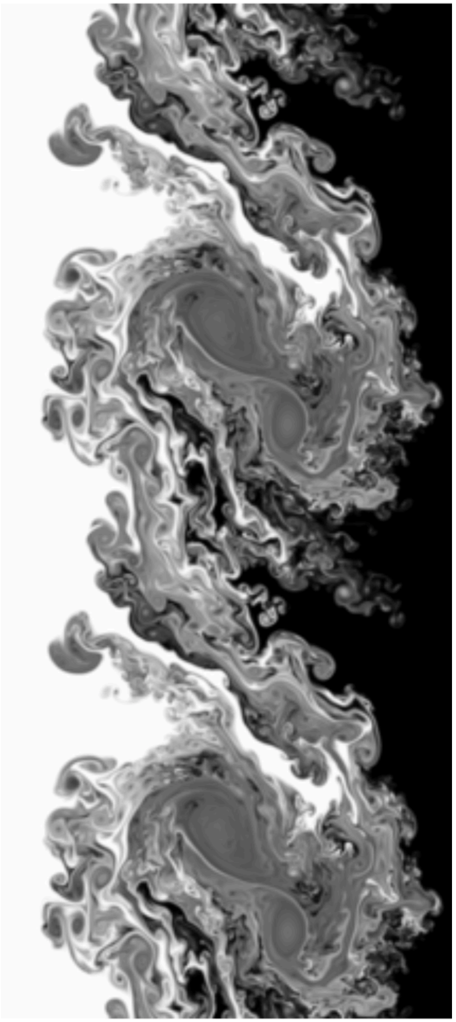
Hierarchical Parcel Swapping (HiPS) Model

Motivation

- A key challenge of turbulent combustion is the wide range of length and timescales
  - DNS costs are extremely high (scales with Re^3).
- LES and RANS require subgrid models of unresolved reaction and transport processes.
  - Models struggle to accurately capture all combustion phenomena under a range of flow conditions.
    - Premixed vs. nonpremixed
    - Flame extinction and ignition
    - Soot and NO_x formation

Models idealize these processes

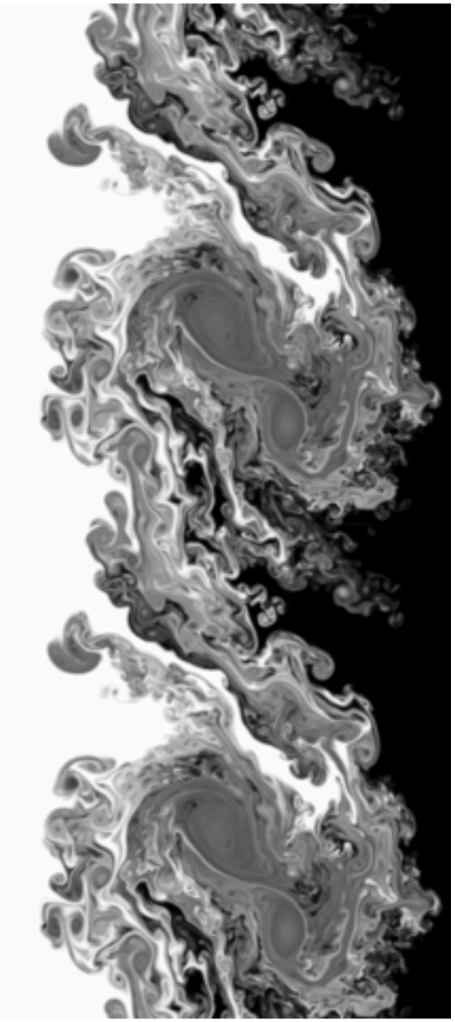
- PDF transport models represent the reaction source but need accurate mixing model closures.



https://en.wikipedia.org/wiki/Kelvin–Helmholtz_instability

Motivation

- Mixing closures often consist of intermixing pairs or groups of notional fluid particles.
  - Interaction by Exchange with the Mean (IEM)
  - Modified Curl (MC)
  - Euclidean Minimum Spanning Trees (EMST)
  - Shadow Position (SP)
- Challenges include not mixing of particles with unphysically dissimilar states.
  - How to define "close" in state space?
  - Thermochemically "close" particles may not be physically close.



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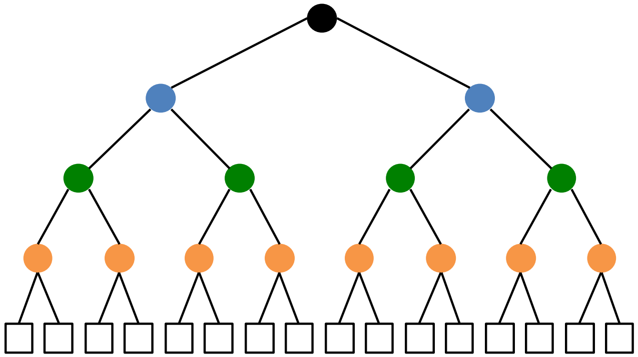
Hierarchical Parcel Swapping (HiPS)

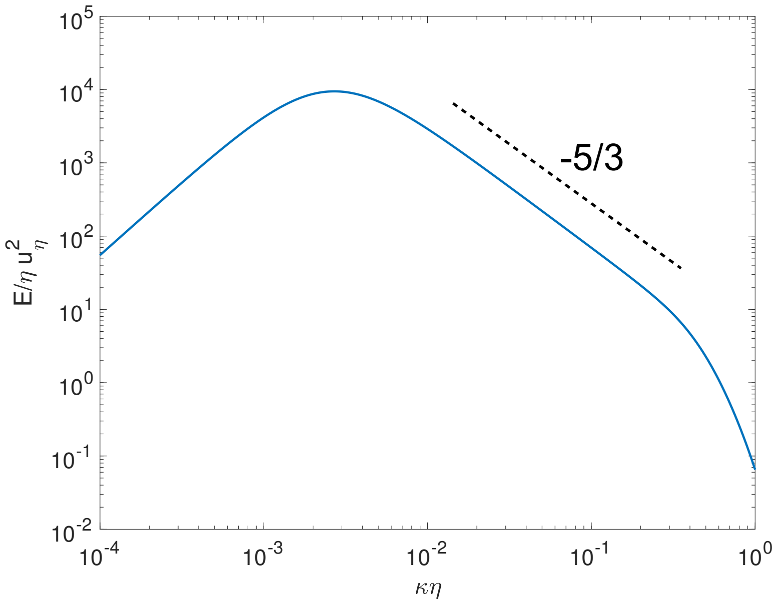
- HiPS is a simulation approach for turbulent mixing
  - A.R. Kerstein, J. Stat. Phys. 153:142-161 (2013)
  - A.R. Kerstein, J. Fluid Mech. 750:421-463 (2014).
- Uses a binary tree structure to define a geometric progression of length scales.
- Fluid elements are defined at the base of the tree and interact as pairs.
- Computationally efficient
- Includes elements of LEM and ODT
  - But does not directly model 1-D diffusion in a physical coordinate
- Can be run standalone or as a flow model
  - Facilitates subgrid wall-models; subgrid jets.



