Scalar Conservation Mapping in Dynamics to Physics Coupling

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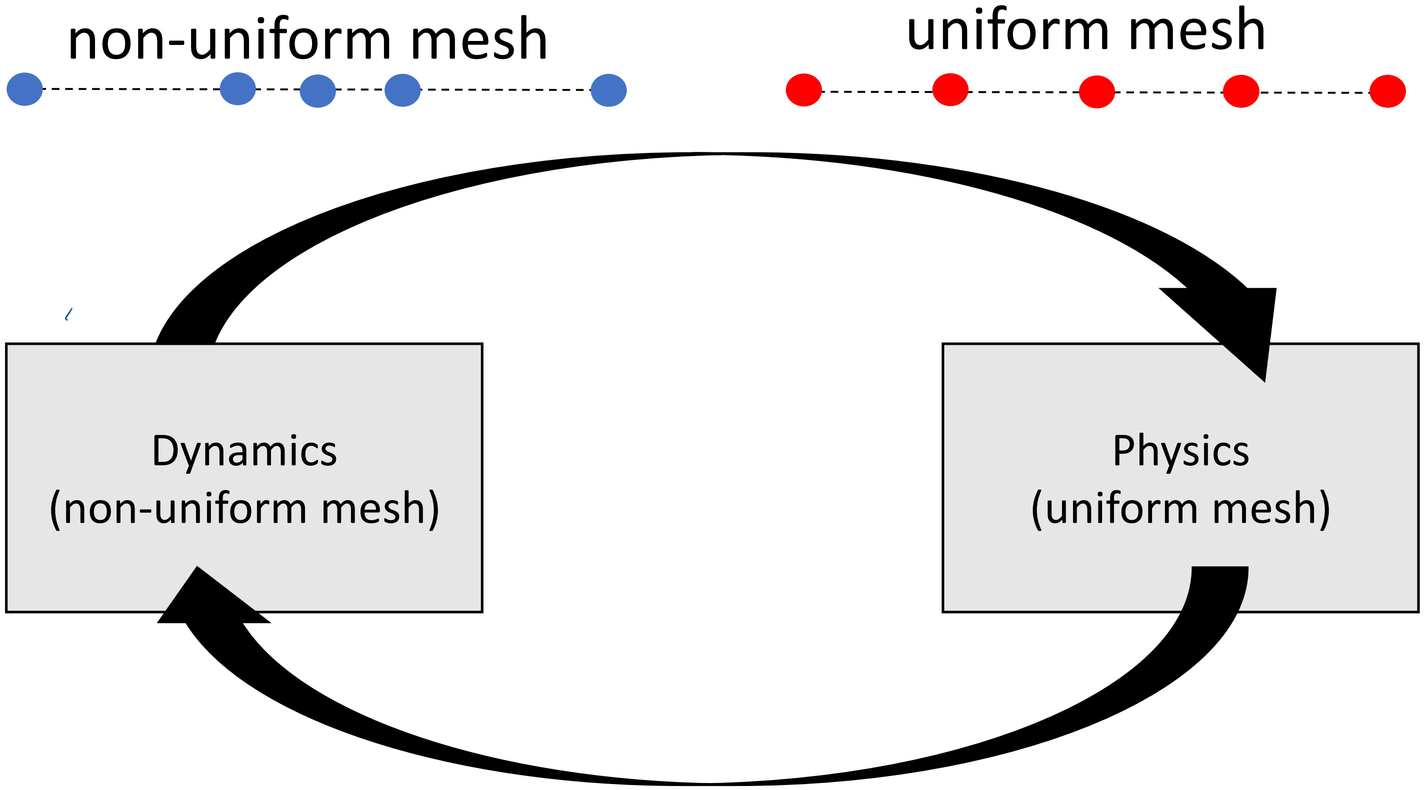
Outline

- Motivation
- Mapping challenges
- Positivity-preserving mapping
- Application results with 1D BOMEX
- Discussion and closing remarks

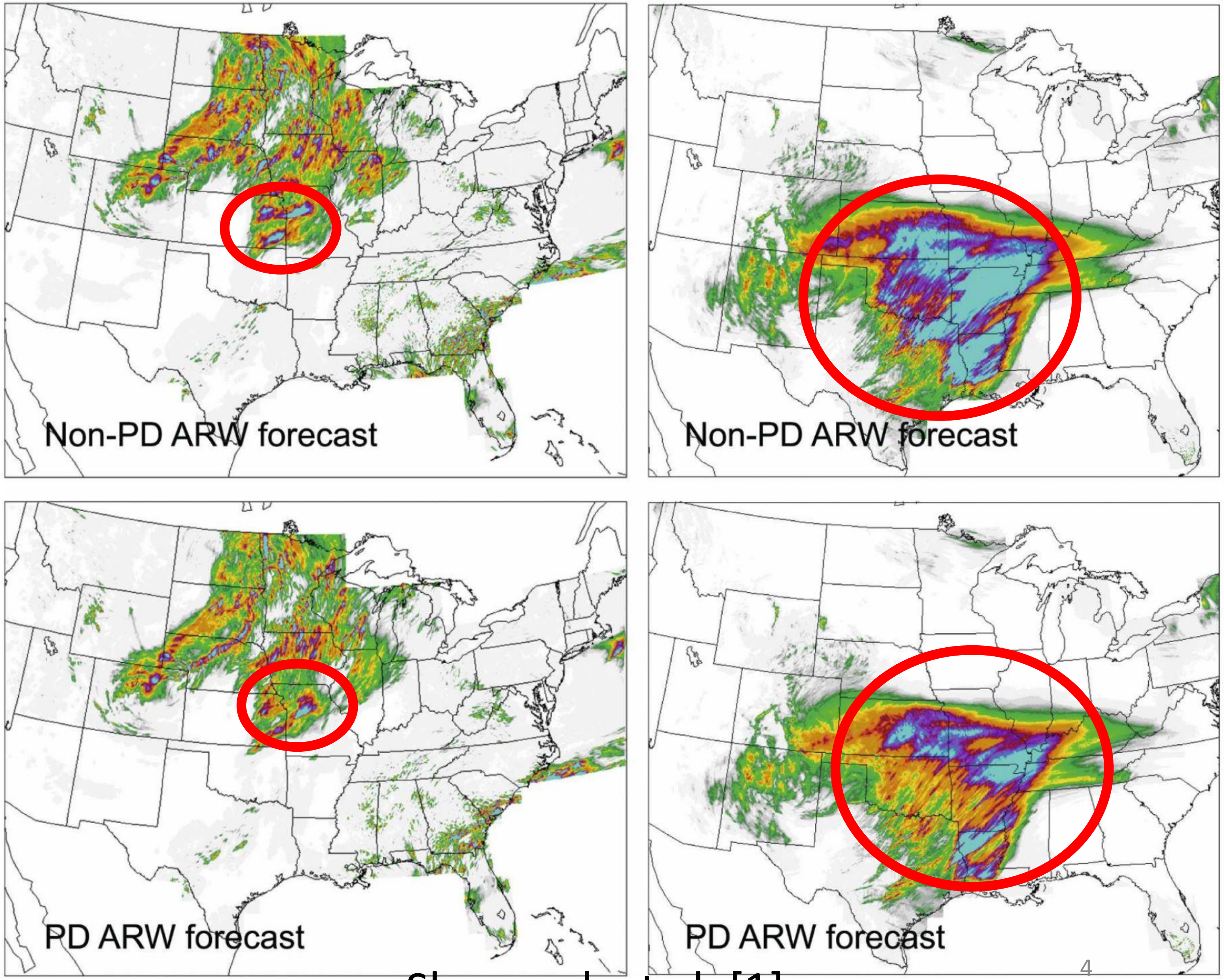
Motivation

- 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.**



Example of Case Studies From Skamrock et al.

