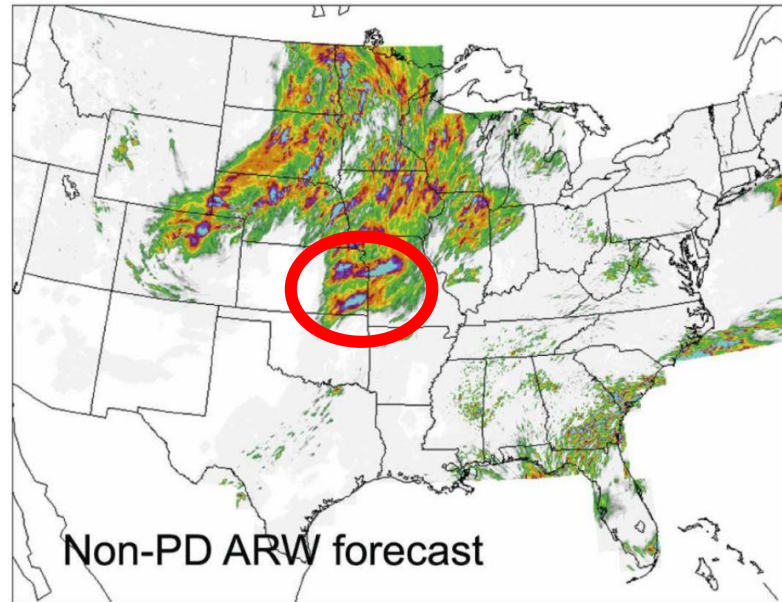
Mapping Challenges

- High-order methods enable high-accuracy and better utilization of compute resource.

- High-order polynomial interpolation may lead to oscillations, especially in the presence of steep gradients.

- Evaluating the polynomial at uniform mesh points may lead to negative values.
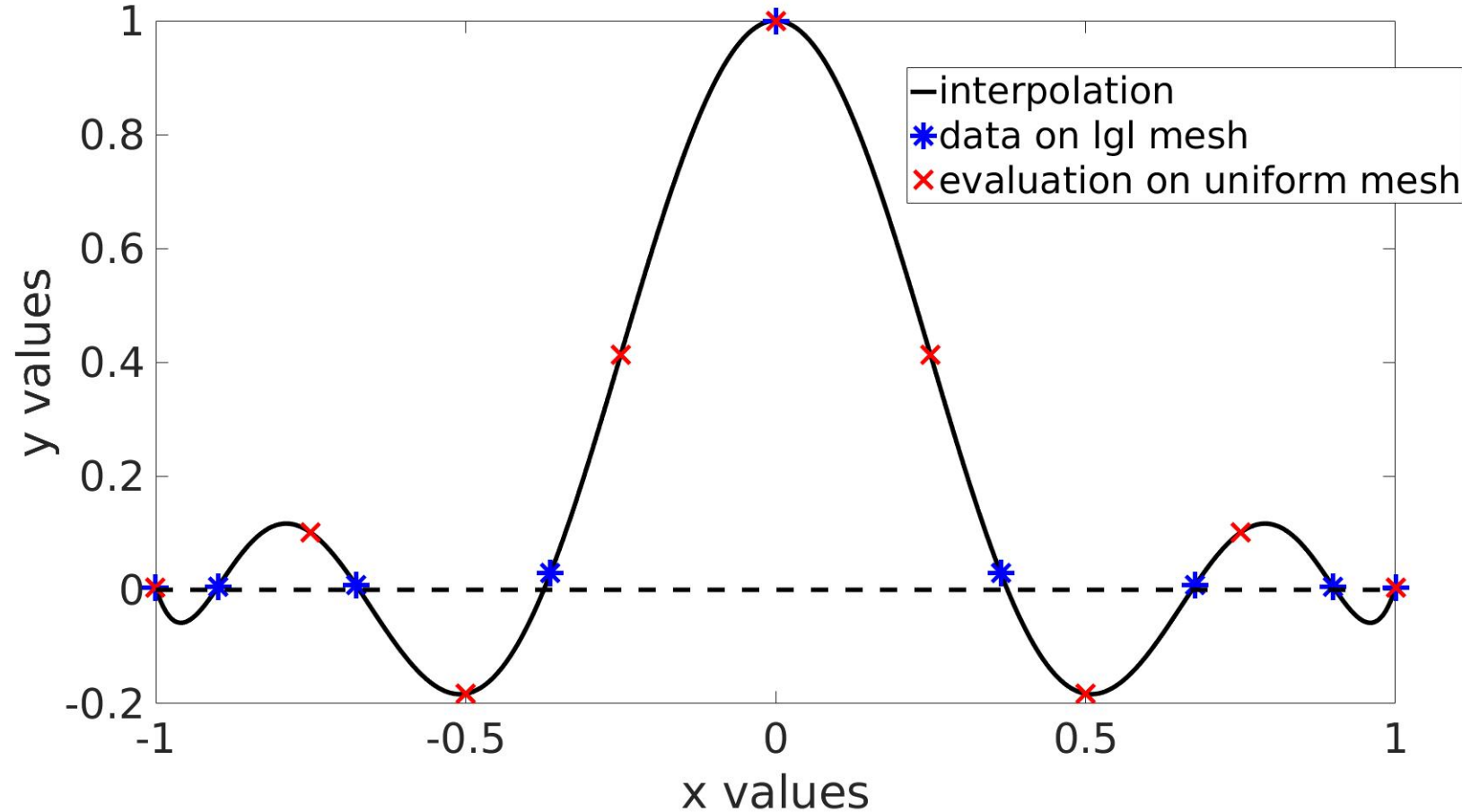
Mapping Challenges

- Now dynamics results in NEPTUNE are rescaled using Limiters by Zhang and Shu [3] and Light and Duran [4] (TMAR).

- Limiters by Zhang and Shu [3] (ZS) and Light and Duran. [4] (TMAR) rescale a given polynomial to ensure positivity at the nodes and conserve mass.

- The ZS or TMAR approach can be used to rescale resulting polynomials from dynamics (mapping from dynamics to physics).

- ZS and TMAR are not applicable for the physics to dynamics mapping because physics produces a set of values but not a polynomial.

- ZS and TMAR conserve mass but may increase oscillations.

Mitigate Mapping Challenges

- Introduce a **positivity-preserving mapping** from physics to dynamics and vice versa for NEPTUNE.
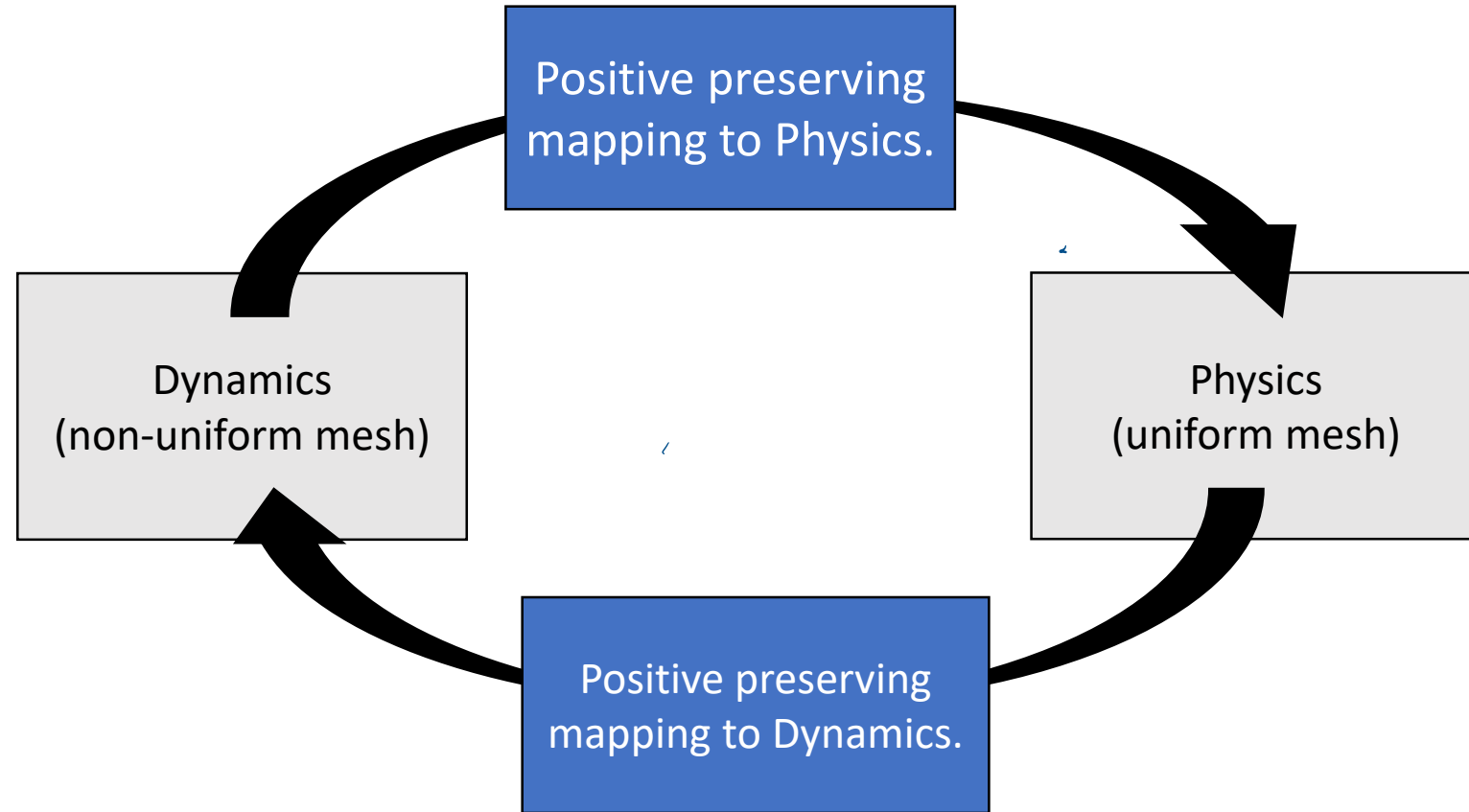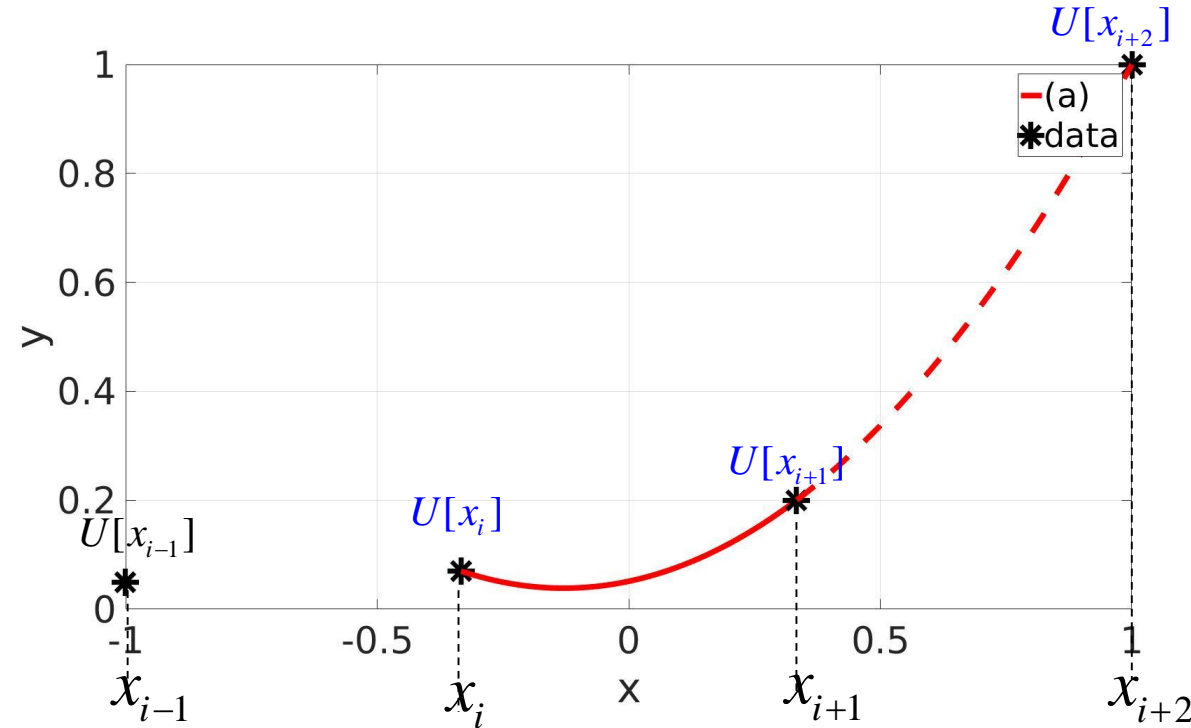
Newton Polynomial