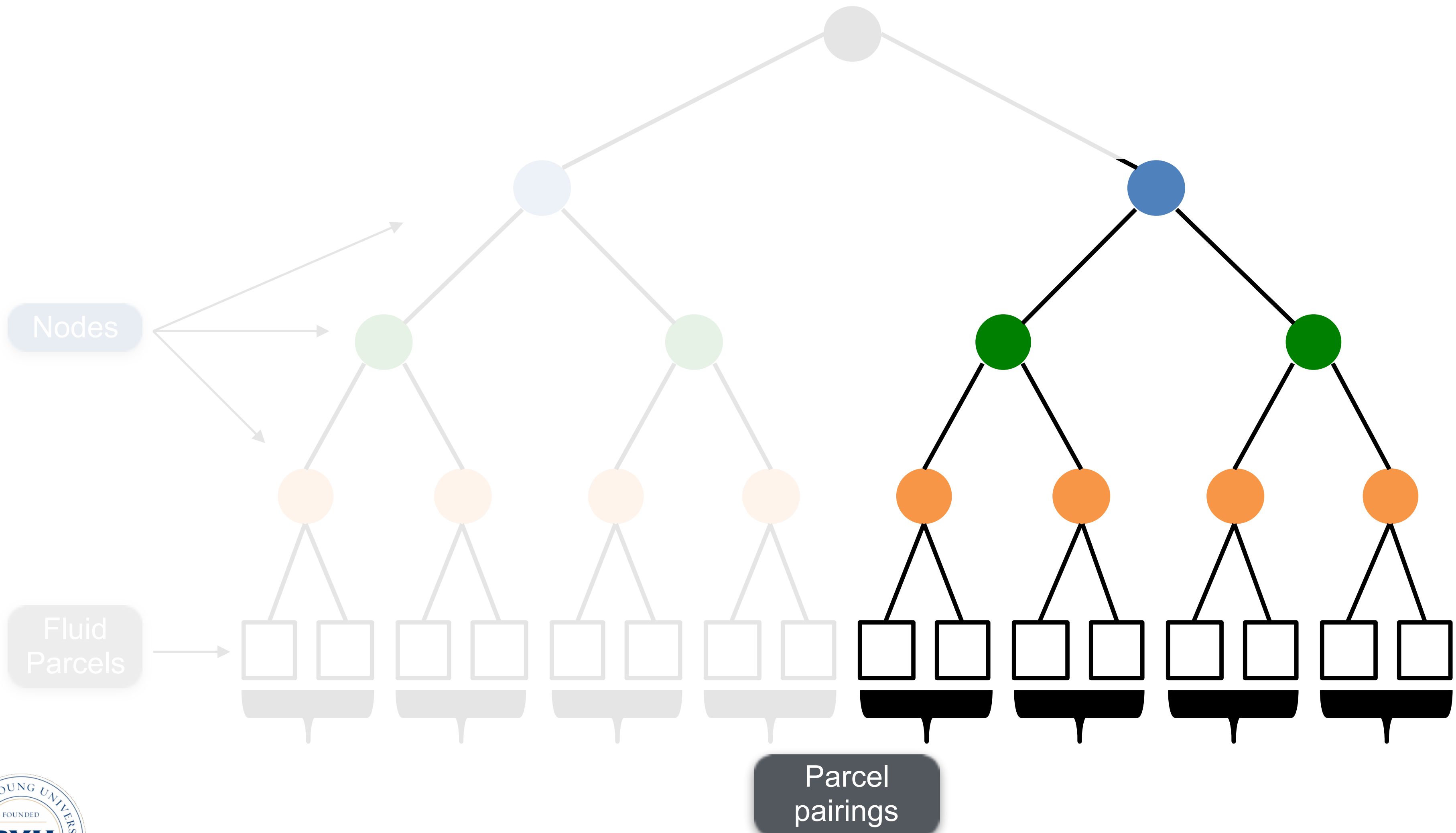
Essentials of Turbulent Mixing

HiPS can be thought of as a *minimal* model of turbulent mixing

- Include a range of scales
- Follow Kolmogorov scaling
- Scale separation
  - Scales interact with local environment
  - Large and small scales are decoupled
- Cascade of scales: large to small
- Increase of initially close parcels



Model Formulation—Binary Tree



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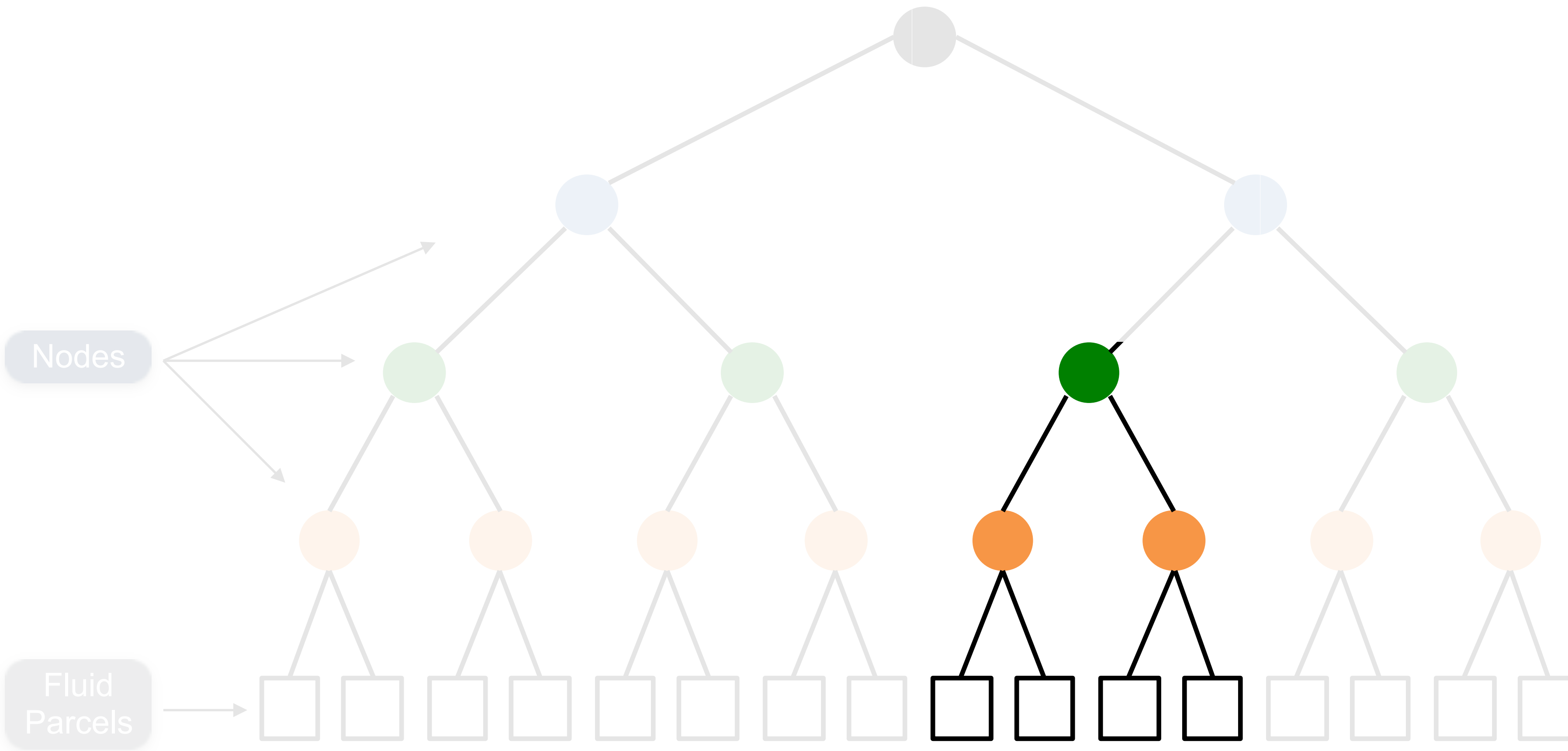

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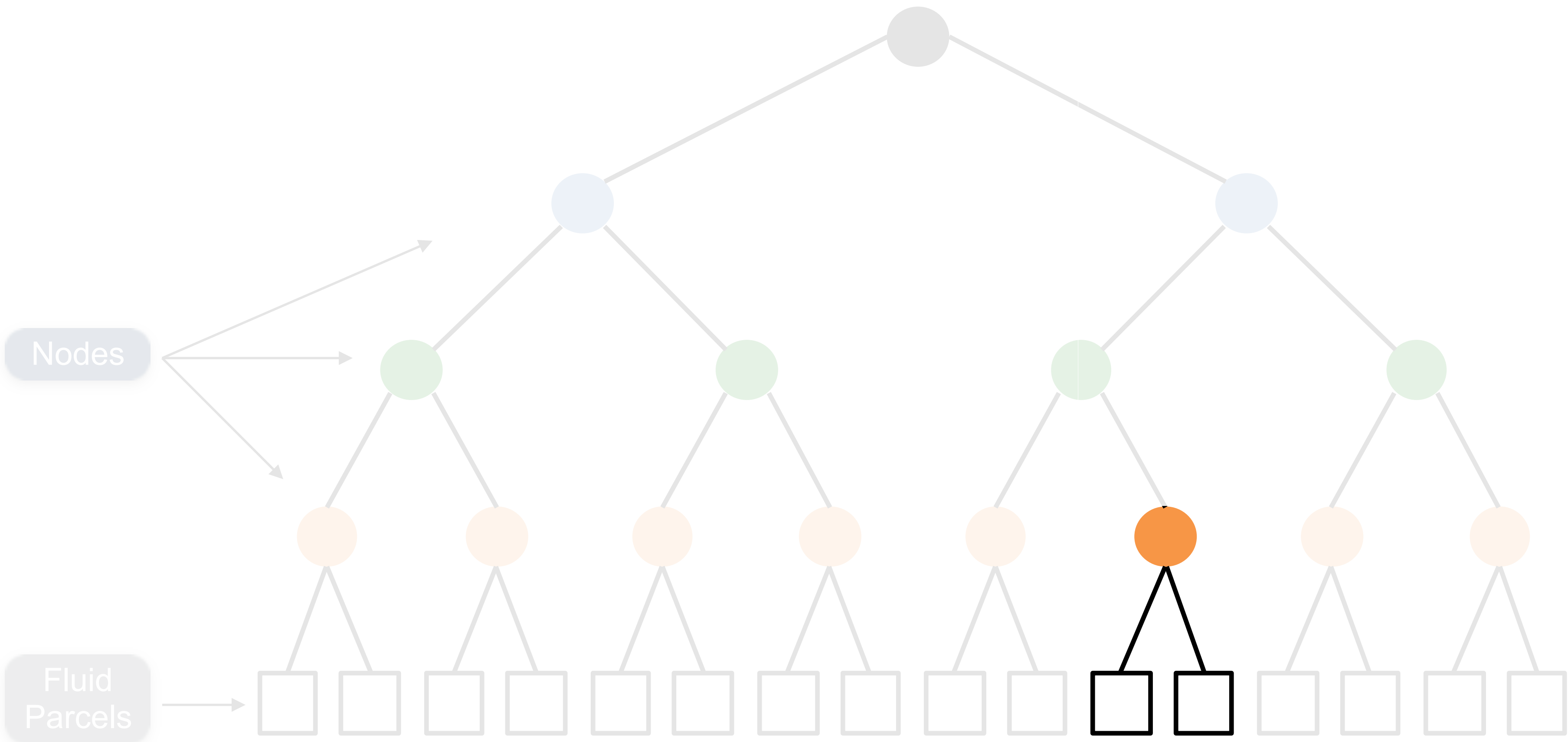