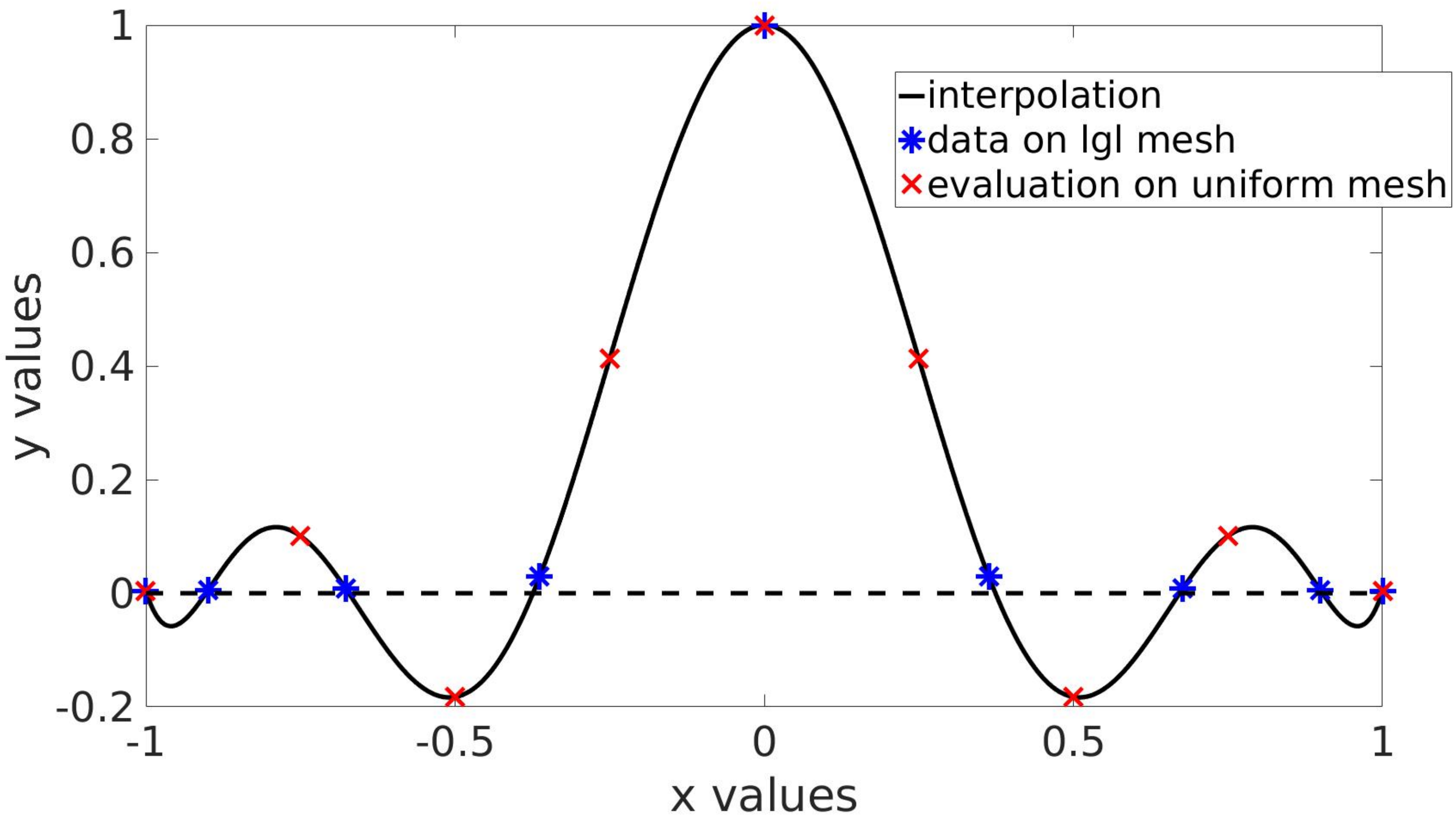
- The top two figures are not positivity preserving and the bottom two are.
- Non positivity-preserving in advection scheme contributes to the large positive bias found in the precipitation forecast.
- The 24-h accumulated precipitation valid at (left) 1200 UTC 5 Jun 2005 and (right) 1200 UTC 14 Apr 2007: (top) 12–36-h ARW non-PD forecasts, and (bottom) 12–36-h ARW PD forecasts.
- Positivity-preserving scheme reduces the moisture.



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.

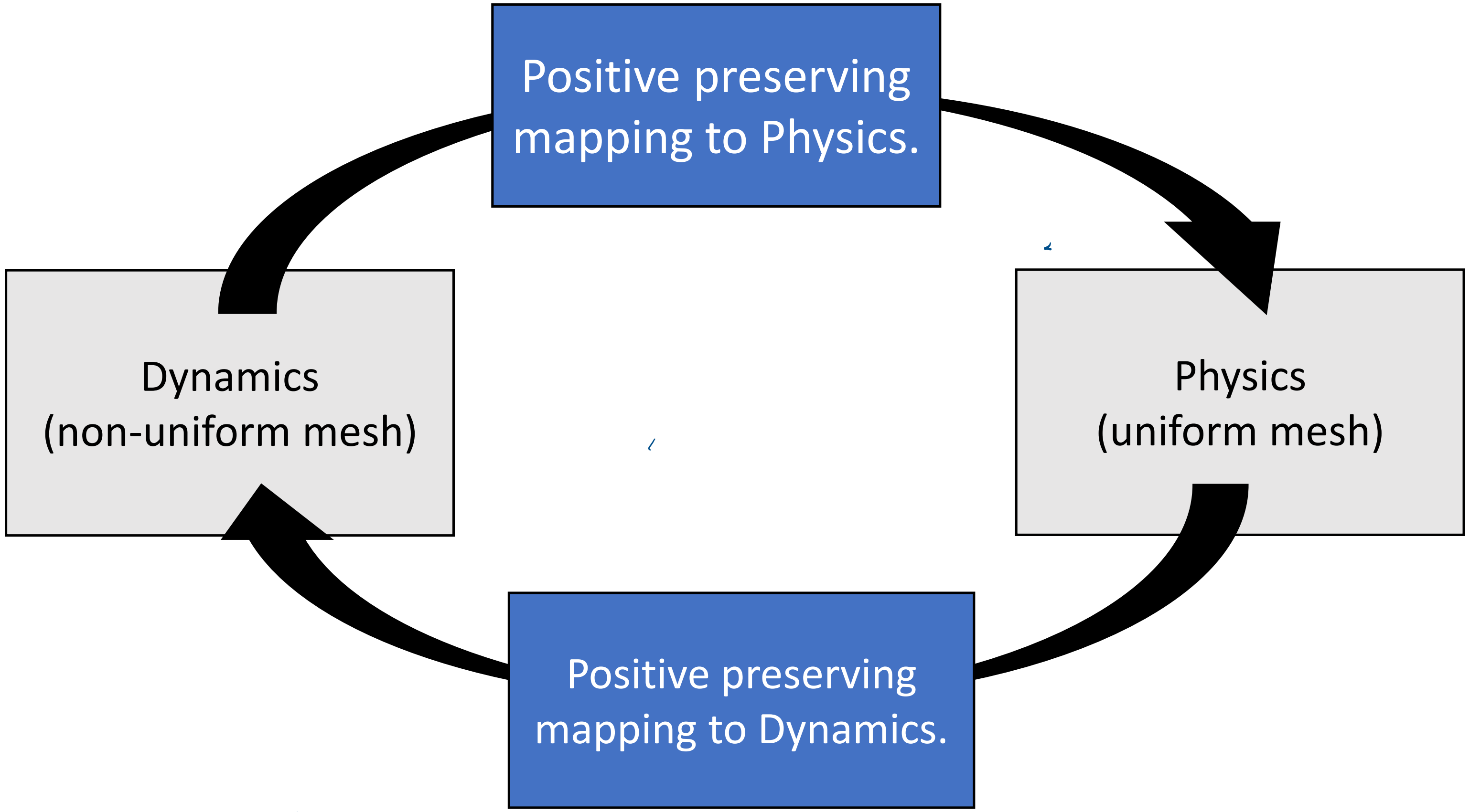


Mapping Challenges

- 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.