(a) $P_N(x) = U[x_i] + (x - x_i)U[x_i, x_{i+1}]$
$+ (x - x_i)(x - x_{i+1})U[x_i, x_{i+1}, x_{i+2}]$

Divided difference: $U[x_i, x_{i+1}] = \dfrac{U[x_{i+1}] - U[x_i]}{x_{i+1} - x_i}$

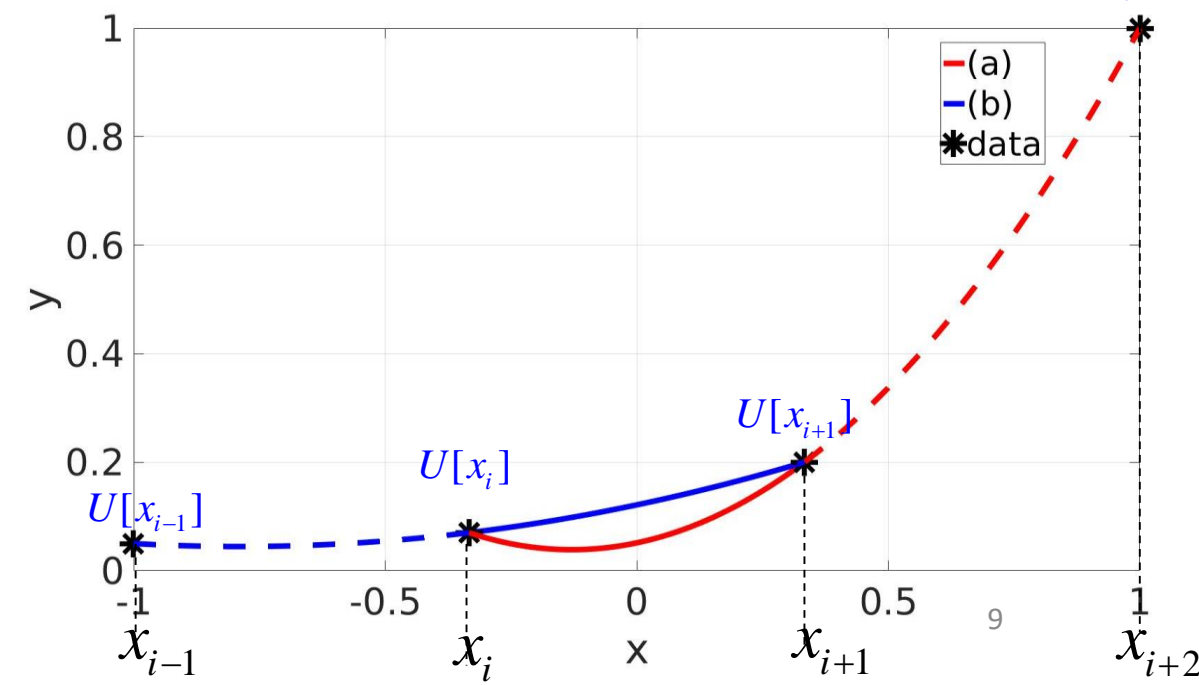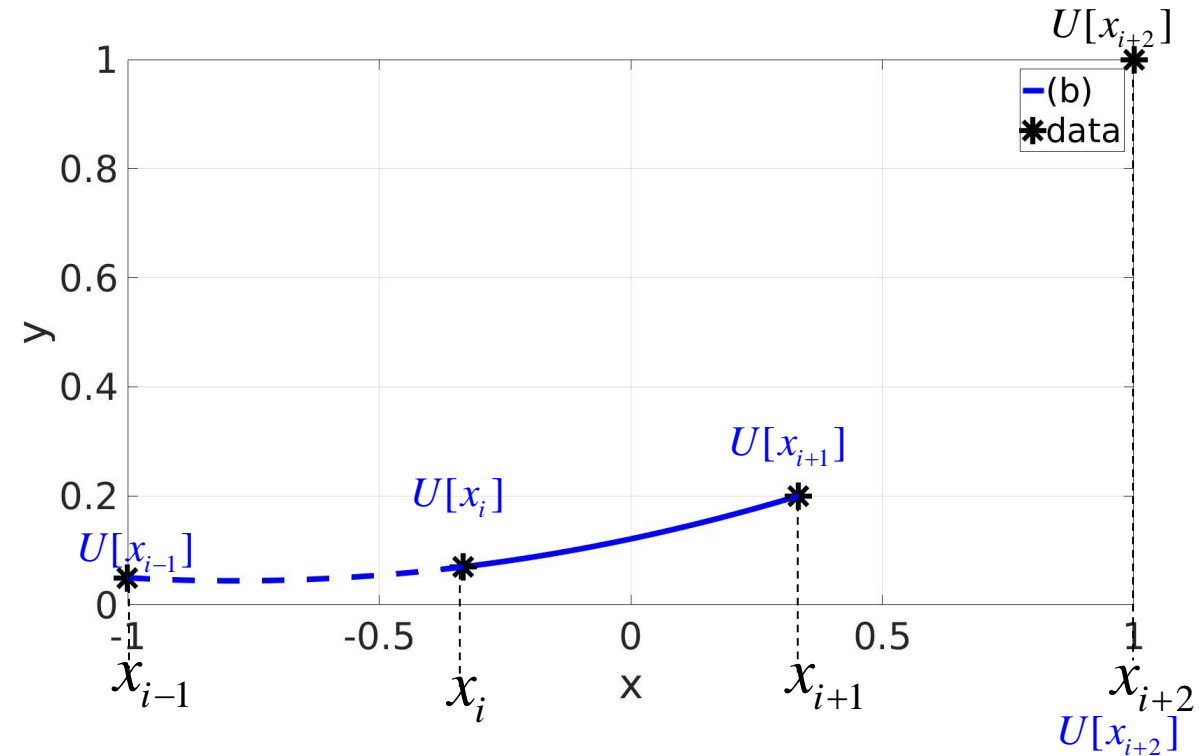$U[x_i, x_{i+1}, x_{i+2}] = \dfrac{U[x_i, x_{i+2}] - U[x_i, x_{i+1}]}{x_{i+2} - x_i}$

General case: $U[x_i, x_{i+1}, ..., x_{i+k}] = \dfrac{U[x_{i+1}, ..., x_{i+k}] - U[x_i, ..., x_{i+k-1}]}{x_{i+k} - x_i}$

Newton Polynomial

(a) $P_N(x) = U[x_i] + (x - x_i)U[x_i, x_{i+1}]$
$+ (x - x_i)(x - x_{i+1})U[x_i, x_{i+1}, x_{i+2}]$

(b) $P_2(x) = U[x_i] + (x - x_i)U[x_i, x_{i+1}]$
$+ (x - x_i)(x - x_{i+1})U[x_{i-1}, x_i, x_{i+1}]$

Data-Bounded

The positivity-preserving method builds on the data-bounded method by Berzins [2].