Model Formulation—Binary Tree

- Mixing—Swap Nodes
  - Select a node
  - Select a grandchild to the right
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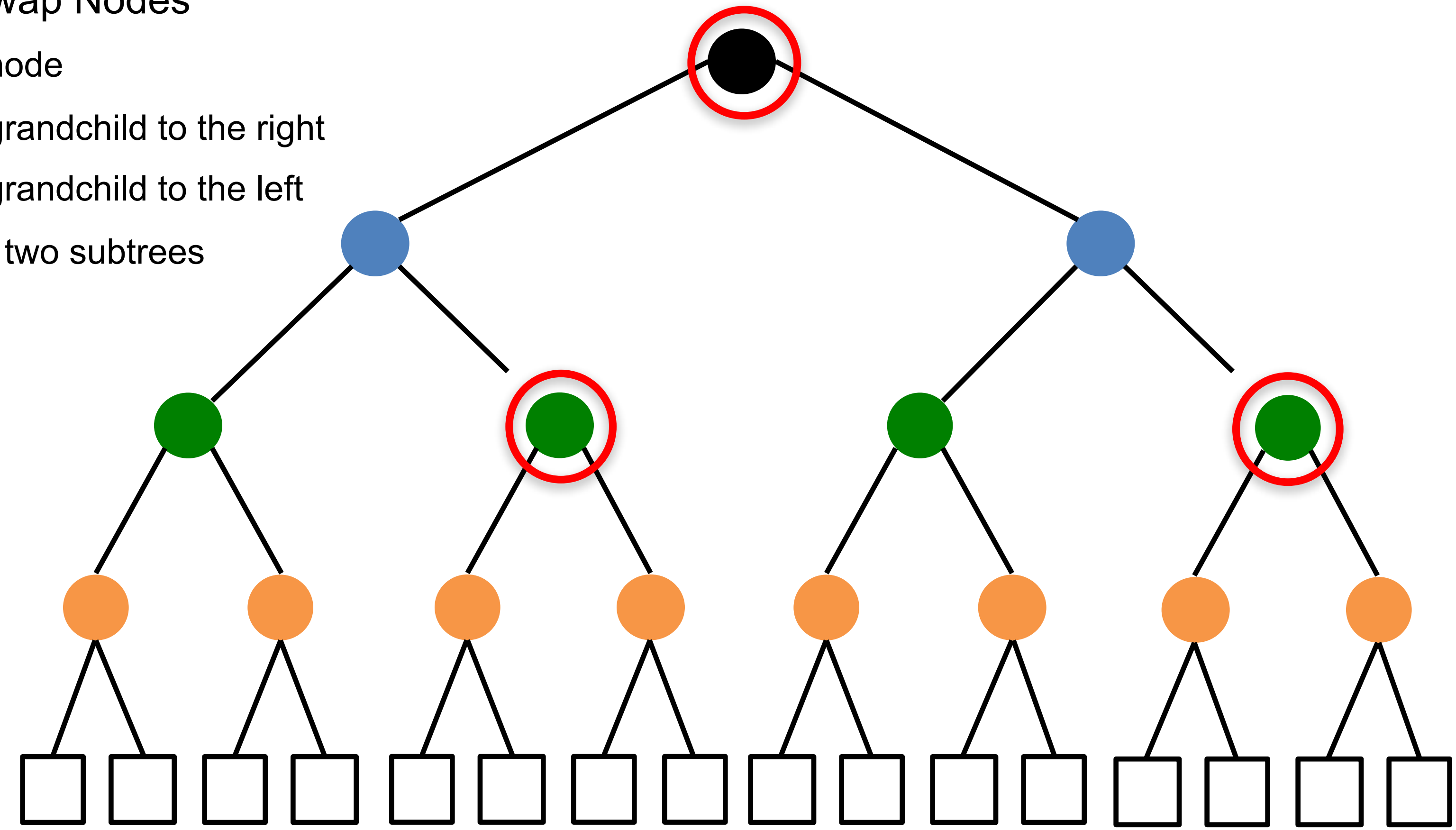
  - Swap the two subtrees



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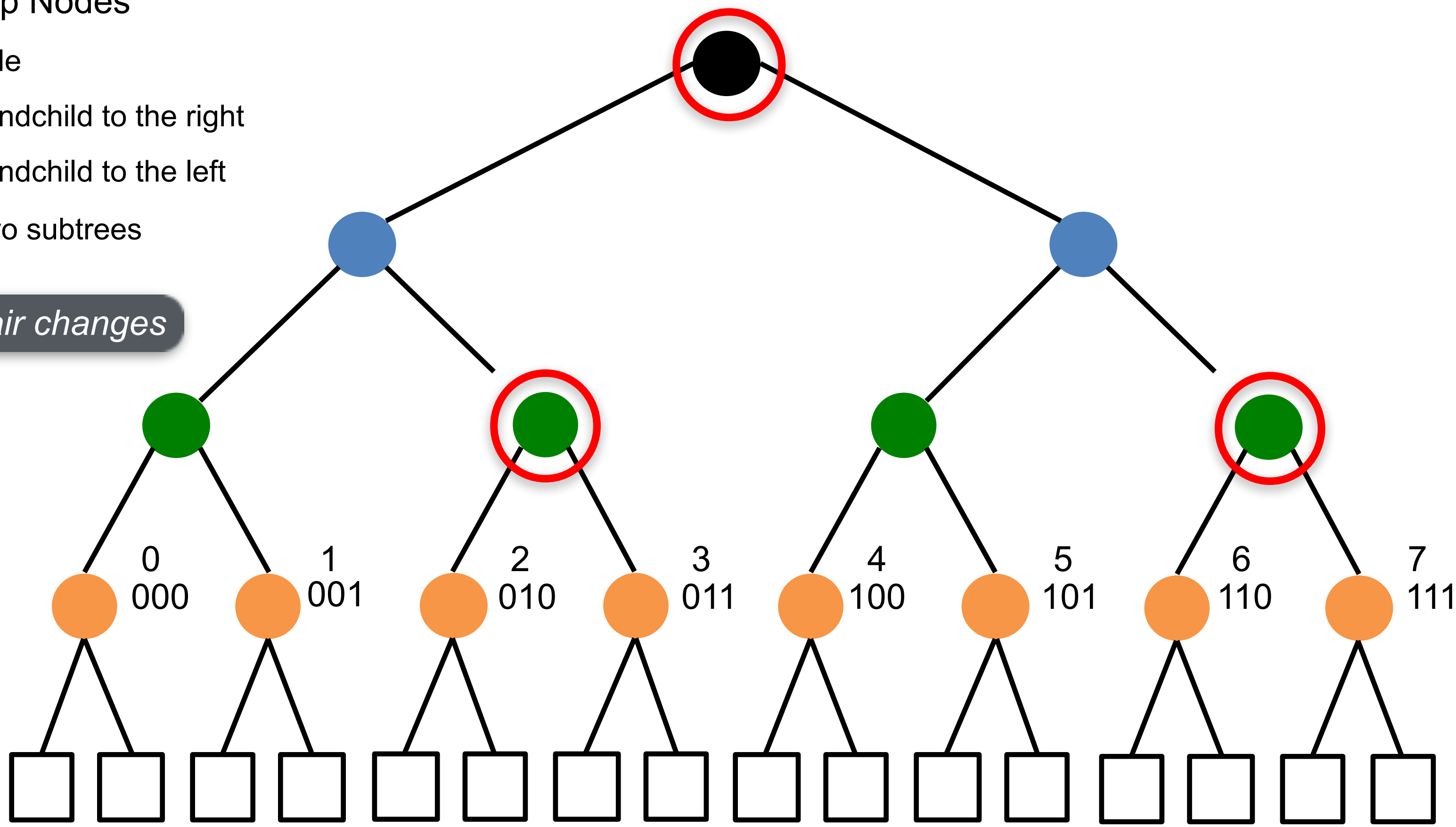
No parcel pair changes