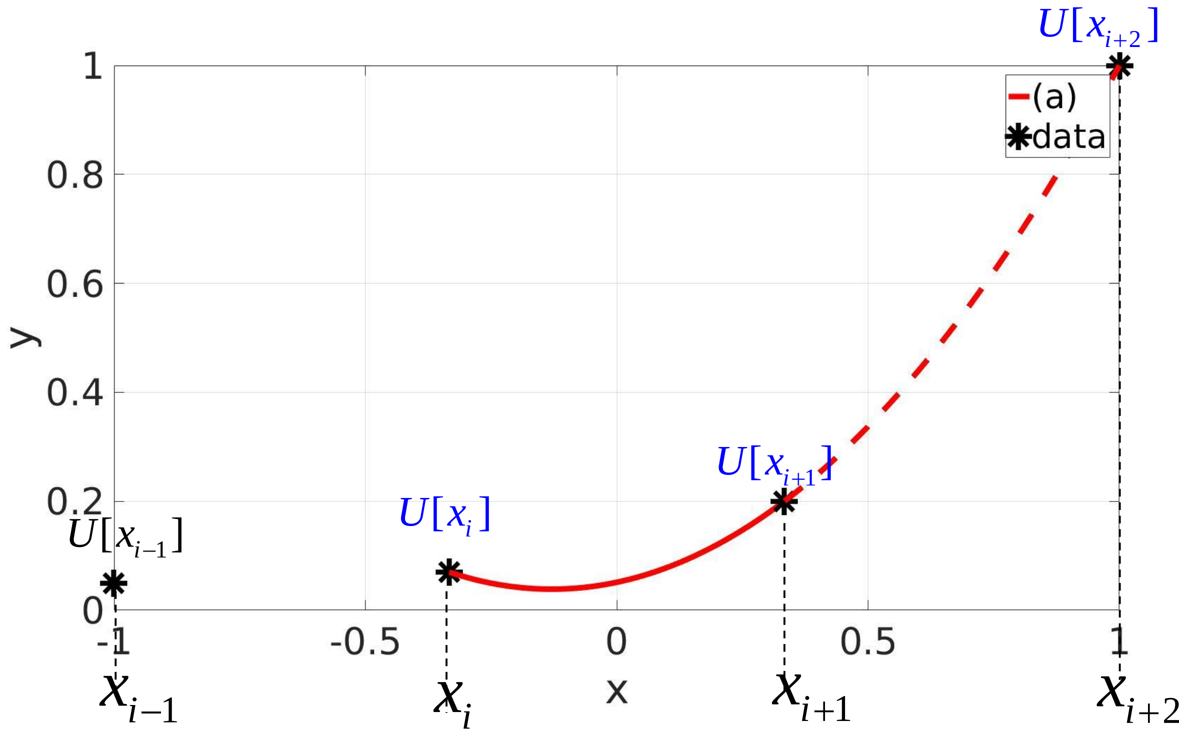
Mitigate Mapping Challenges

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

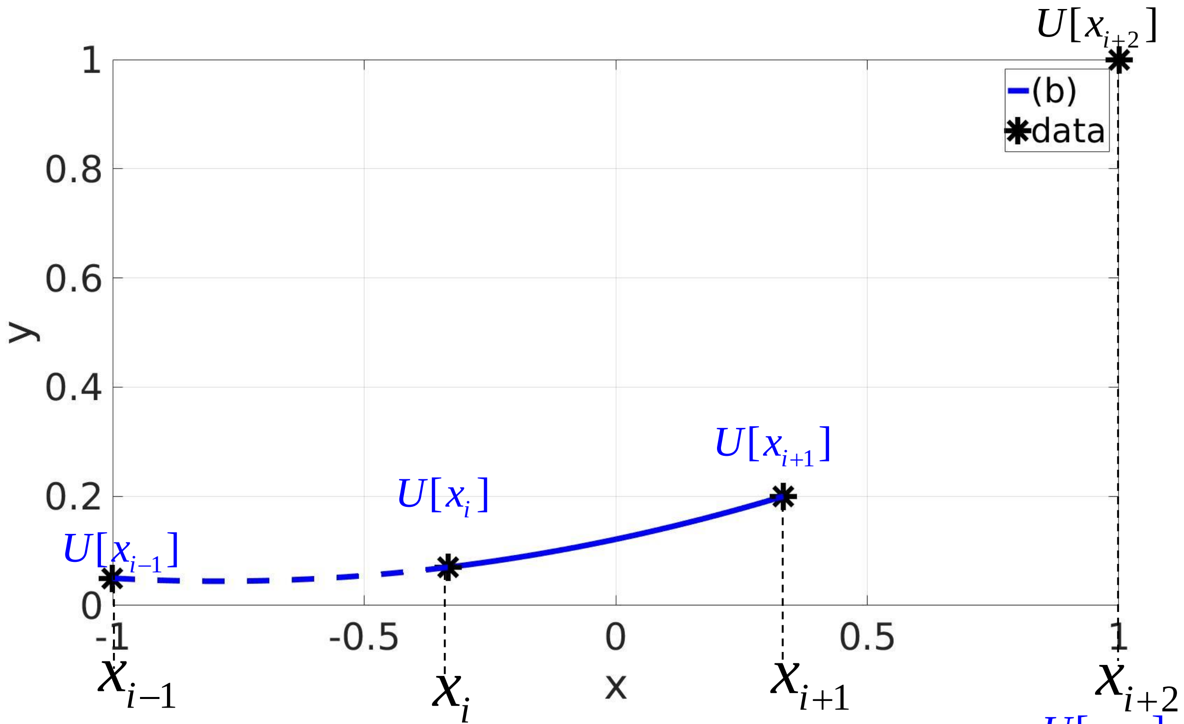
$$U[x_i, x_{i+1}, x_{i+2}] = \frac{U[x_i, x_{i+2}] - U[x_i, x_{i+1}]}{x_{i+2} - x_i}$$