(b) $P_2(x) = U[x_i] + (x - x_i)U[x_i, x_{i+1}]$
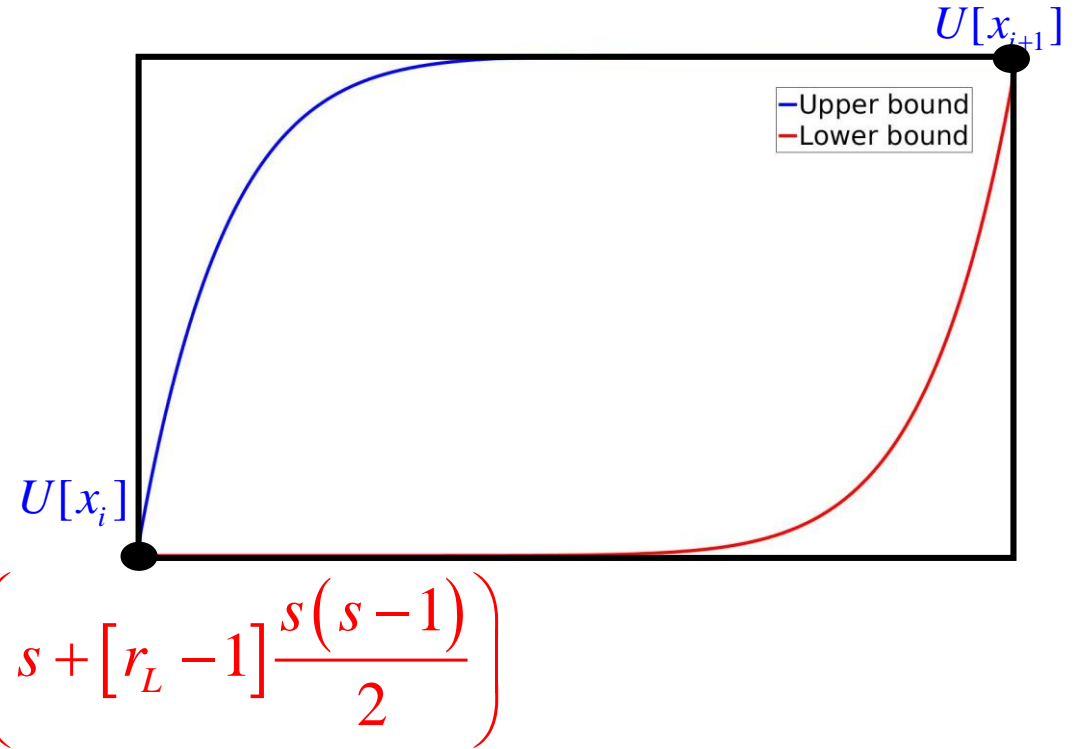
$\qquad + (x - x_i)(x - x_{i+1})U[x_{i-1}, x_i, x_{i+1}]$

Upper bound
Lower bound

$U[x_{i+1}]$

$U[x_i]$

can be written as $P_2(x) = U[x_i] + \left(U[x_{i+1}] - U[x_i]\right)\left(s + [r_L - 1]\dfrac{s(s-1)}{2}\right)$

with $0 \le s = \dfrac{(x - x_i)}{(x_{i+1} - x_i)} \le 1$ and $r_L = \dfrac{U[x_{i-1}, x_i]}{U[x_i, x_{i+1}]}$

$P_2(x)$ bounded between $U[x_{i+1}], U[x_i]$ requires $\boxed{0 \le S_2 = \left(s + [r_L - 1]\dfrac{s(s-1)}{2}\right) \le 1 \Rightarrow 0 \le r_L \le 1}$

Data-bounded method chooses the points so that the ratio of divided difference is bounded.

$0 \le r_L \le 1 \ or \ 0 \le r_R = \dfrac{U[x_{i+1}, x_{i+2}]}{U[x_i, x_{i+1}]} \le 1.$

Positivity-Preserving

The positivity-preserving method builds on the data-bounded method [2].

The positivity-preserving method is essentially relaxing

the bounds on the divided difference ratio r_R [5].
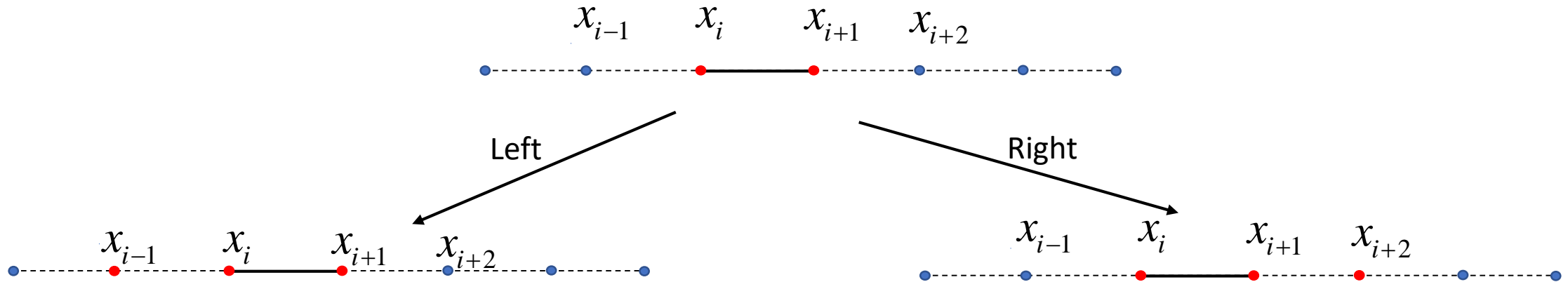
Positivity-preserving method requires

$$\Rightarrow -\frac{U[x_i]}{U[x_{i+1}]-U[x_i]} \leq r_L \leq -\frac{U[x_{i+1}]}{U[x_{i+1}]-U[x_i]} + 1 \text{ with } r_L = \frac{U[x_{i-1},x_i]}{U[x_i,x_{i+1}]}$$

$$\text{or } -\frac{U[x_{i+1}]}{U[x_{i+1}]-U[x_i]} - 1 \leq r_R \leq \frac{U[x_i]}{U[x_{i+1}]-U[x_i]} \text{ with } r_R = \frac{U[x_{i+1},x_{i+2}]}{U[x_i,x_{i+1}]}$$

Paper in preparation [5].

Adaptive Polynomial Interpolation
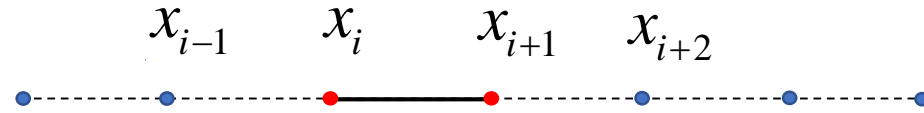
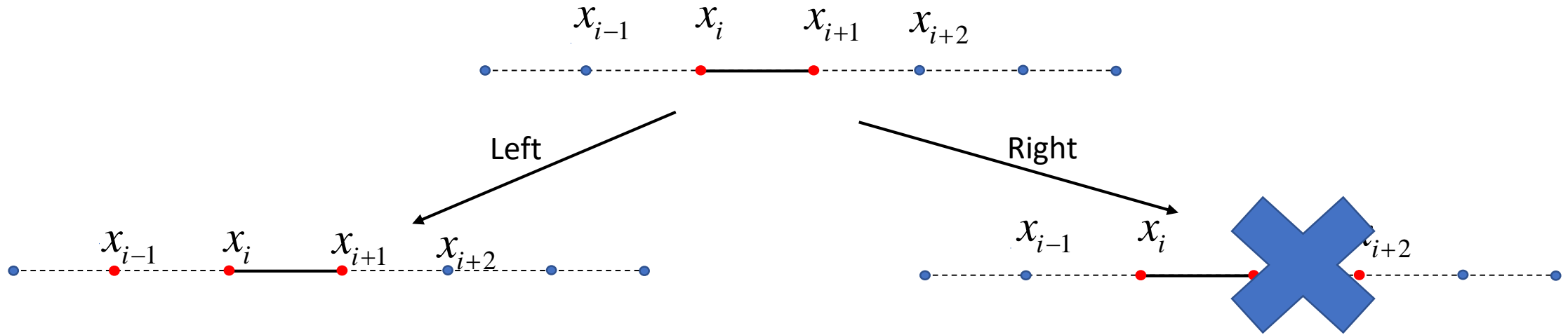$$x_{i-1} \qquad x_i \qquad x_{i+1} \qquad x_{i+2}$$