i0q i1r

i0qs ⟷ i1rs

Sweeping of small scales by large scales

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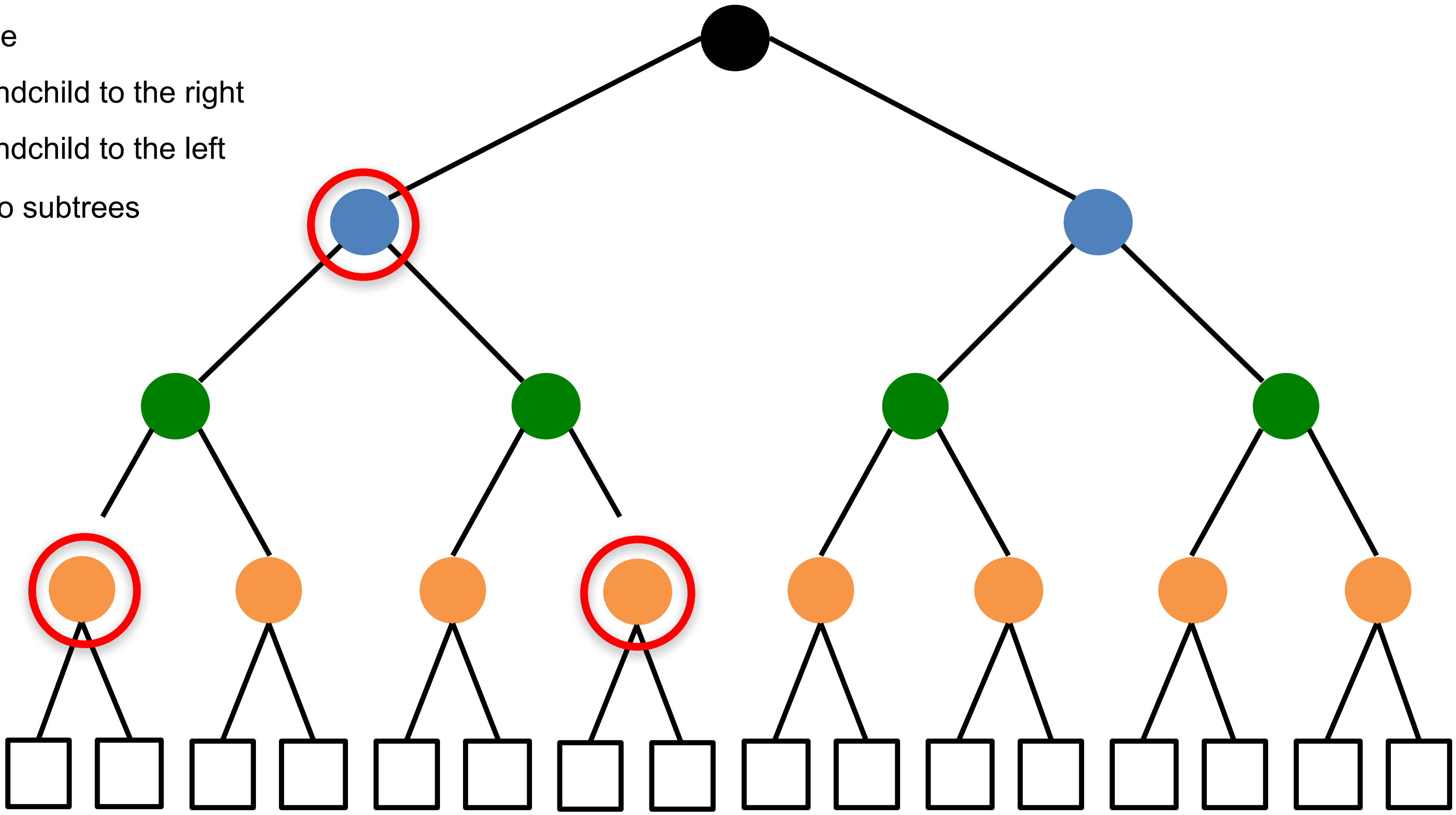

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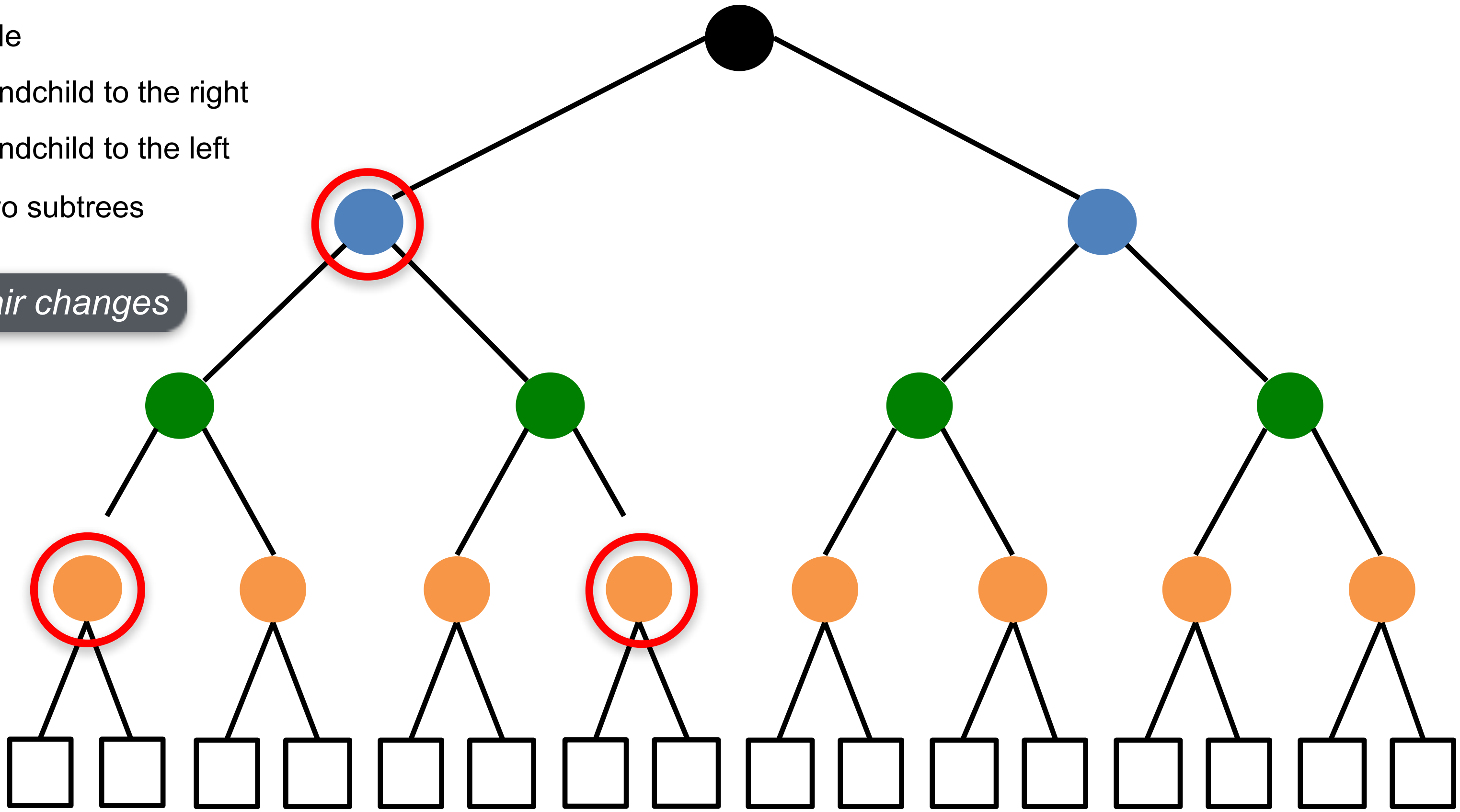

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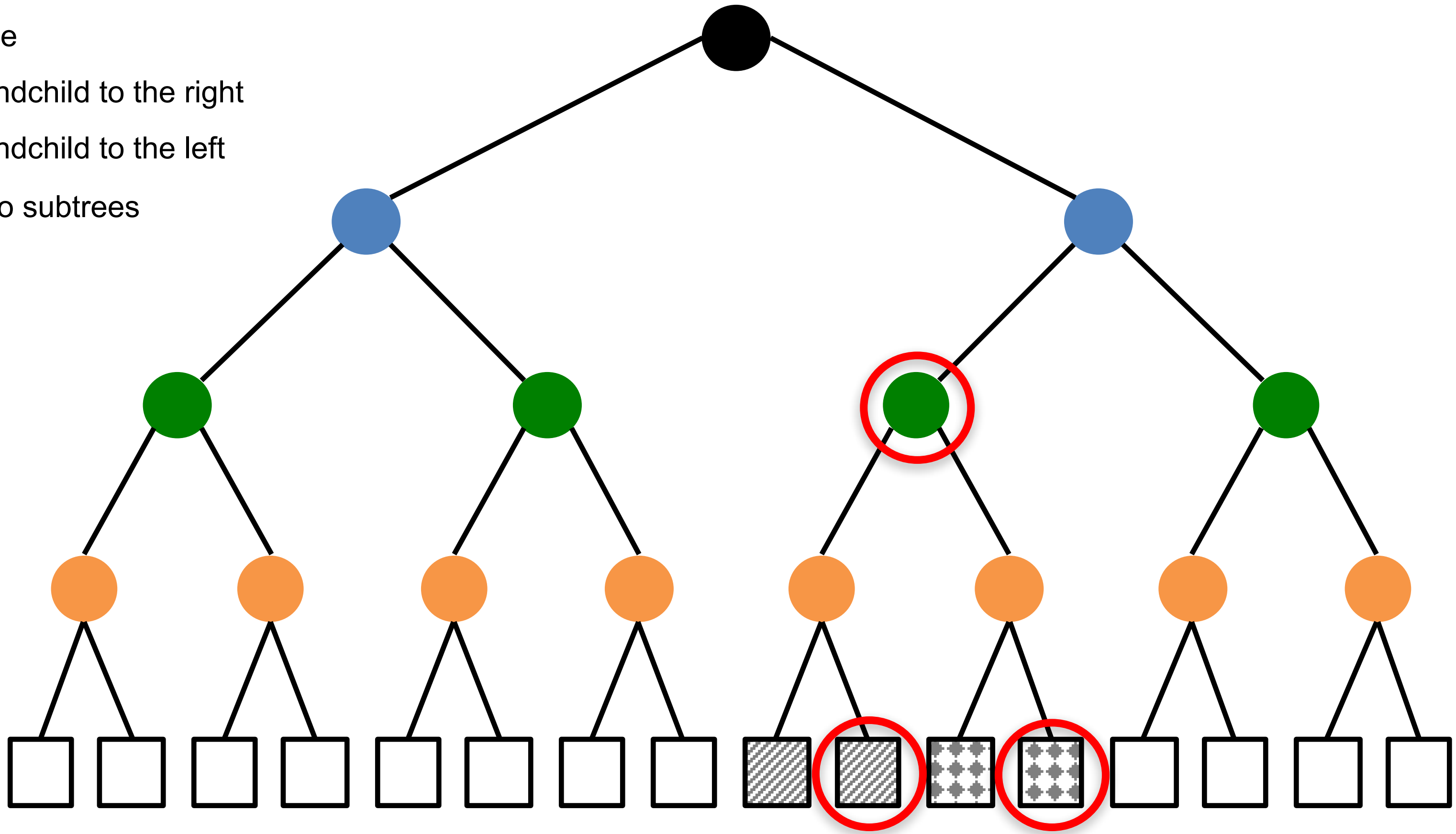