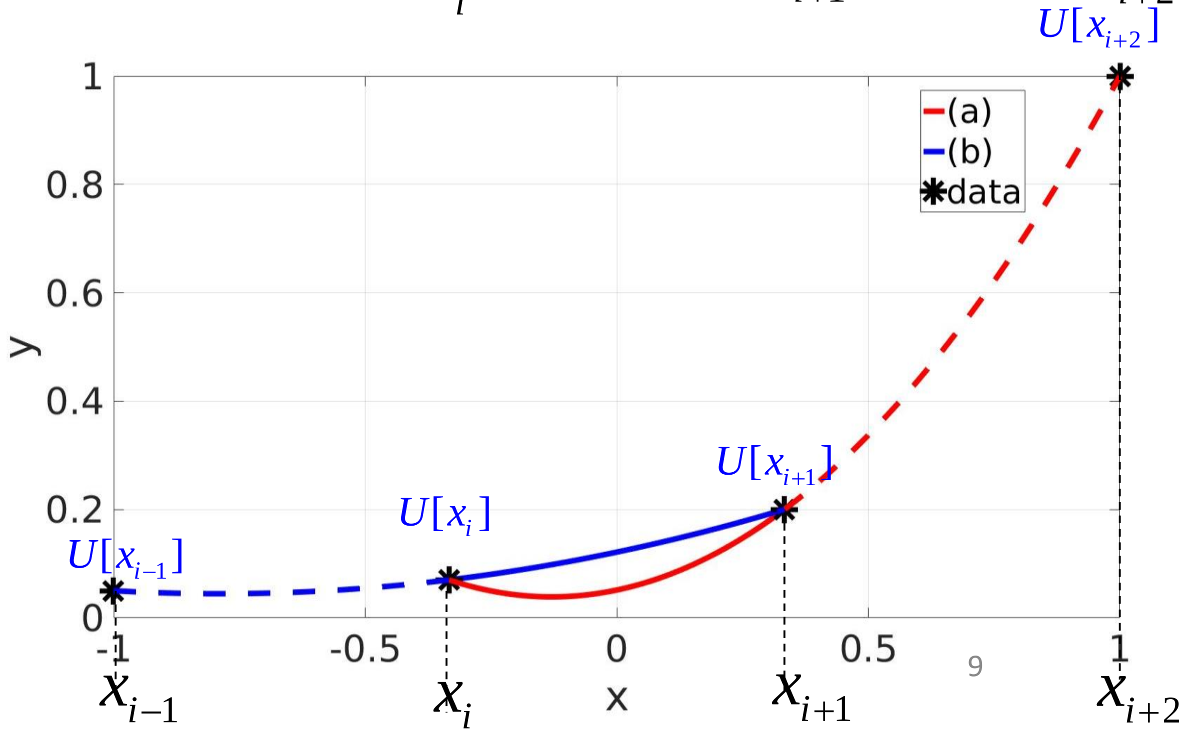
General case: $U[x_i, x_{i+1}, \ldots, x_{i+k}] = \dfrac{U[x_{i+1}, \ldots, x_{i+k}] - U[x_i, \ldots, x_{i+k-1}]}{x_{i+k} - x_i}$

Newton Polynomial

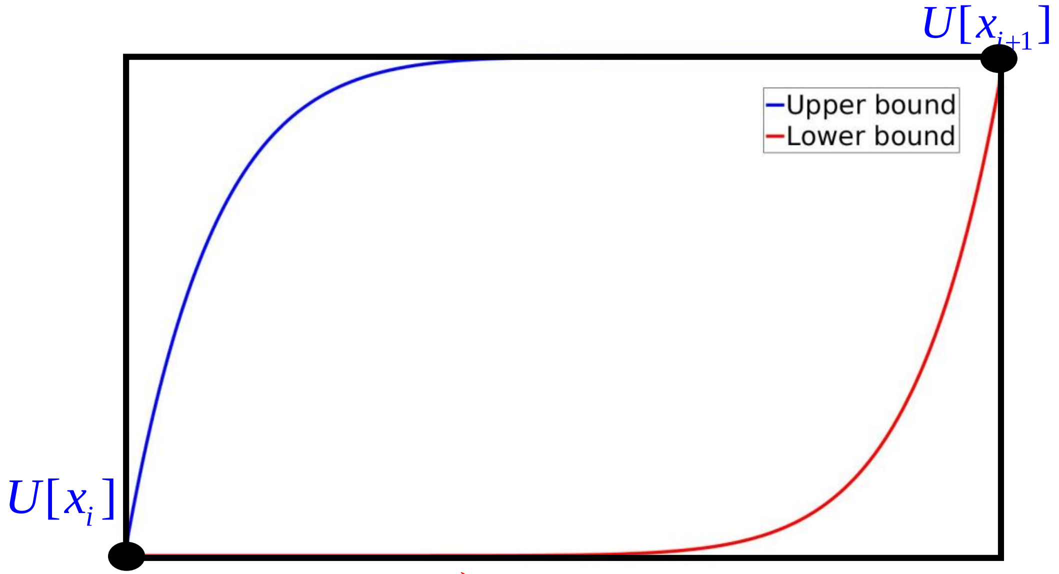
(a) $P_N(x) = U[x_i] + (x - x_i)U[x_i, x_{i+1}]$
$+ (x - x_i)(x - x_{i+1})U[x_i, x_{i+1}, x_{i+2}]$

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

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

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

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

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

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

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].

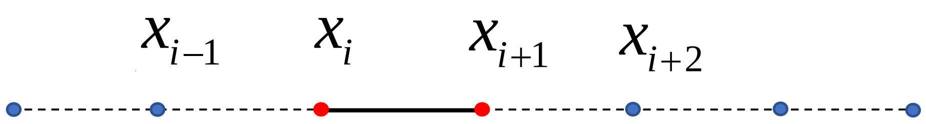
Positivity-preserving method requires

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

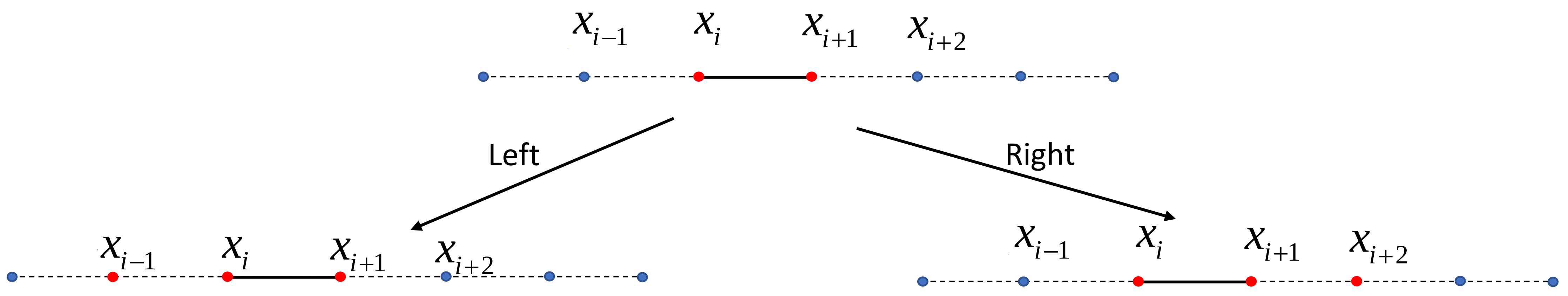
$$\text{or } -\frac{U[x_{i+1}]}{U[x_{i+1}]-U[x_i]}-1 \le r_R \le \frac{U[x_i]}{U[x_{i+1}]-U[x_i]} \text{ with } r_R = \frac{U[x_{i+1},x_{i+2}]}{U[x_i,x_{i+1}]}$$

Paper in preparation [5].