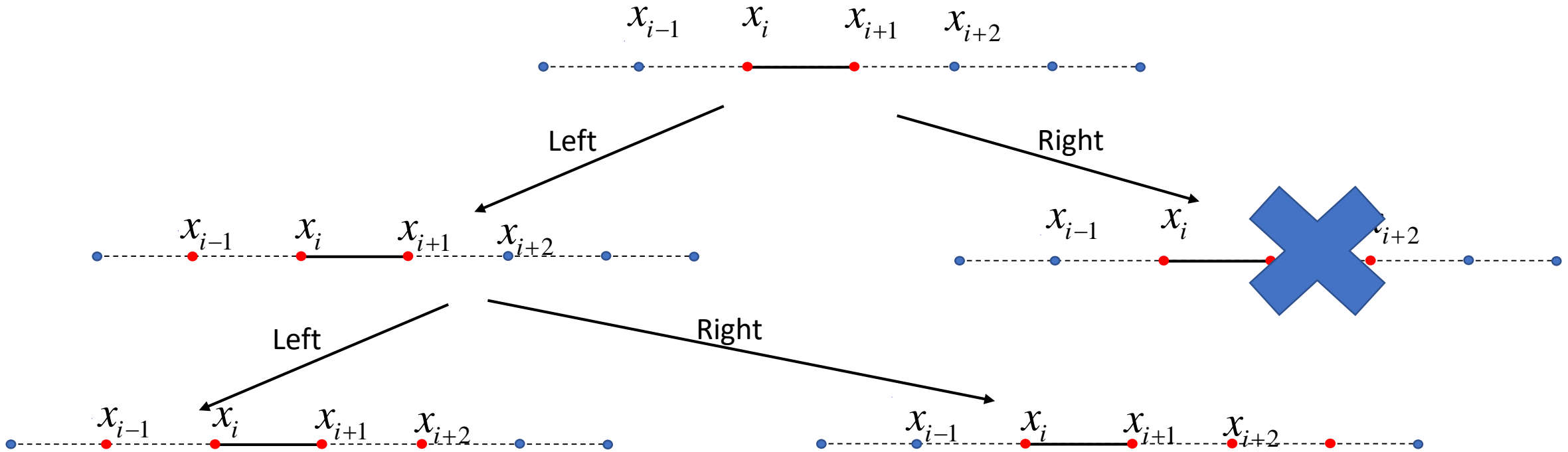# Adaptive Polynomial Interpolation

- Choose the direction with the smallest divided difference.

Adaptive Polynomial Interpolation

- Choose the direction with the smallest divided difference.
- Pick left because $\left| U[x_{i-1},...,x_{i+1}] \right| \leq \left| U[x_i,...,x_{i+2}] \right|$
- Check for positivity-preserving requirement.

Adaptive Polynomial Interpolation

- Choose the direction with the smallest divided difference.
- Pick left because $\left| U[x_{i-1}, \ldots, x_{i+1}] \right| \leq \left| U[x_i, \ldots, x_{i+2}] \right|$
- Check for positivity-preserving requirement.
- Repeat the process for the next degree.

Mapping Challenges

- The rescaled polynomial using TMAR ensures positivity at the nodes.

- Rescaling with TMAR conserves mass.

- The rescaled polynomial may increase oscillations.

- Rescaling requires a polynomial.

- The new positivity-preserving ensures positivity over the entire interval.

High Order Interpolation

Legend:
— Polynomial
— TMAR
— Pos. Pres.
∗ Data at lgl
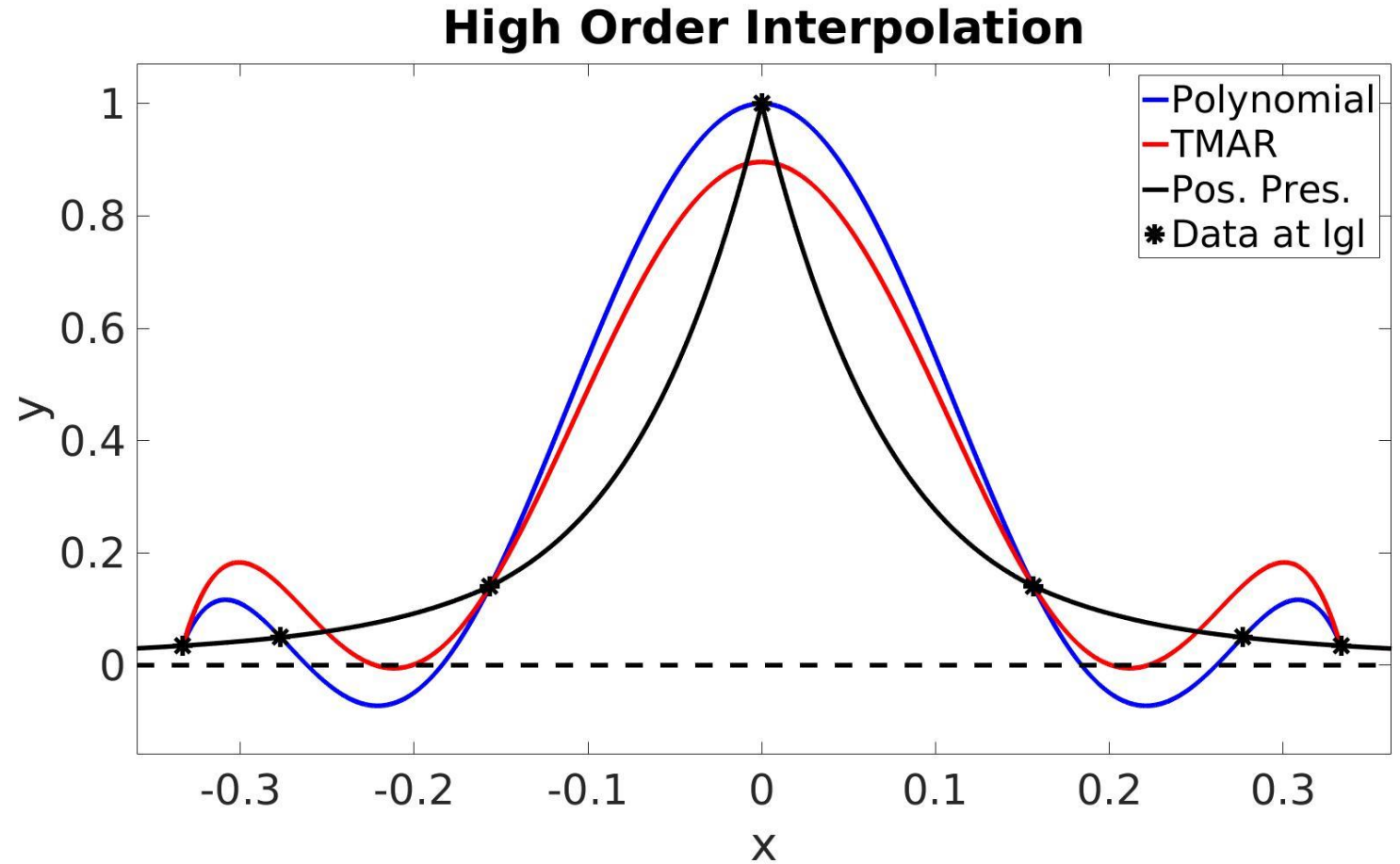
BOMEX Test Case

- The 1D Barbados Oceanographic and Meteorological Experiment (BOMEX) is a simulation developed to measure and study the rate of the properties of heat, moisture, and momentum.

- This work focuses on moisture, because "cloud mixing ratio" mapping between dynamics and physic leads to negative values.

- This simulation uses a 5th degree polynomial for each element.

$$\frac{\partial \overline{\phi}}{\partial t} = \left(\frac{\partial \overline{\phi}}{\partial t} \right)_{\mathrm{mod}\, el / dynamics} + \left(\frac{\partial \overline{\phi}}{\partial t} \right)_{forcing / physics}$$

Where ϕ is dependent on (θ, q, u, v) that are respectively

water potential temperature, total water scpecific humidity,

and the velocity components.

Positivity-Preserving Interpolation In BOMEX Code

- The pseudo code indicates where positivity-preserving interpolation is applied in the BOMEX test case.

- The positivity-preserving interpolation enables a positivity-preserving mapping from dynamics to physics and vice versa.

- *While(t <=tf)*
  - *Bomex_ls_forcing(...)   !!dynamics*
  - ***Positve_preserv_interpolation(....)***
  - *Run_scm_physics(...)   !! physics*
 - ***Positve_preserv_interpolation(....)***
- *end*