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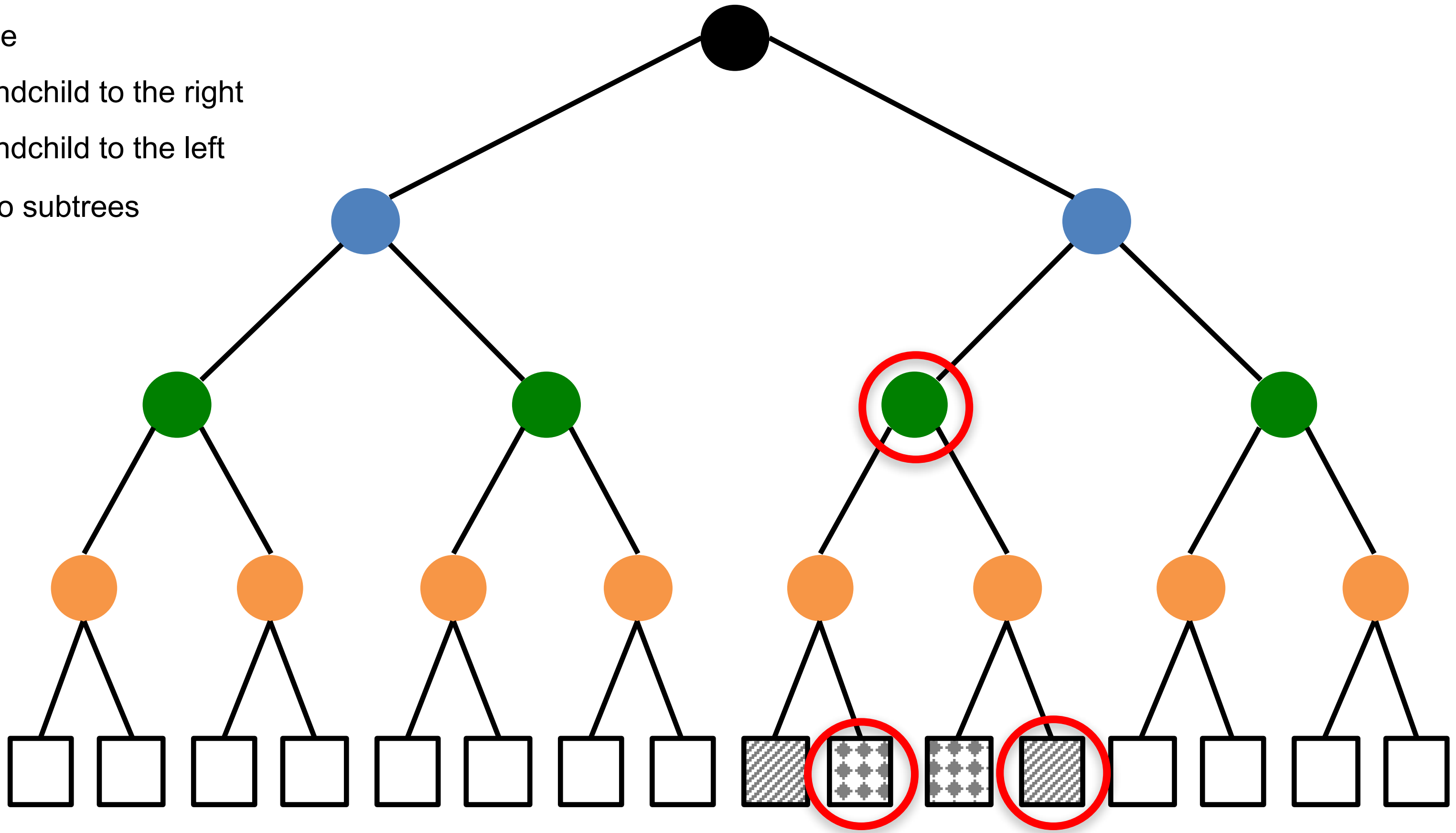


Parcel pairing changes

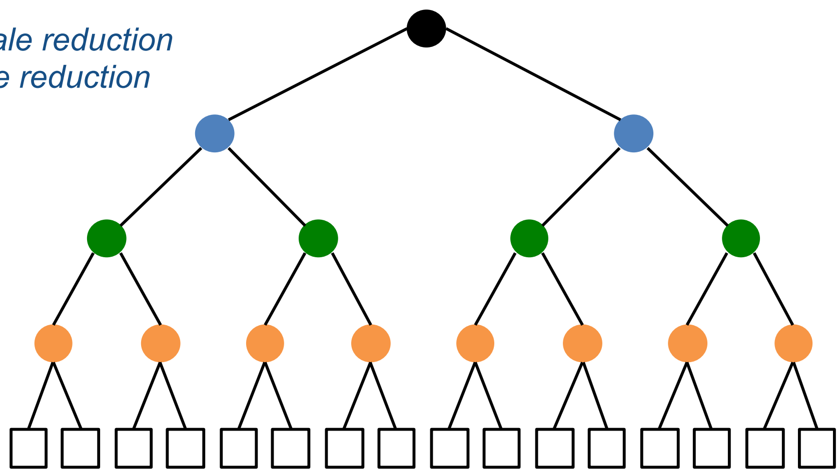
Model Formulation—Tree Scales

- Specify length scales at each level
  - Top level is the tree length scale L_0
  - L_0 is user-defined
  - Each level decreases length scale by factor A<1.
  - If parcels occupy fluid volume, then for a binary tree, each subtree occupies half the volume as the tree above, with a length scale ratio of A.

$$A = \frac{1}{2^{1/3}}$$ *cube of length scale reduction A matches volume reduction*

$$A = \frac{1}{2^{1/D}}$$ *for D dimensions*

$$A = \frac{1}{2}$$ *D=1 assumed*

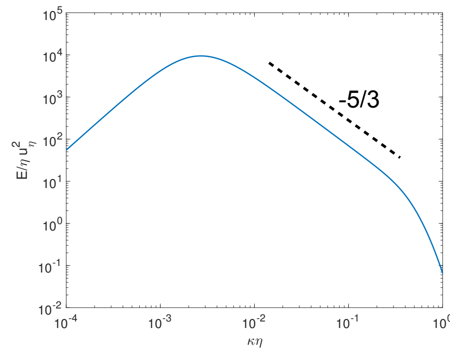


Level	Length scale
0	L_0
1	$L_0/2$
2	$L_0/4$
i	$L_0/2^i$
n-1	$L_0/2^{n-1}$

Parcel "proximity" is the node level of the nearest node connecting two parcels. This is used to define a parcel separation based on the corresponding length scale.

Model Formulation—Tree Scales

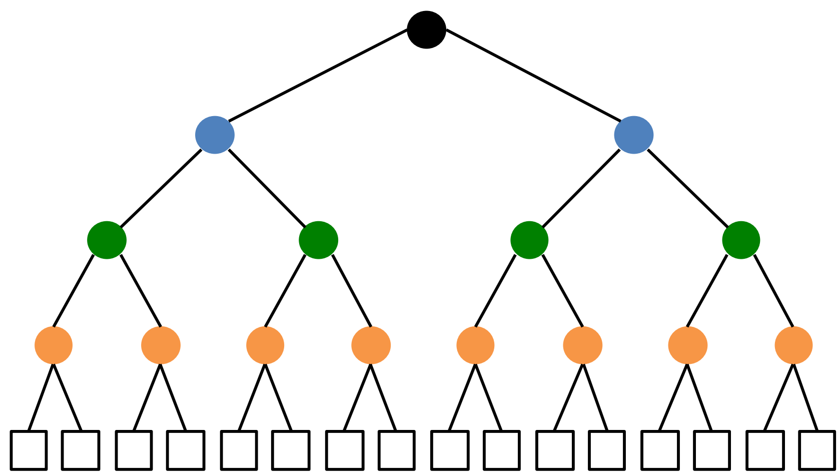
- Specify time scales at each level
  - Top level is the tree length scale τ_0
  - τ_0 is user-defined
  - Use inertial range scaling
    - ε is constant
    - scales depend on ε