Adaptive Polynomial Interpolation

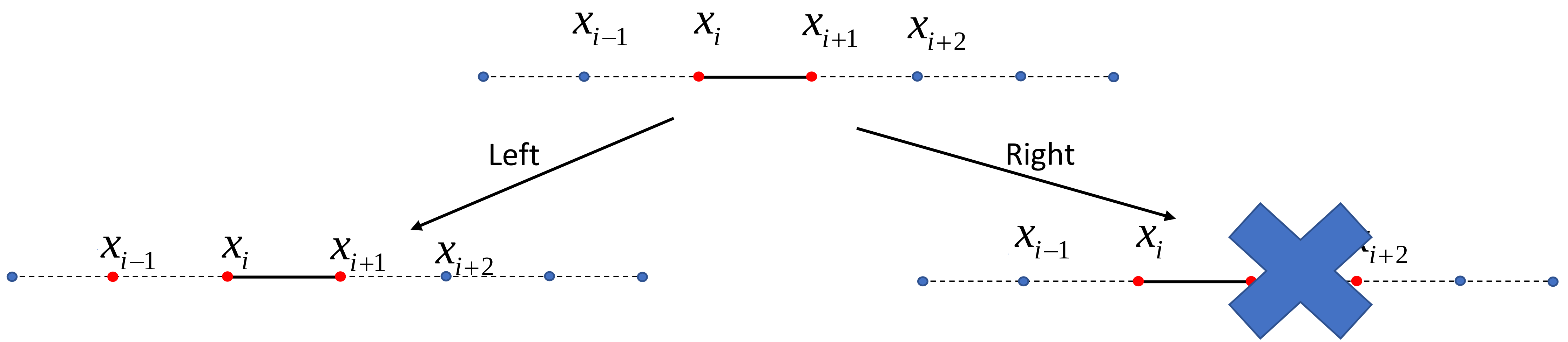


Adaptive Polynomial Interpolation



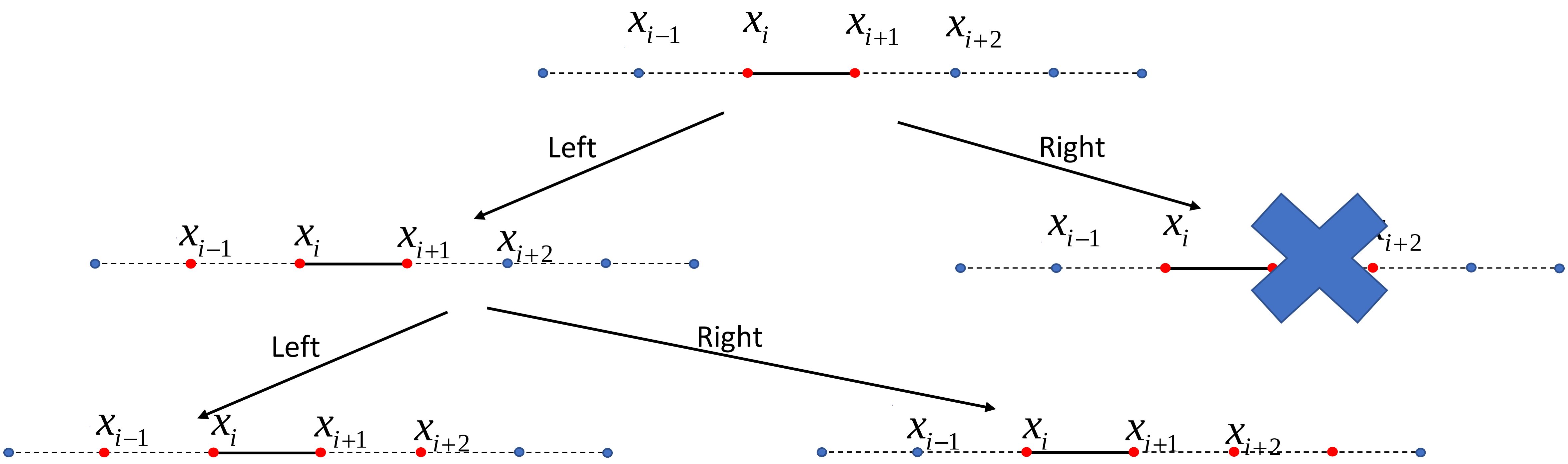
- Choose the direction with the smallest divided difference.

Adaptive Polynomial Interpolation



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

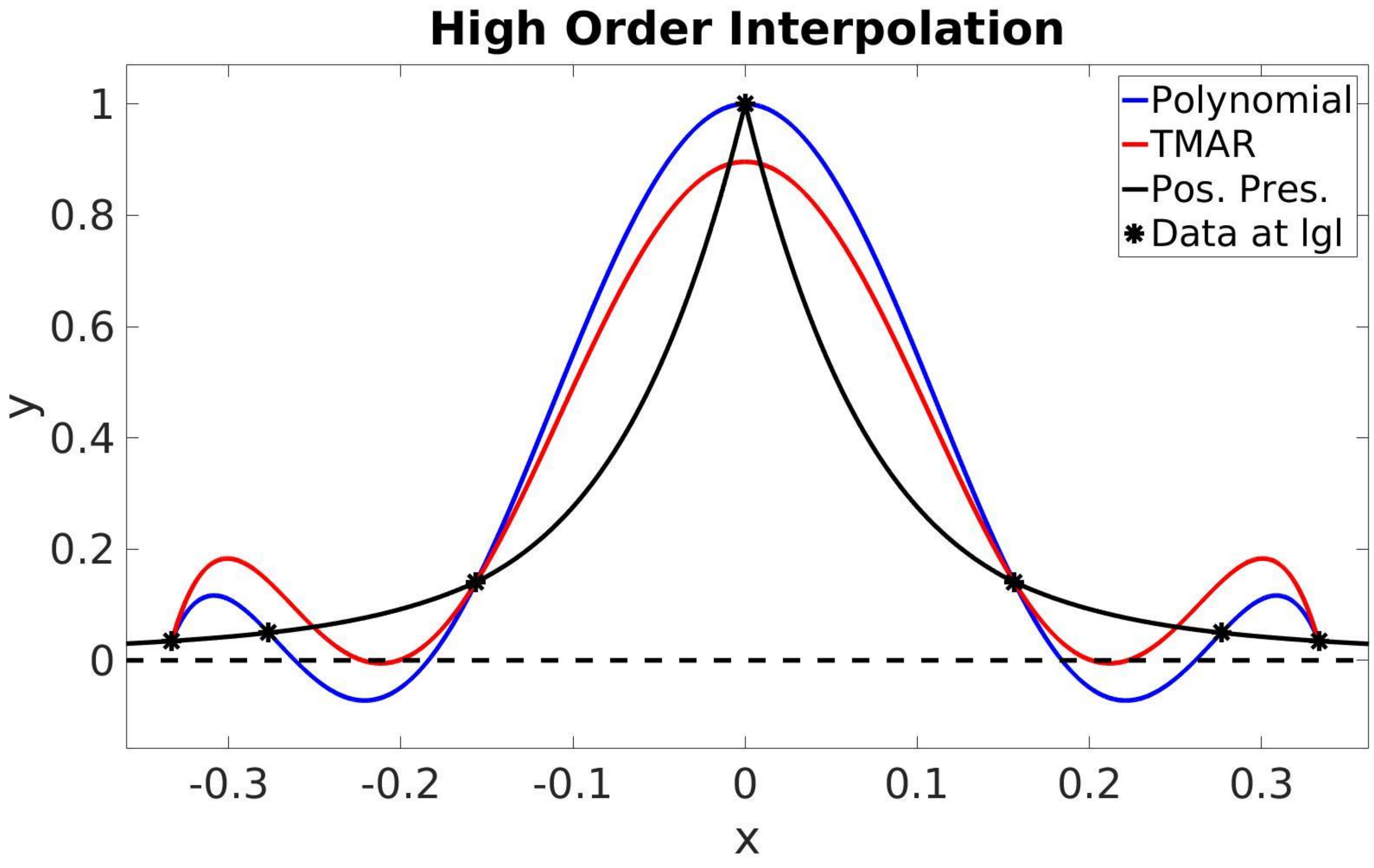
Adaptive Polynomial Interpolation



- 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.



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.