BOMEX (No Limiter)
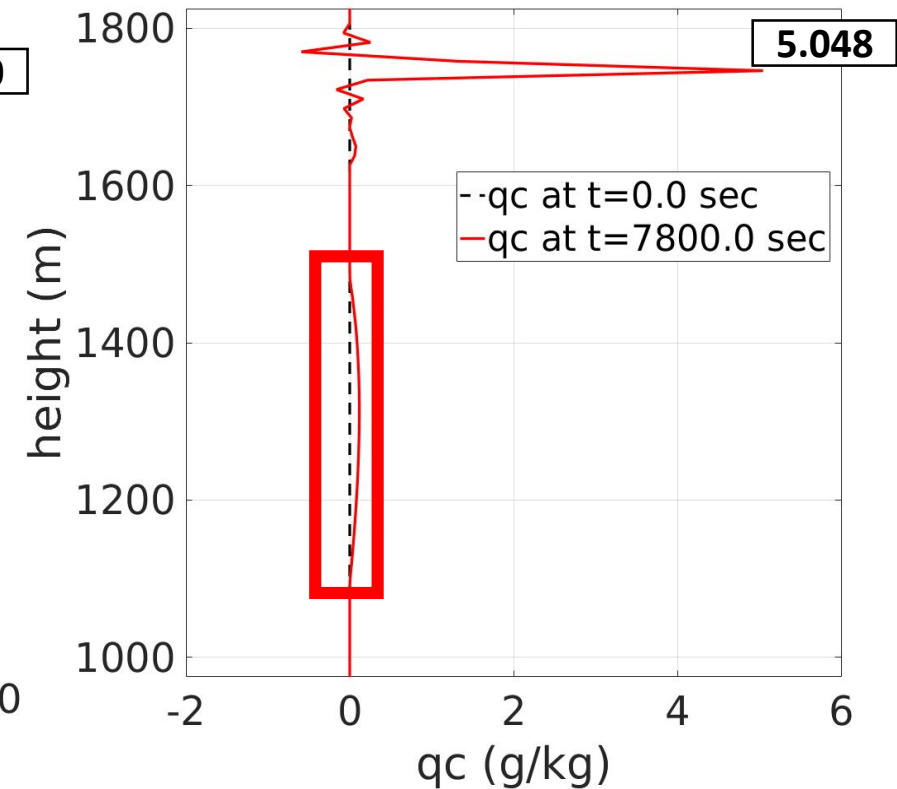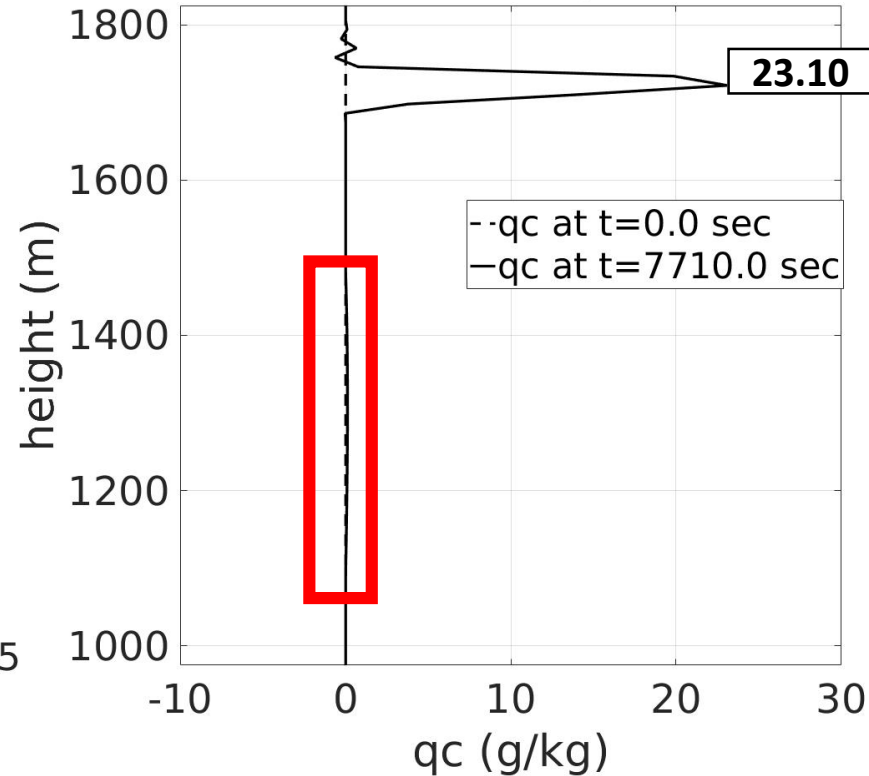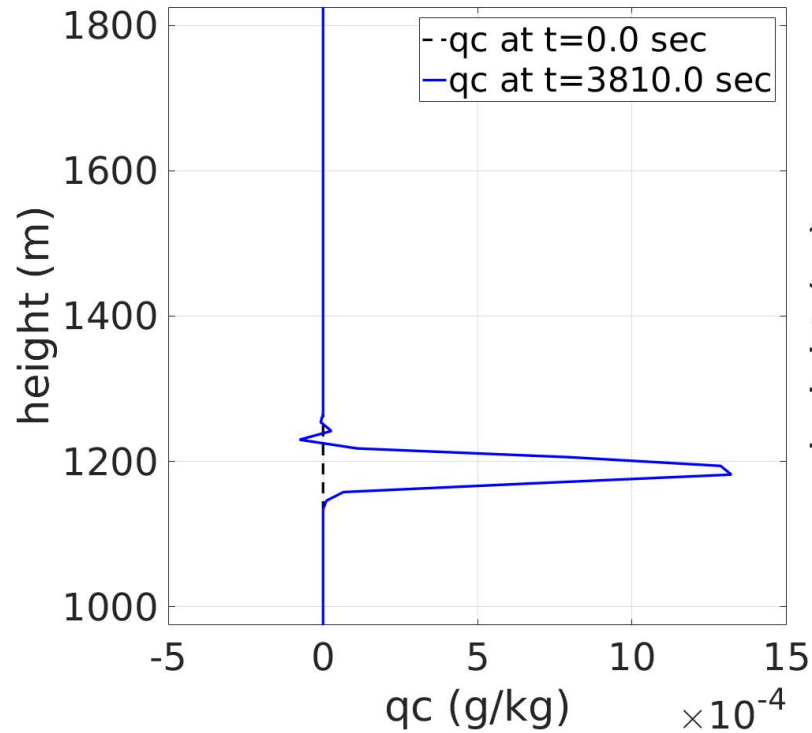
- The negative values (started at t= 3810 sec) and oscillations are picked up by the physics, causing false peaks at t = 7710.0. sec and t=7800 sec.

- Unphysical values cause the simulation to crash before the final time step t=21600.0

- The red box indicates the interval [1150, 1500] where the cloud-mixing ratio should be observed.

BOMEX (No Limiter)
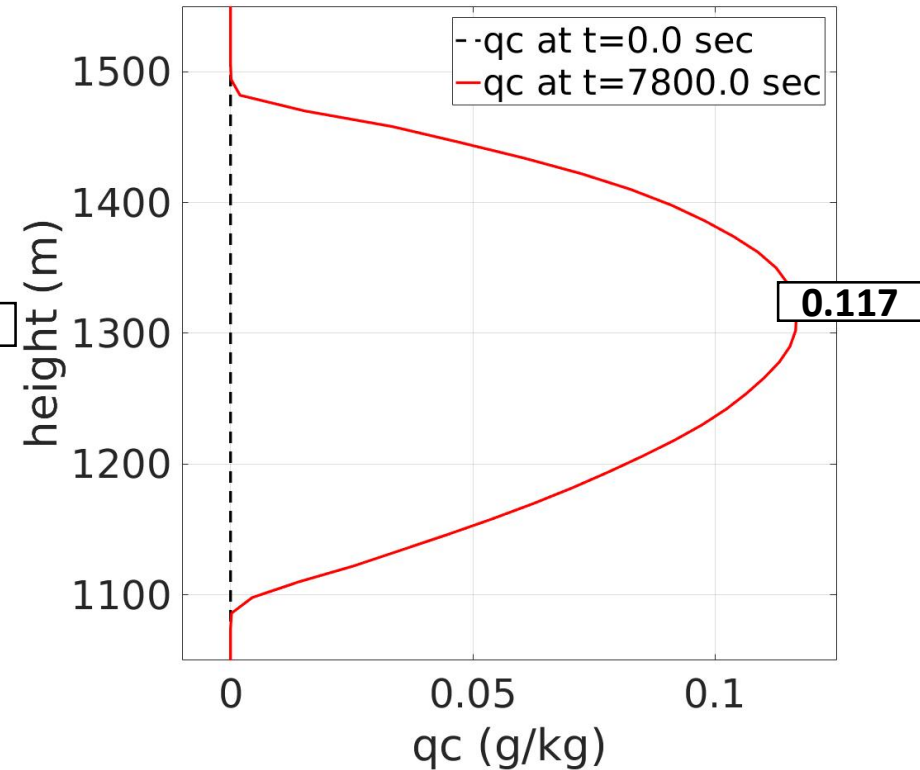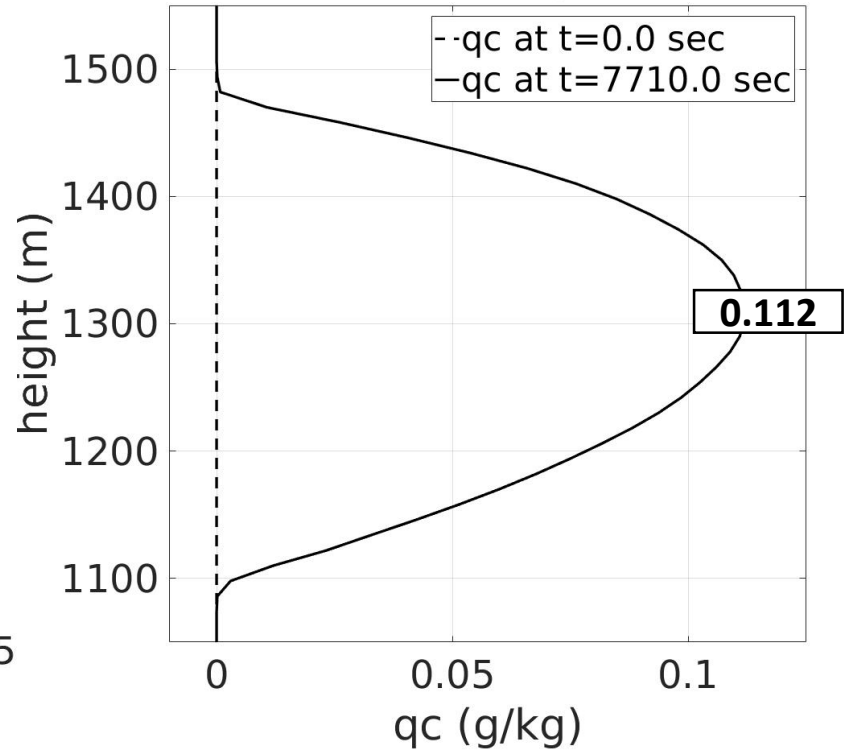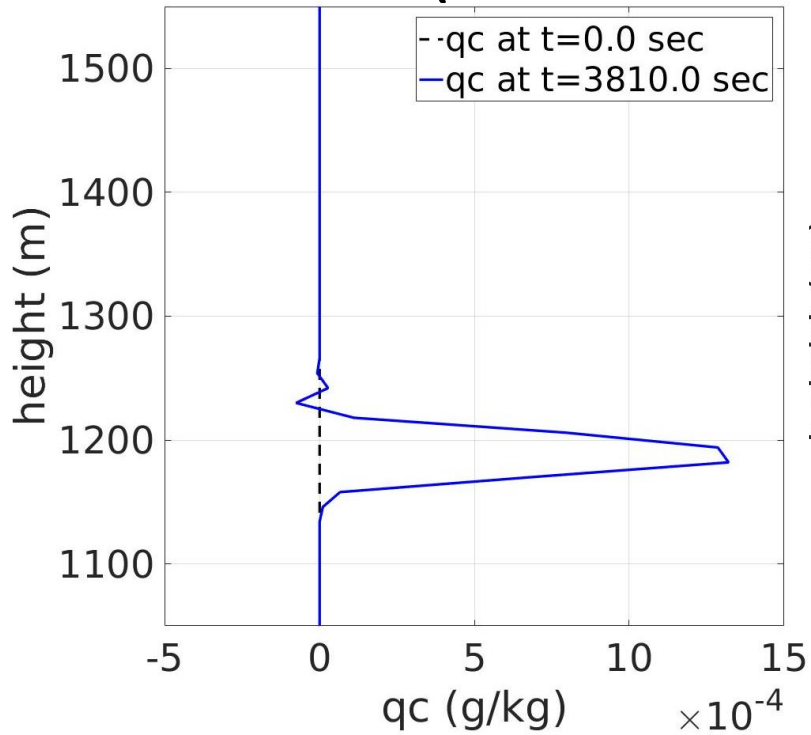
- A close look at the interval [1050, 1500] indicates more reasonable peaks.
- The blue plot is early in the simulation when not much of the cloud mixing-ratio is produced.