Kolmogorov's second similarity hypothesis. In every turbulent flow at sufficiently high Reynolds number, the statistics of the motions of scale L in the inertial subrange have a universal form that is uniquely determined by ε. —Pope, *Turbulent Flows*

$$\epsilon \sim \frac{u^2}{\tau} \sim \frac{l^2}{\tau^3}$$
$$\tau \sim l^{2/3}$$
$$\tau = \tau_0 \left(\frac{l}{L_0}\right)^{2/3}$$

$$\chi \sim \frac{\theta^2}{\tau}$$
$$\theta^2 \sim l^{2/3}$$
$$E \sim \frac{\theta^2}{k} \sim \theta^2 l \sim k^{-5/3}$$



Level	Length scale	Time scale
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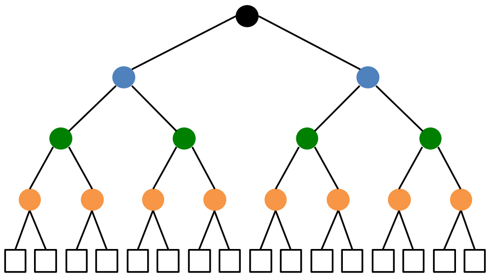
n-1	$L_0/2^{n-1}$	$\tau_0\left(\frac{1}{2^{n-1}}\right)^{2/3}$

Model Formulation—Eddy Events

- Tree swaps = "eddy events"
- Eddy rate at each level computed from time scales

$$\lambda_i = \frac{1}{\tau_i} \cdot 2^i$$

2^i factor is # nodes at level i



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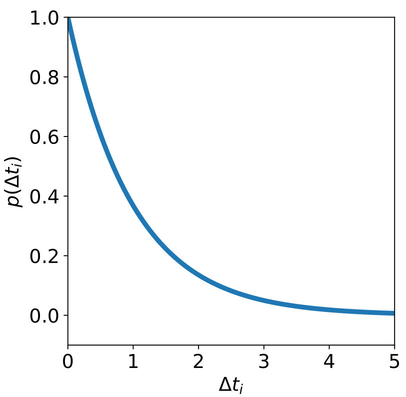
- Eddy event times at each level are sampled as a Poisson process with mean rate λ_i.

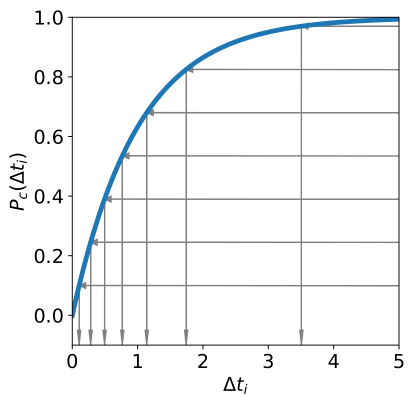
$$p(\Delta t_i) = \lambda_i e^{-\lambda_i \Delta t_i}$$

$$P_c(\Delta t_i) = \int_0^{\Delta t_i} p(\Delta t_i) d\Delta t_i$$

$$P_c(\Delta t_i) = 1 - e^{-\lambda_i \Delta t_i}$$

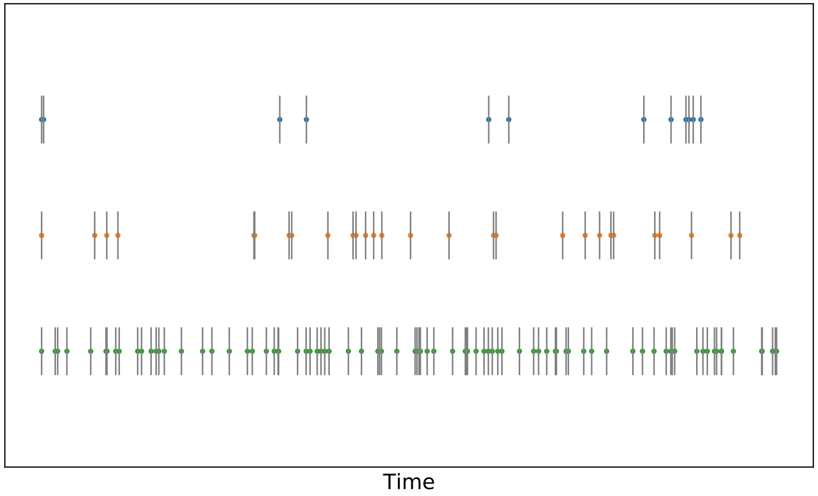
$$\Delta t_i = -\frac{\ln(P)}{\lambda_i} \qquad P \rightarrow r \in [0,\ 1]$$

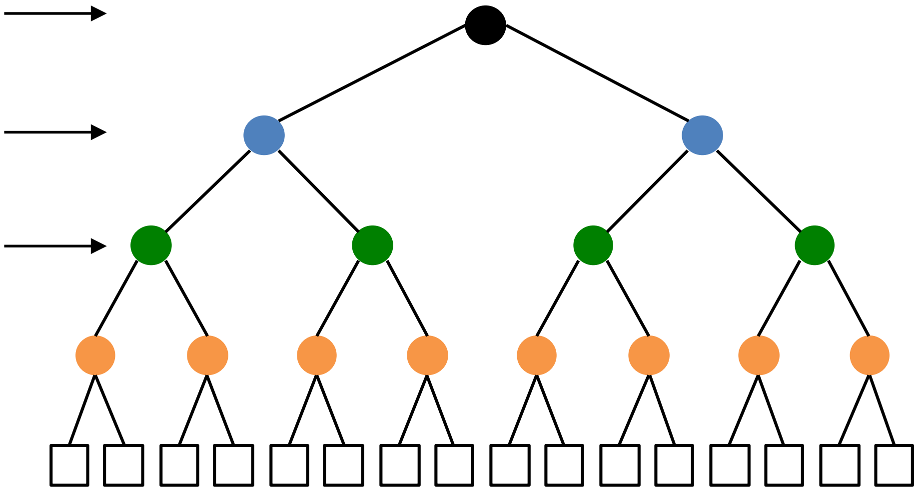




Model Formulation—Eddy Events

Eddy occurrence times at three levels

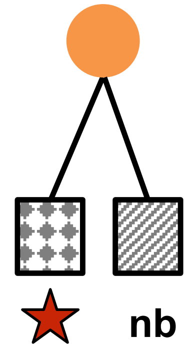




- Combine the times for the three levels
- Make a list of the levels for each eddy event time.
- Advance mixing and reaction processes for each parcel between eddy events.

Model Formulation—Mixing/Reaction

- **Two mixing models**
  - **Fast mixing:**
    - Eddy events instantaneously mix the state
    - Solve separate evolution equations for chemical reaction
  - **Rate equation:**
    - Semi-implicit, semi-analytic solution approach
    - Also works well with a second order Strang splitting



Fast mixing

$$\phi_{mix} = \frac{1}{2}(\phi + \phi_{nb})$$

$$\frac{d\phi}{dt} = \frac{\dot{m}'''_{\phi}}{\rho}$$

Solve reaction equations implicitly

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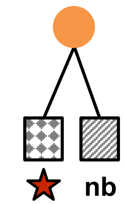


$$\frac{d\phi}{dt} = \frac{\dot{m}'''_{\phi}}{\rho}$$

Solve reaction equations implicitly

Rate Equation

$$\frac{d\phi}{dt} = \frac{-1}{\tau_m}(\phi - \phi_{nb}) + \frac{\dot{m}'''_{\phi}}{\rho}$$

Analytic solution

Mixing only

$$\frac{d\phi}{dt} = \frac{-1}{\tau_m}(\phi - \phi_{nb}) \longrightarrow \phi(t) = \frac{1}{2}\phi_0(1 - e^{-2t/\tau_m}) + \frac{1}{2}\phi_{nb,0}(1 - e^{-2t/\tau_m})$$