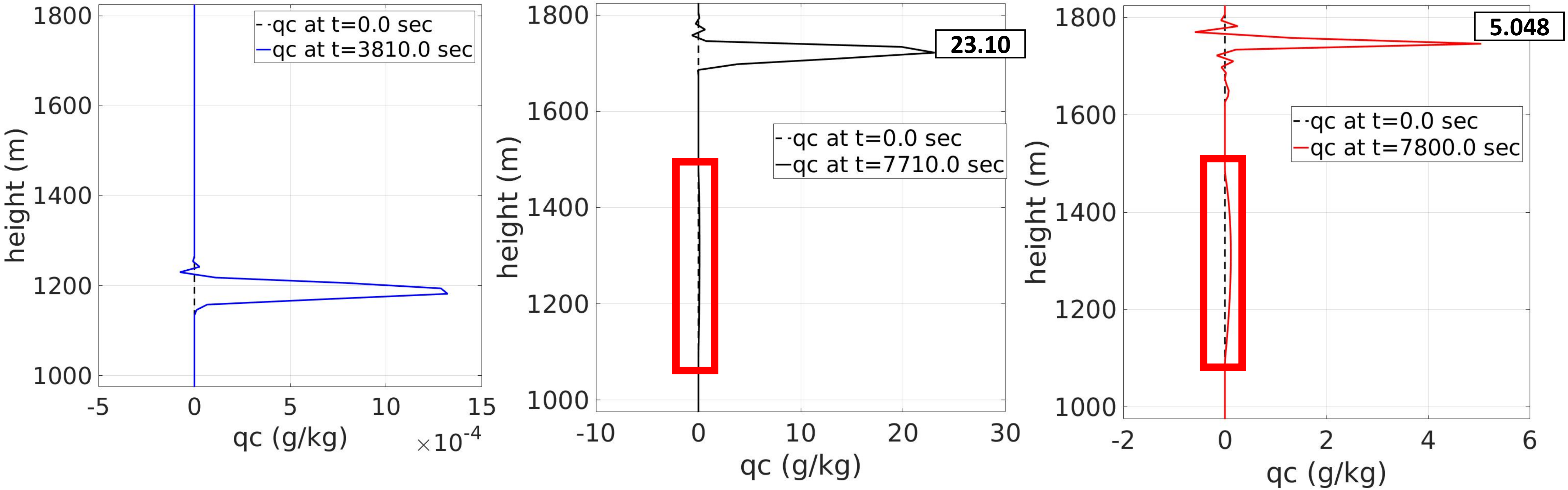
Positivity-Preserving Interpolation In BOMEX Code

- 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.

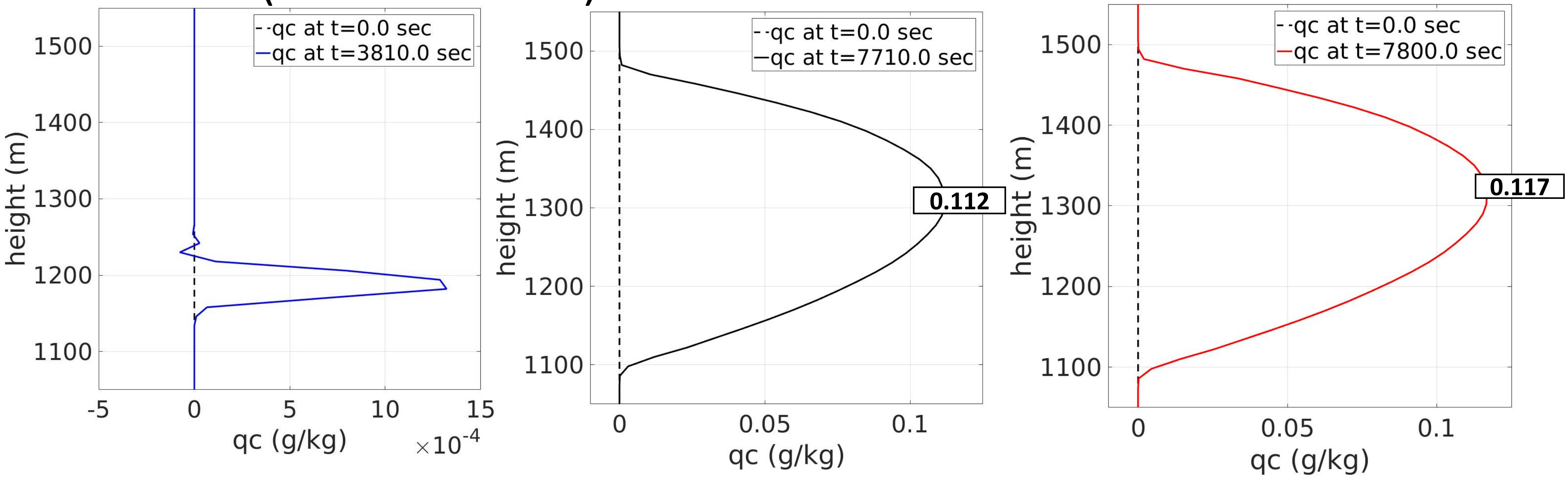
- *While(t <=tf)*
  - *Bomex_ls_forcing(…)   !!dynamics*
  - ***Positve_preserv_interpolation(….)***
  - *Run_scm_physics(…)   !! physics*
  - ***Positve_preserv_interpolation(….)***
- *end*

BOMEX (No Limiter)



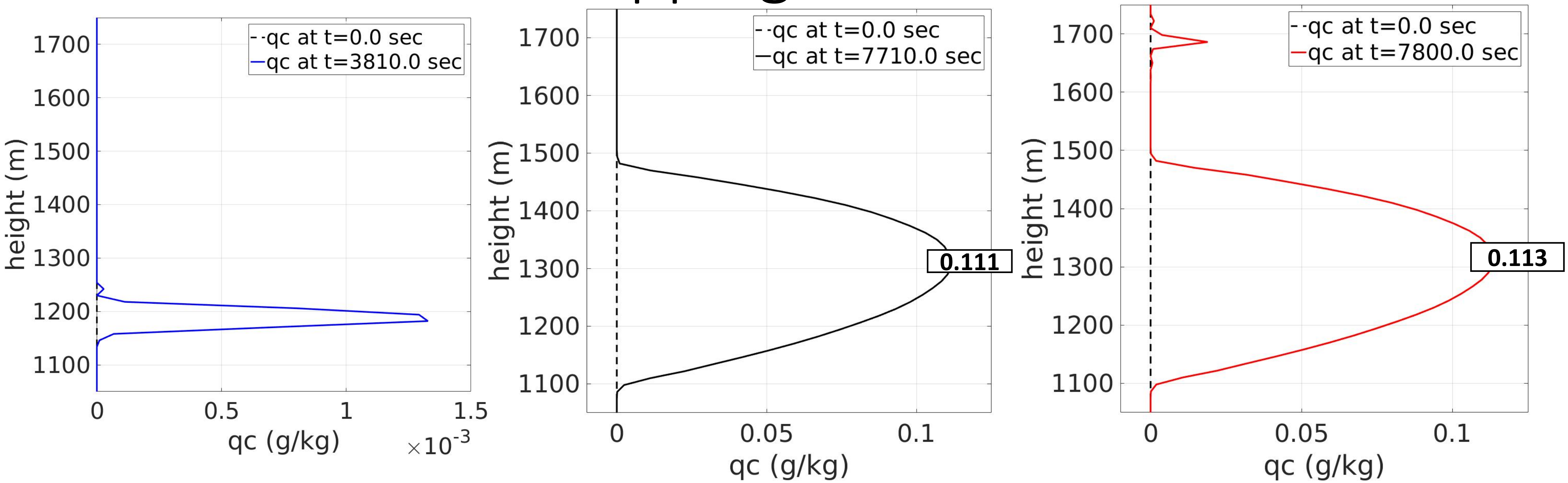
- The negative values (started at t= 3810 sec) and oscillations are picked up by the physics, causing false peaks at t = 7710.0. sec and t=7800 sec.
- Unphysical values cause the simulation to crash before the final time step t=21600.0
- The red box indicates the interval [1150, 1500] where the cloud-mixing ratio should be observed.