BOMEX With "Clipping"
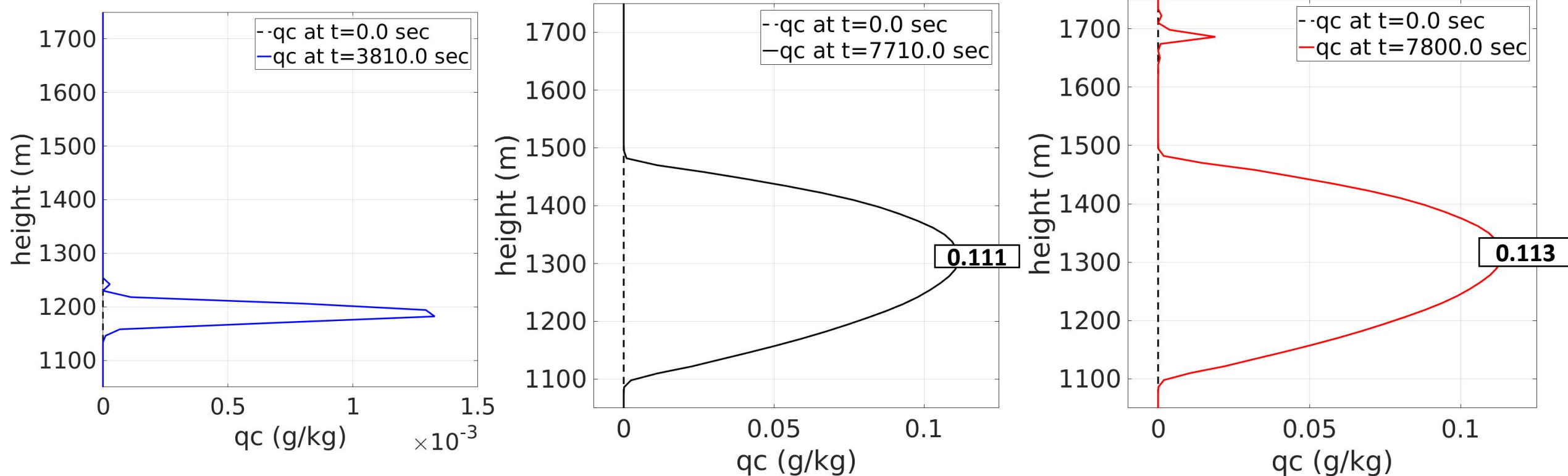
- "Clipping" corresponds to truncating negative values by setting them to zero.
- The values of qc do not blow up, and the simulation does not crash.
- Oscillations cause a secondary peak as shown with the red plot at t = 7800.0 sec.

Positivity Preserving Interpolation
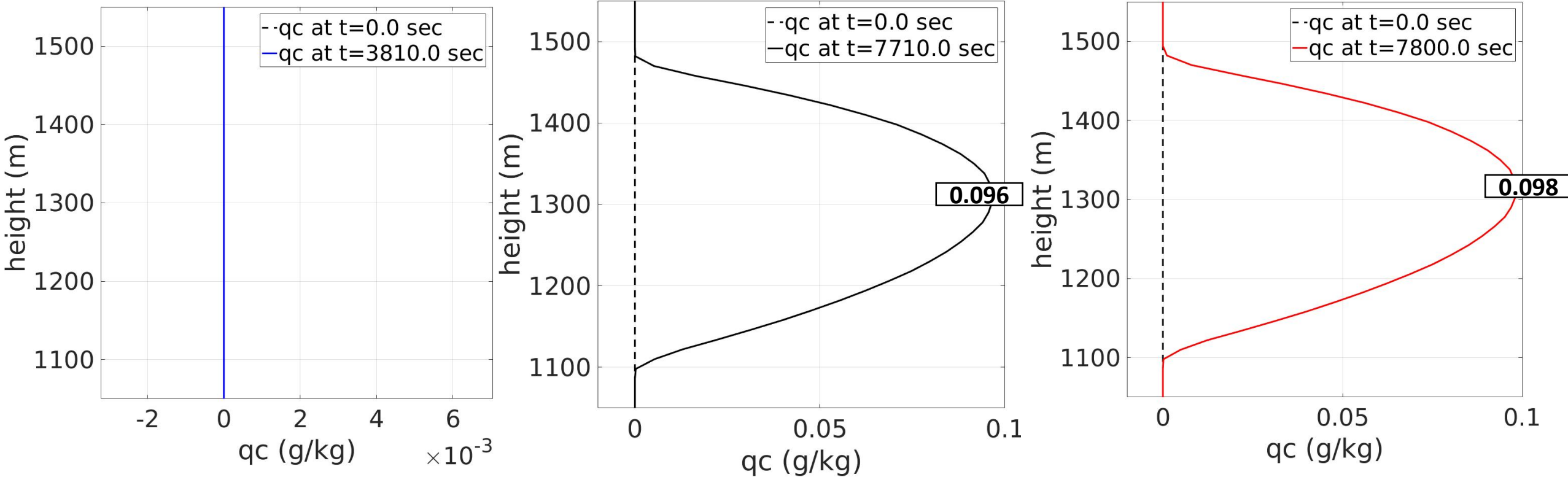
- The cloud-mixing ratio remains positive over the entire simulation.

- The cloud-mixing ratio peak is **qc=0.098** g/kg at t=7800 sec, which is less than all the previous cases. Positivity-preserving interpolation reduces the positive bias in the cloud-mixing ratio prediction.

Polynomial Degree Distribution (preliminary results)

- The two figures show preliminary results on the polynomials degrees for the different sub-interval.

- More investigation is required to better understand the distribution.

- The histogram shows the polynomials degrees distribution at t = 7800.0 sec.