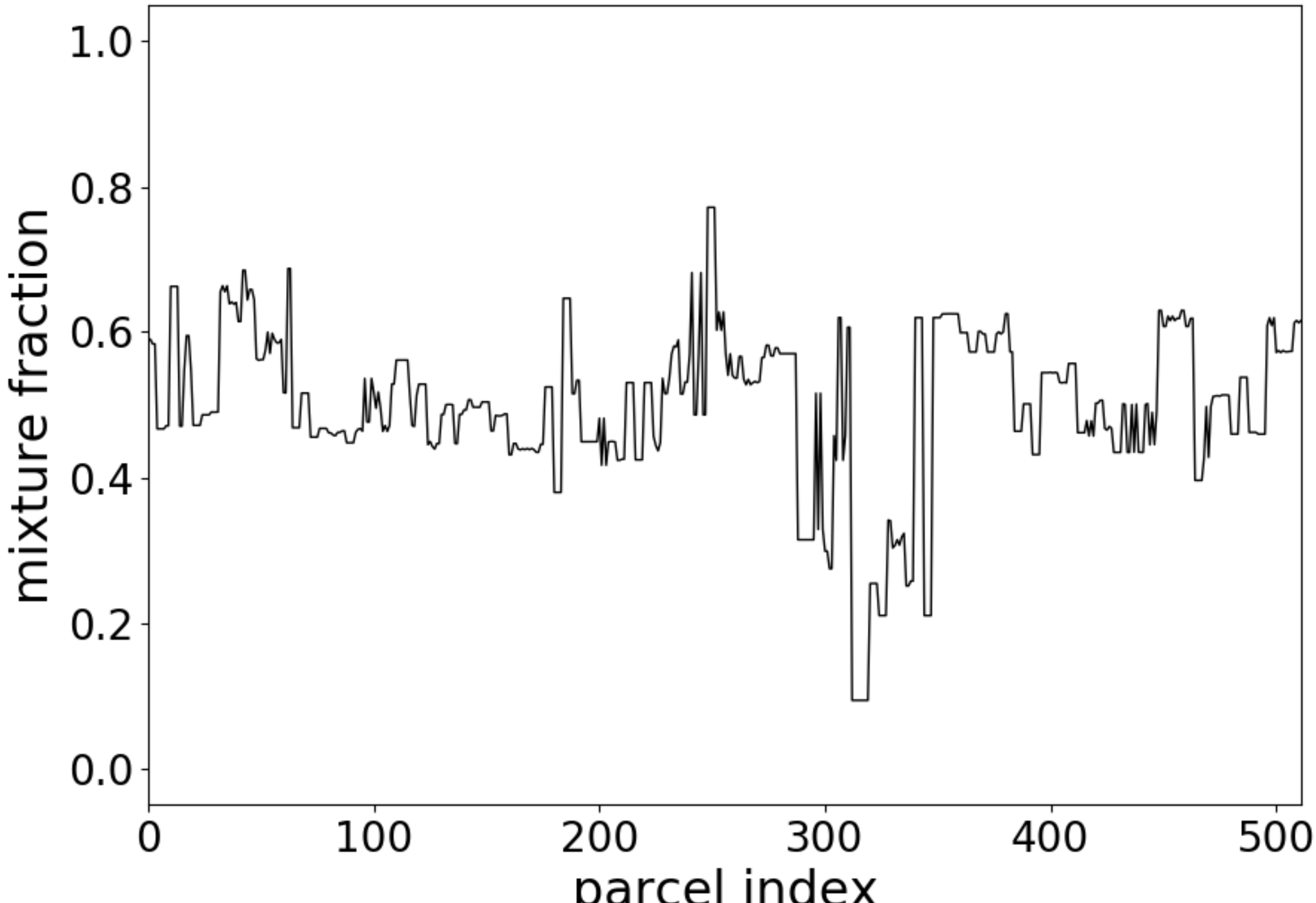
1-step mixing rate

$$R_{mix} = \frac{\phi(t + \Delta t) - \phi(t)}{\Delta t}$$

Implicit solve to t+Δt using constant R_{mix}

$$\frac{d\phi}{dt} = R_{mix} + \frac{\dot{m}'''_{\phi}}{\rho}$$

Results—Simple Mixing



Parallel Reactions

$$A + B \rightarrow R$$
$$A + R \rightarrow P$$

Take R as the desired product

$$M_A = M_B = 1$$

$$Da = \frac{\tau_{mix}}{\tau_{rxn}} = \frac{\text{reaction rate}}{\text{mixing rate}}$$

$$S = \frac{Y_R}{Y_R + Y_P}$$

$$\frac{dY_A}{dt} = -Da_1 Y_A Y_B - \frac{1}{2} Da_2 Y_A Y_R$$

$$\frac{dY_B}{dt} = -Da_1 Y_A Y_B$$

$$\frac{dY_R}{dt} = 2 Da_1 Y_A Y_B - Da_2 Y_A Y_R$$

$$\frac{dY_P}{dt} = \frac{3}{2} Da_2 Y_A Y_R$$

Parallel Reactions

$$A + B \rightarrow R$$
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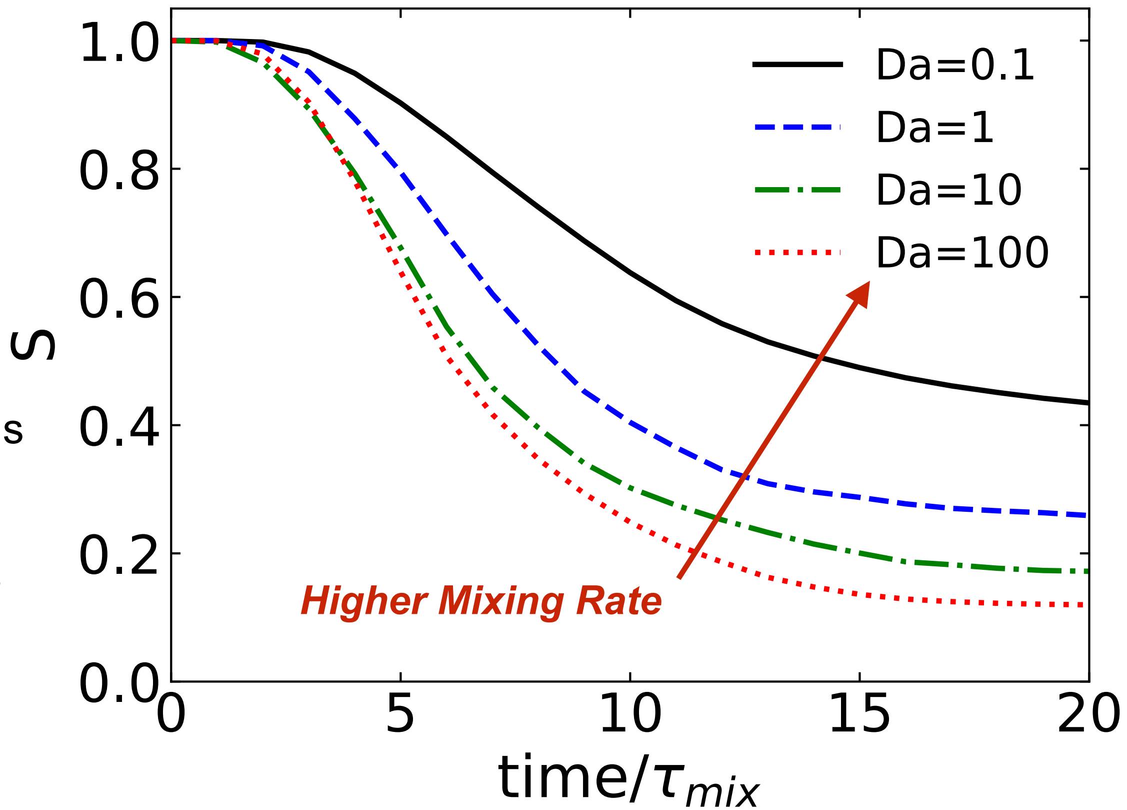
$$\frac{dY_P}{dt} = \frac{3}{2} Da_2 Y_A Y_R$$

- Initially segregated reactants, 9 levels
- **Re = 1625 (645, 256)**
- Vary τ_{mix} with constant reaction rates
- Higher mixing rate favors desired product R.
  - Mixing dilutes R, reducing its concentration, hence the reaction rate forming P



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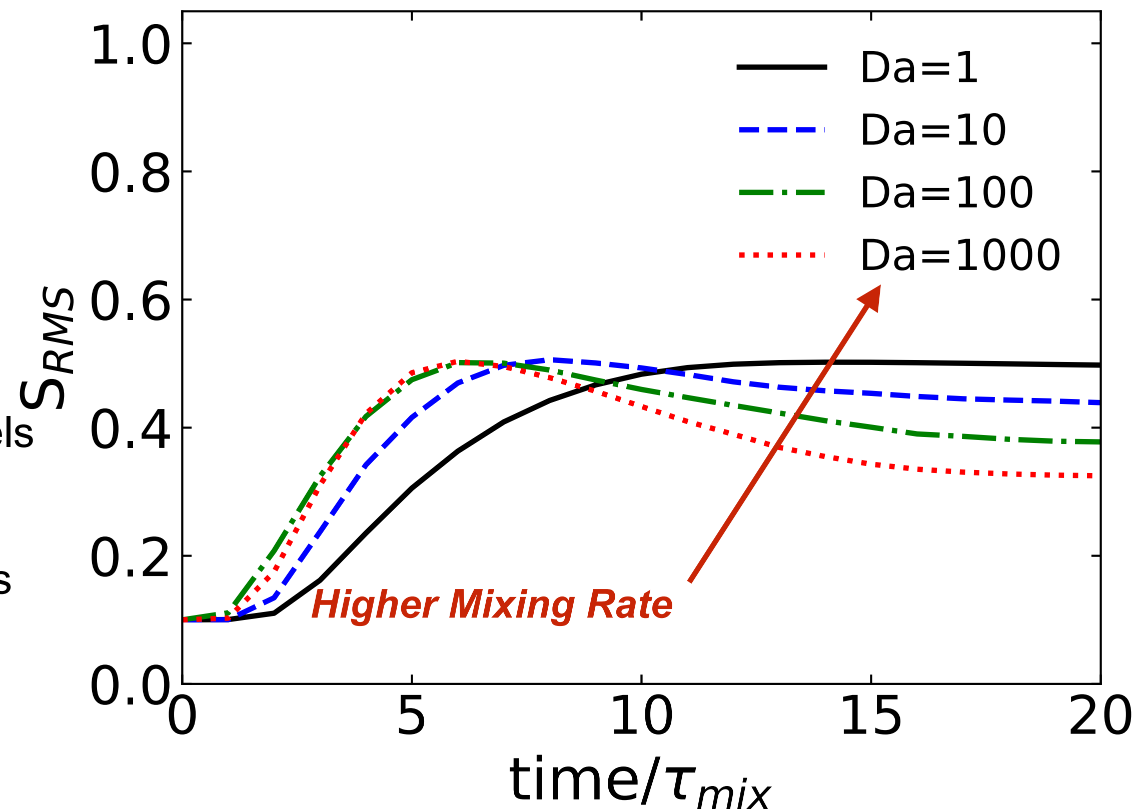
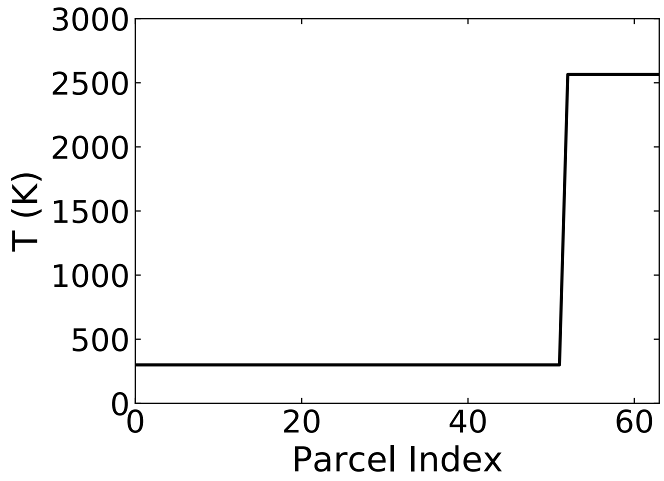