BOMEX (No Limiter)



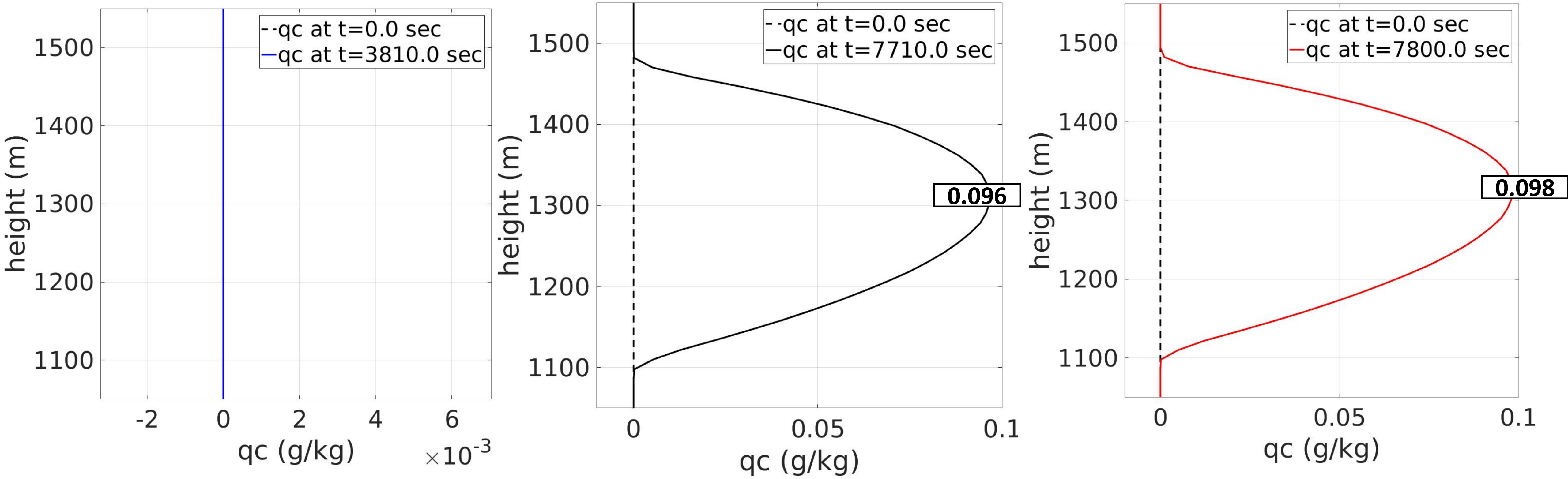
- A close look at the interval [1050, 1500] indicates more reasonable peaks.
- The blue plot is early in the simulation when not much of the cloud mixing-ratio is produced.

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.

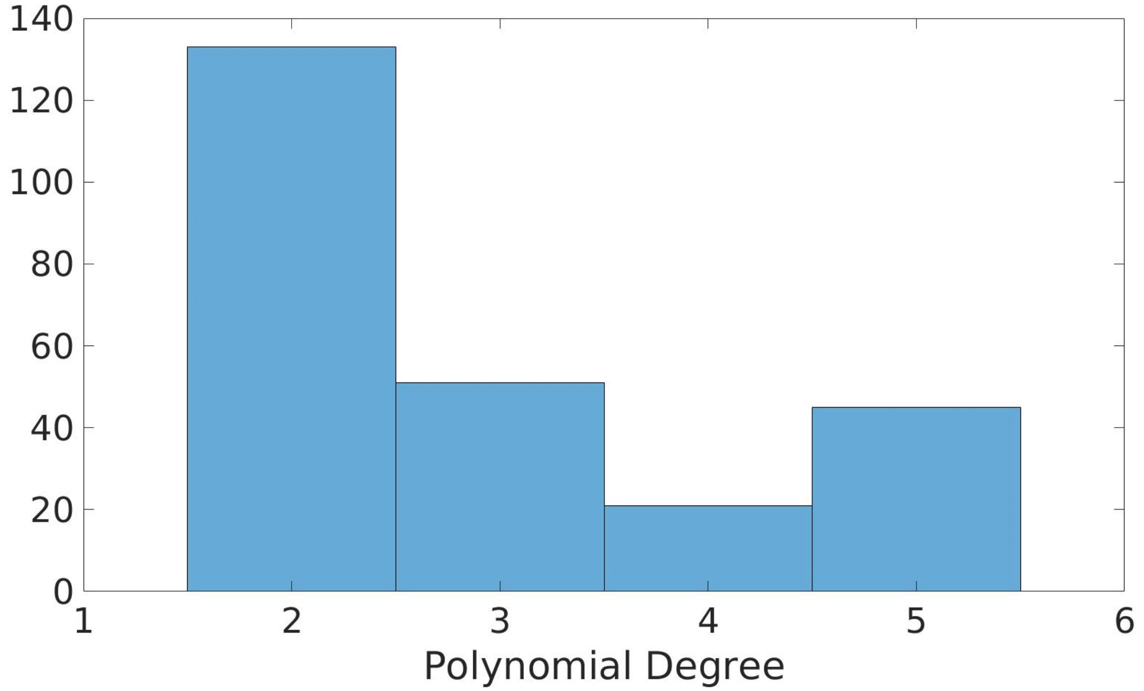
Positivity Preserving Interpolation

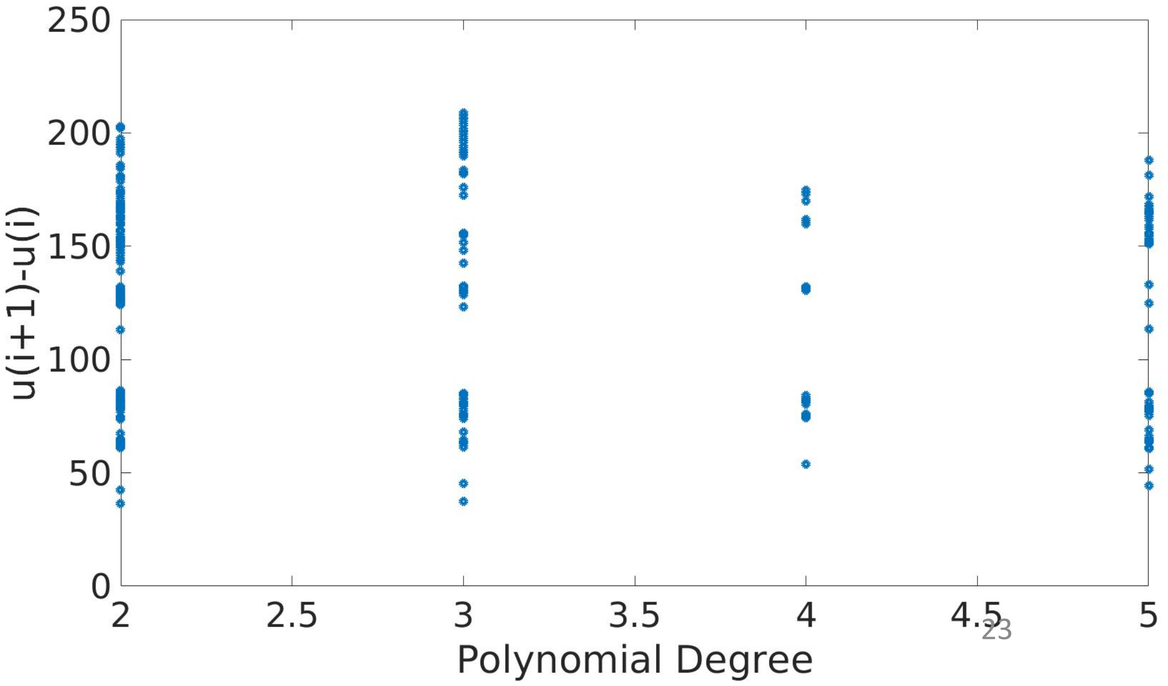


- The cloud-mixing ratio remains positive over the entire simulation.
- The cloud-mixing ratio peak is **qc=0.098** g/kg at t=7800 sec, which is less than all the previous cases. Positivity-preserving interpolation reduces the positive bias in the cloud-mixing ratio prediction.