- The figure to the bottom shows the range (subinterval range) in terms of the polynomials degrees.
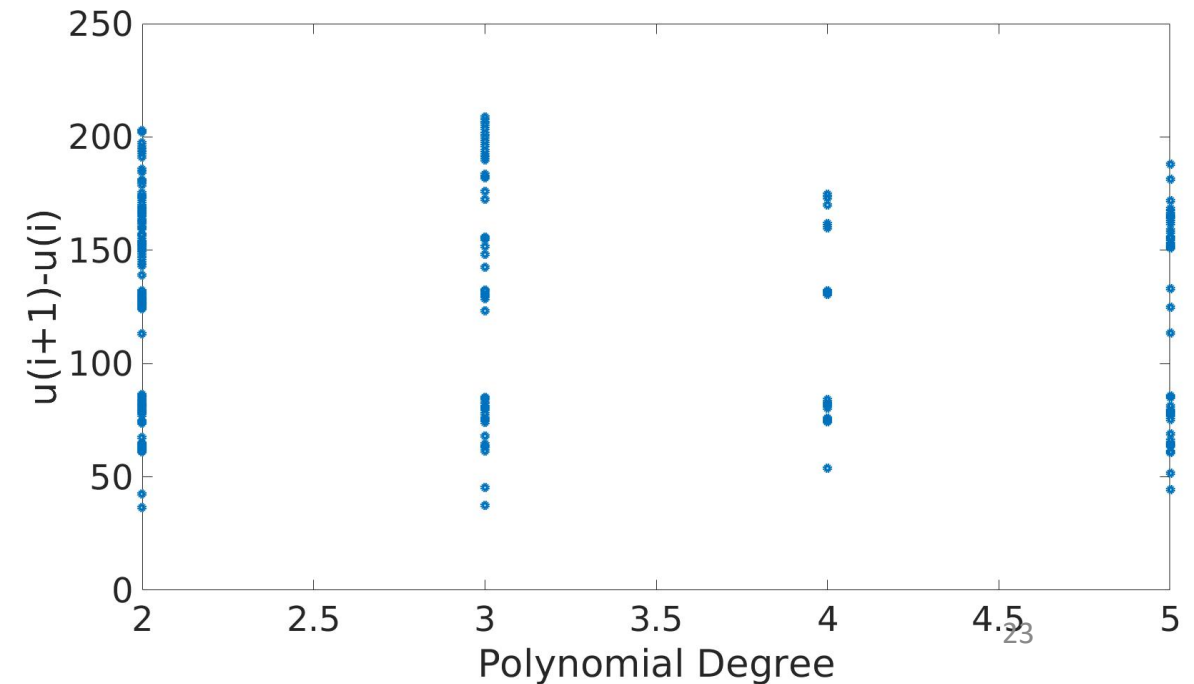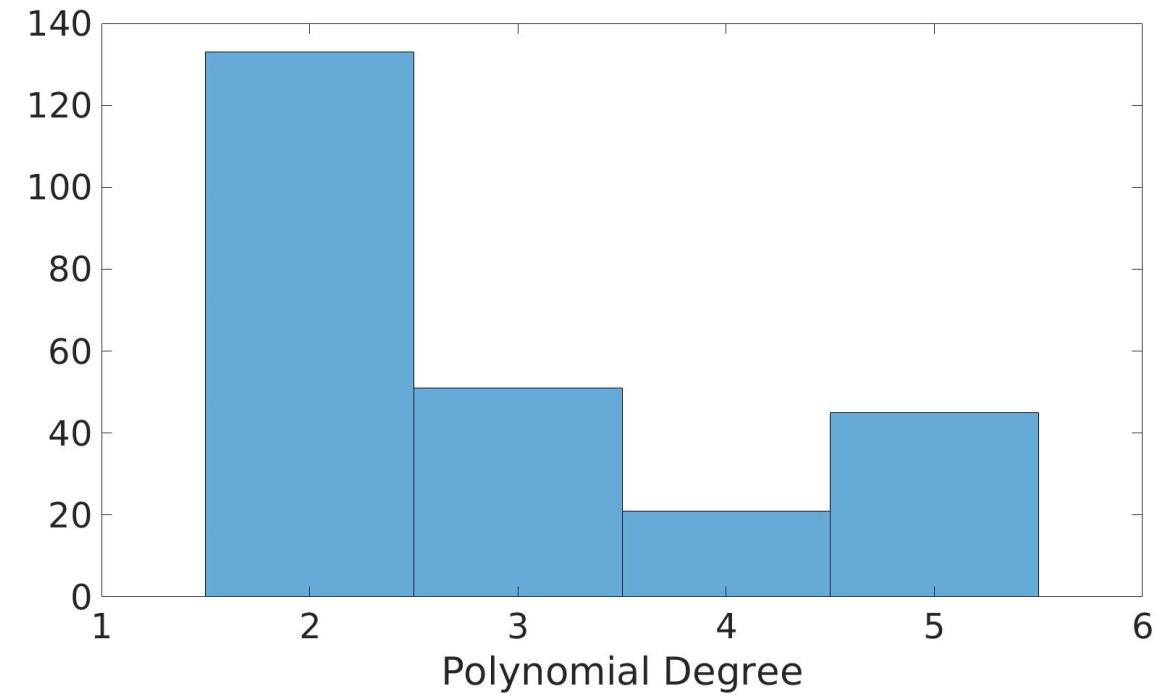
Discussion

- High-order interpolation may lead to oscillations and negative values.

- Non positivity-preserving leads to positive bias in the cloud-mixing ratio prediction.

- "Clipping" removes the negatives values but does not reduce the positive bias in the cloud-mixing ratio prediction.

- The positivity-preserving is less restrictive than the data-bounded interpolation and reduces oscillations.

- The positivity-preserving interpolation reduces the positive bias in the cloud-mixing ratio prediction.

- In some cases ensuring positivity may require the use of low-order polynomial.

Future Work/Conclusion

- Investigate the 3D case in the context of NEPTUNE.

- Mathematical formulation of the positivity-preserving interpolation for non-uniform mesh.

- **Acknowledgements:**
  - Intel Parallel Computing Center.

References

[1] Skamarock, William C., and Morris L. Weisman. "The impact of positive-definite moisture transport on NWP precipitation forecasts." *Monthly Weather Review* 137.1 (2009): 488-494.

[2] Berzins, Martin. "Adaptive polynomial interpolation on evenly spaced meshes." *SIAM review* 49.4 (2007): 604-627.

[3] Zhang, Xiangxiong, and Shu Chi-Wang. "Maximum-principle-satisfying and positivity-preserving high-order schemes for conservation laws: survey and new developments." *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*. Vol. 467. No. 2134. The Royal Society, 2011.

[4] Light, Devin, and Dale Durran. "Preserving Non negativity in Discontinuous Galerkin Approximations to Scalar Transport via Truncation and Mass Aware Rescaling (TMAR)." *Monthly Weather Review* 144.12 (2016): 4771-4786.

[5] T.A.J Ouermi, Robert M. Kirby, Martin Berzins, Positivity Preserving Interpolation (paper in preparation)

Thank you !!

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Adaptive Polynomial Interpolation

Let $\{x_0, x_1, x_2, \ldots, x_N\}$ be a mesh with corresponding data values $\{y_0, y_1, y_2, \ldots, y_N\}$

The Newton polynomial passing through the set N data values can be represented as

$$P_N(x) = u_0 + u_1 L_1(x) + u_2 L_2(x) + \ldots + u_n L_N(x)$$

where u_i Represents divided differences and L_i the newton basis functions

The polynomial can be rewritten as

$$P_N(x) = U[x_0] + (x - x_0)U[x_0, x_1]\left(1 + \frac{(x - x_1)}{(x_1^r - x_1^l)}\lambda_2 \times \left(1 + \frac{(x - x_1)}{(x_2^r - x_2^l)}\lambda_3 \times \left(1 + \frac{(x - x_3^e)}{(x_3^r - x_3^l)}\lambda_4 \times \ldots \times \left(1 + \frac{(x - x_{N-1}^e)}{(x_2^r - x_2^l)}\lambda_N\right)\ldots\right)\right)\right)$$

where λ_i is a function of the divided difference u_i

Data-Bounded and Positivity

$$\lambda_{k+1} = \left(1 - r_{[x_i,...,x_{i+k}]}^{[x_{i-1},...,x_{i+k}-1]}\right)$$ For choosing the next stencil point to be on the left

$$\lambda_{k+1} = \left(r_{[x_i,...,x_{i+k}]}^{[x_{i+1},...,x_{i+k+1}]} - 1\right)$$ For choosing the next stencil point to be on the right

where $$r_{[x_i,...,x_{i+k}]}^{[x_{i+1},...,x_{i+k+1}]} = \frac{U[x_{i+1},...,x_{i+k+1}]}{U[x_i,...,x_{i+k}]}$$

- Non-oscillatory and positivity are ensured by enforcing constraints on λ_{k+1}

Data-Bounded Interpolation

- Data bounded interpolation with 50 elements.

- The cloud-mixing remains positive over the entire simulation.

- The data bounded limiter is applied at every time step.

- The cloud mixing ratio peak qc=0.0707 at t = 7800.0.
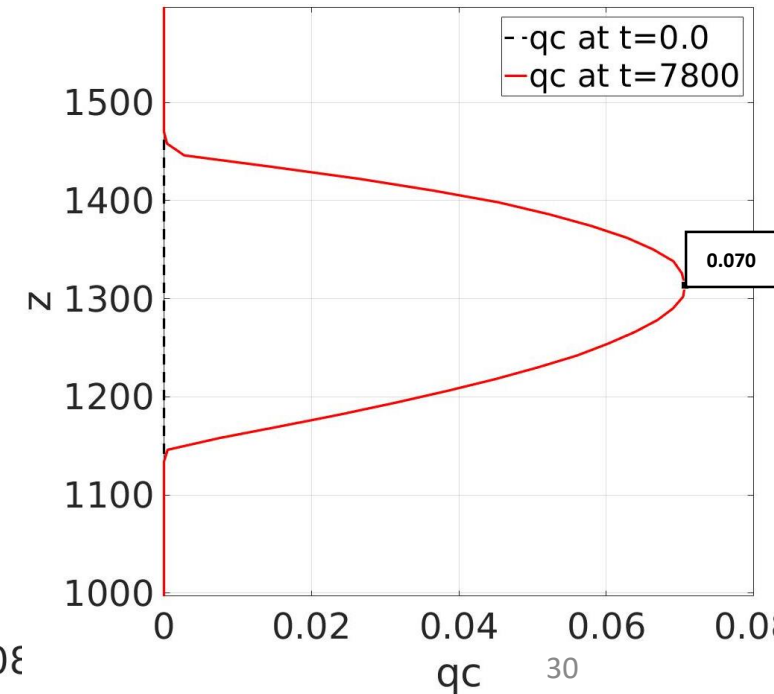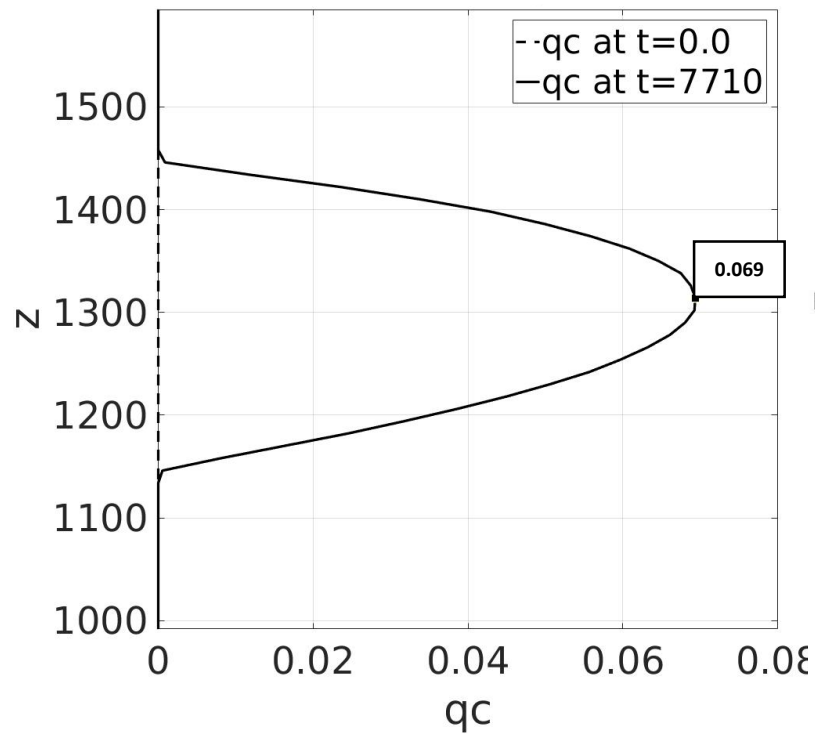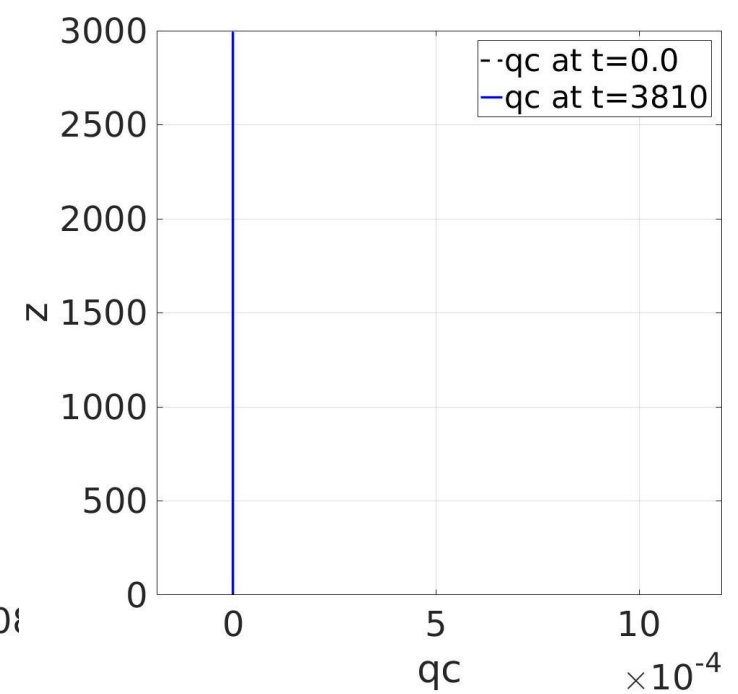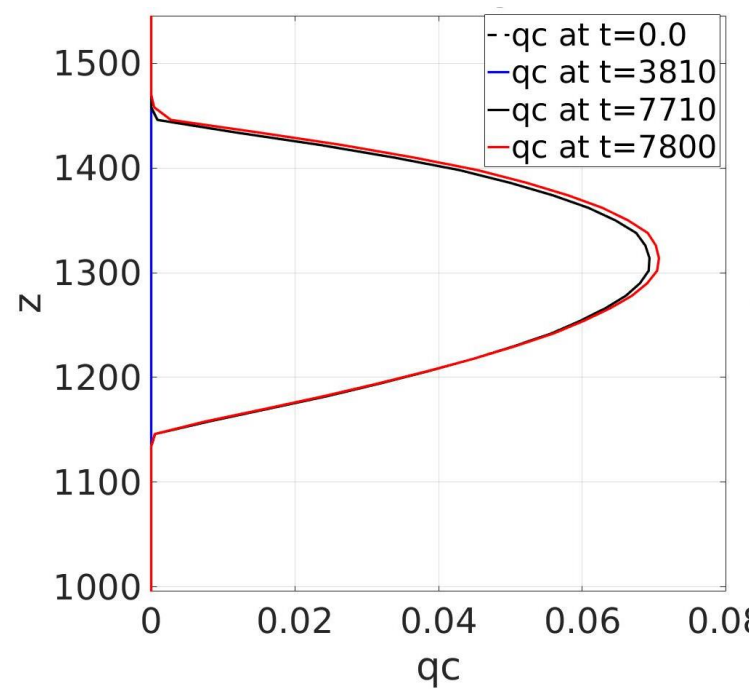
New Positivity-Preserving Interpolation

- Relaxed bounds for interpolation compared to the data-bounded interpolation.
- Preserves positivity over the entire interval.
- Does not necessarily keep high-order for each subinterval.

High Order Interpolation

Legend:
- Data Bounded
- Pos. Pres.
- Data at lgl
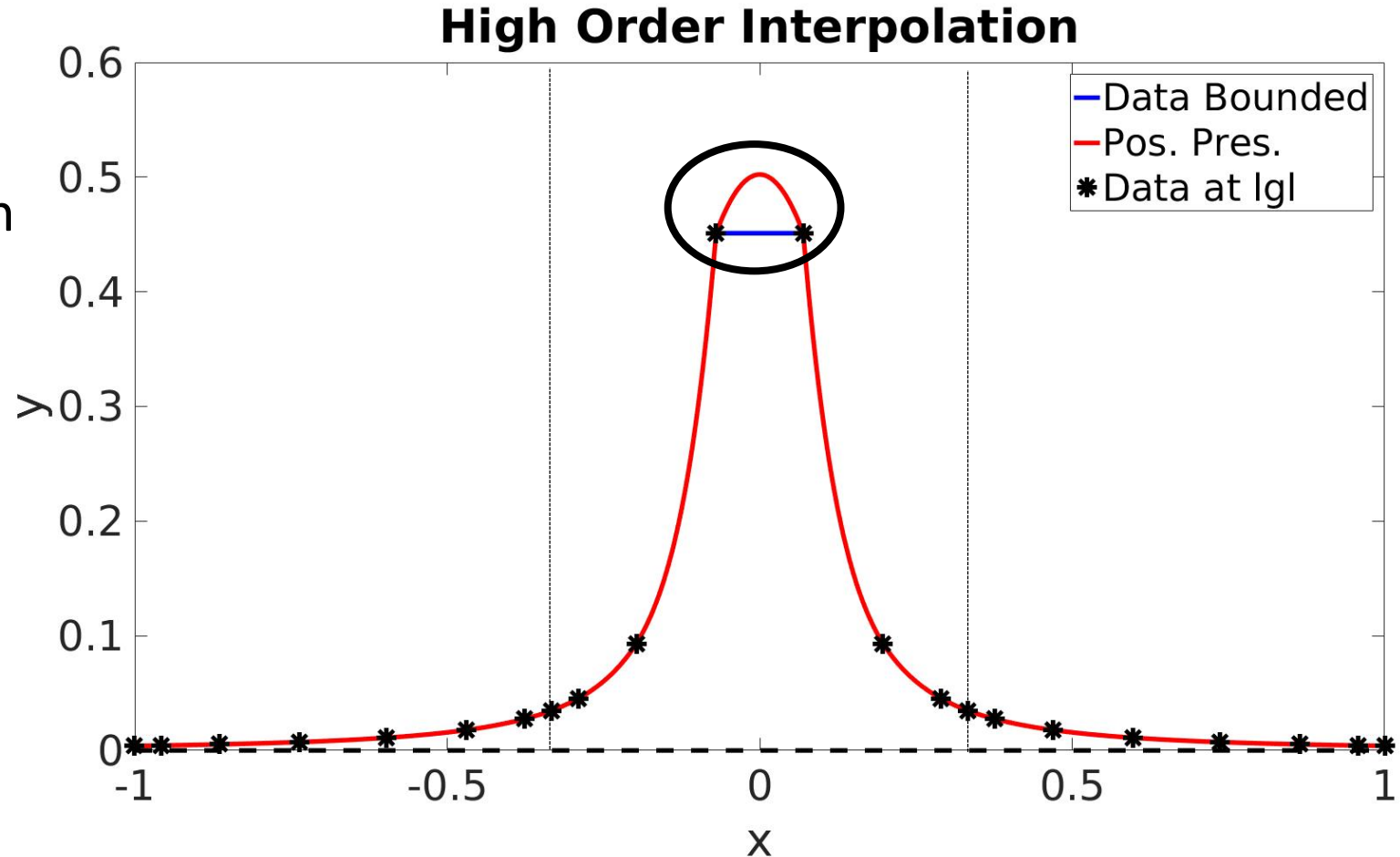
Data-Bounded and Positivity-preserving

$$P_N(x) = U[x_0] + (x - x_0)U[x_0, x_1]\left(1 + \frac{(x - x_1)}{(x_1^r - x_1^l)}\lambda_2 \times \left(1 + \frac{(x - x_1)}{(x_2^r - x_2^l)}\lambda_3 \times \left(1 + \frac{(x - x_3^e)}{(x_3^r - x_3^l)}\lambda_4 \times ... \times \left(1 + \frac{(x - x_{N-1}^e)}{(x_2^r - x_2^l)}\lambda_N\right)...\right)\right)\right)$$

- Choose the stencil with smallest divided difference at each stage

- Alter the polynomial by limiting λ_i to ensure positivity or data-boundedness

$\left|\overline{\lambda}_i\right| \leq 1$ For Data bounded

$\left|\overline{\lambda}_i\right| \leq M$ For positivity

with $\overline{\lambda}_i = \lambda_1 \times \lambda_2 \times ... \times \lambda_i$