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

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

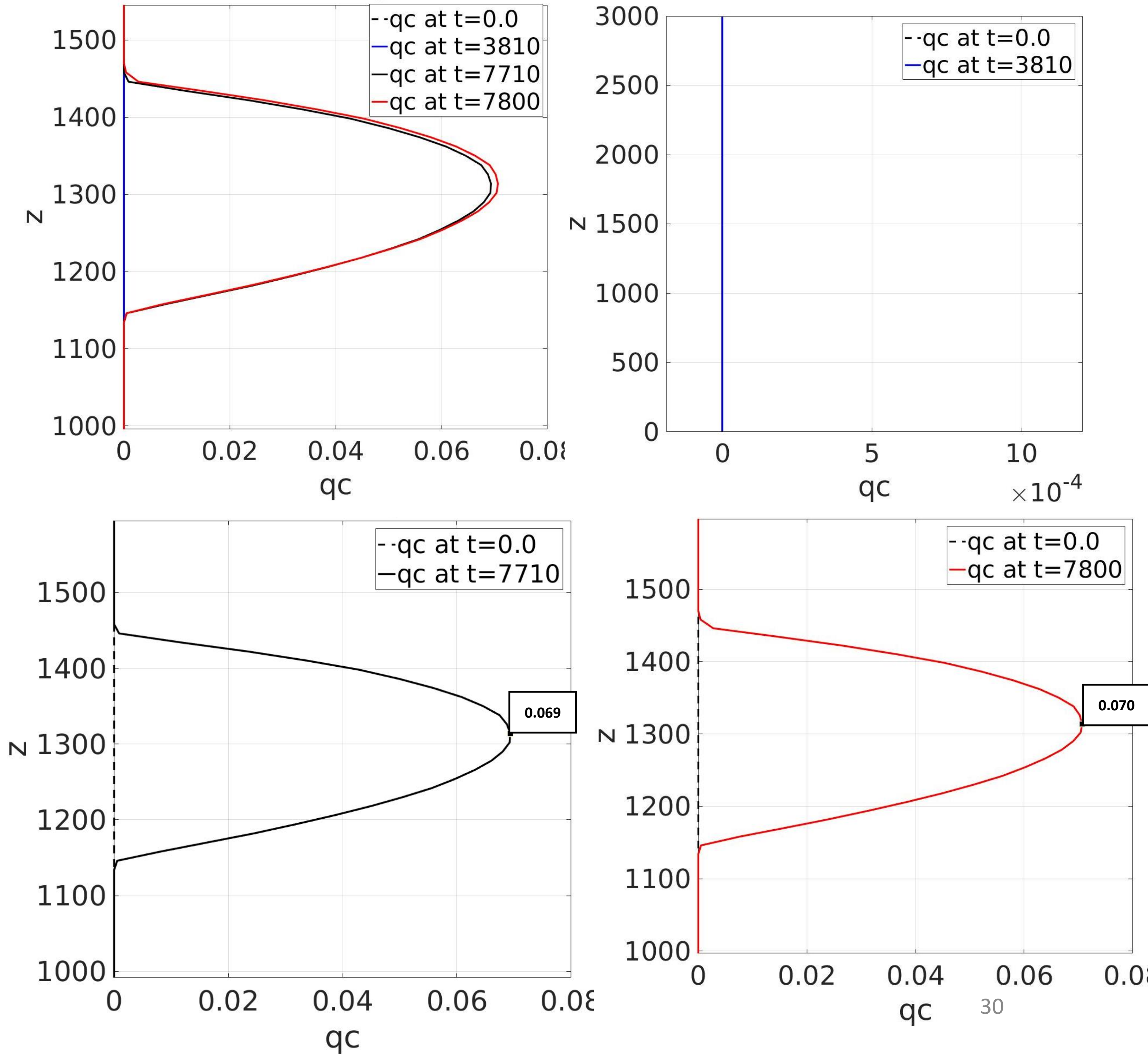
$$\lambda_{k+1} = \left(r_{[x_i,\dots,x_{i+k}]}^{[x_{i+1},\dots,x_{i+k+1}]} - 1\right)$$ For choosing the next stencil point to be on the right

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

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

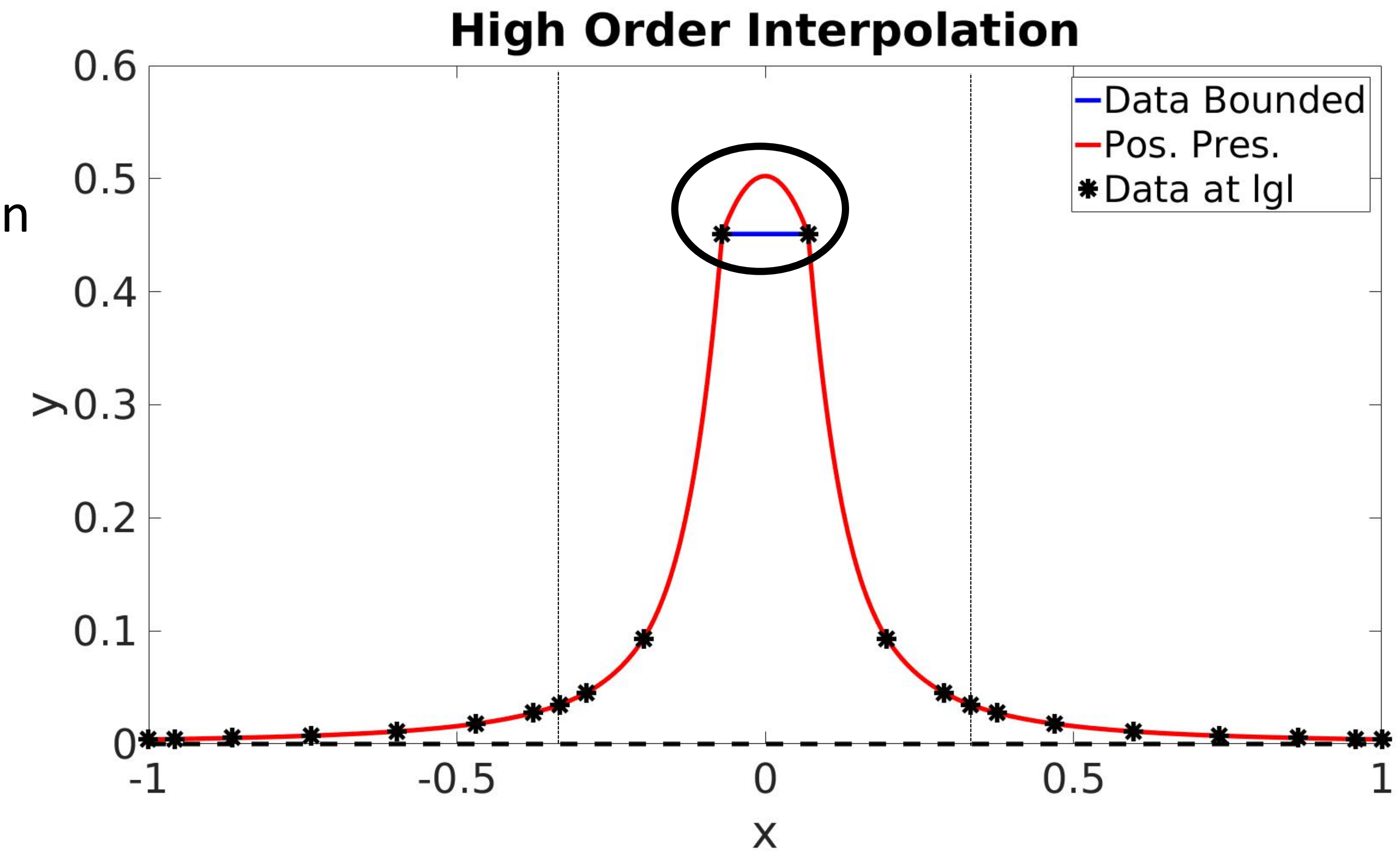
Data-Bounded Interpolation

- 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.



Data-Bounded and Positivity-preserving

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

- Choose the stencil with smallest divided difference at each stage
- Alter the polynomial by limiting λ_i to ensure positivity or data-boundedness

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

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

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