Ethylene flame

- Turbulent premixed ethylene flame
- Initialize 20% of the parcels to be burnt, 80% to be fresh reactants
- Vary the mixing rate
- High mixing results in flame extinction
  - Reactants are mixed into the products faster than reaction occurs.
  - This reduces temperature and quenches the reaction.



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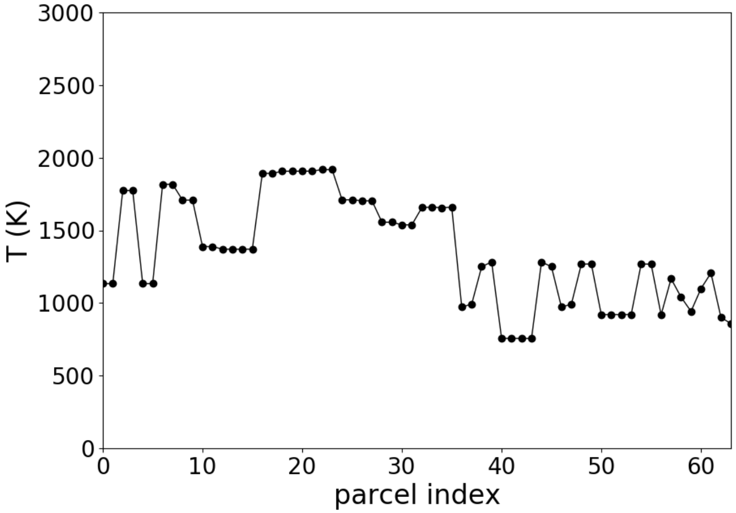
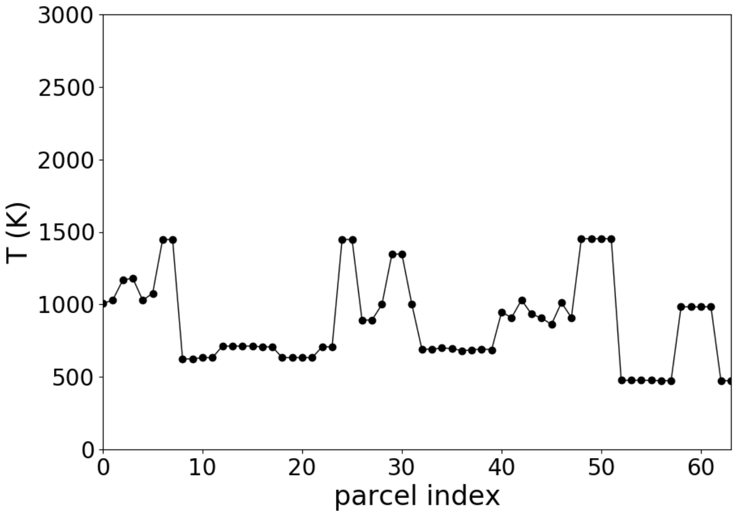


Extinguishes



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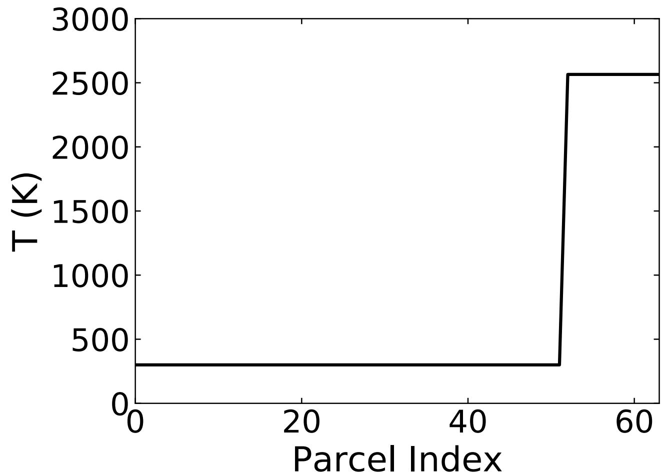

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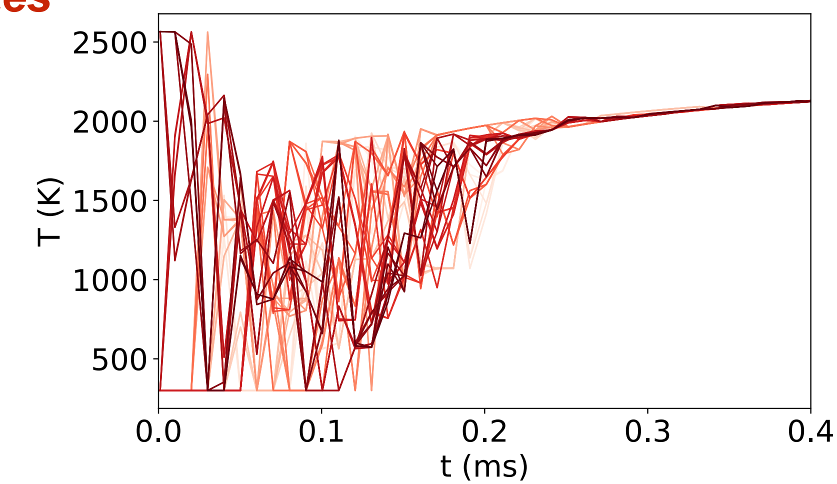

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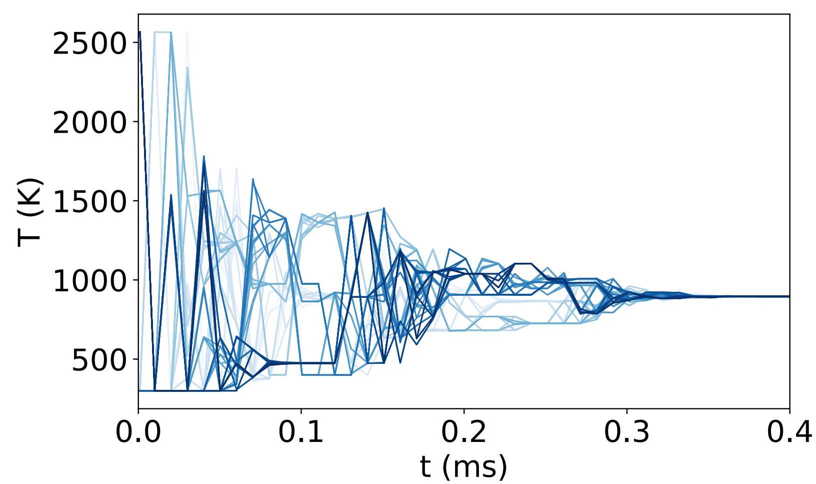

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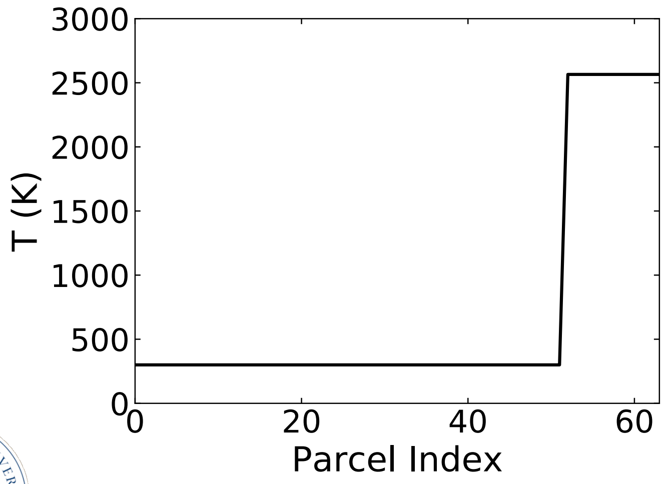

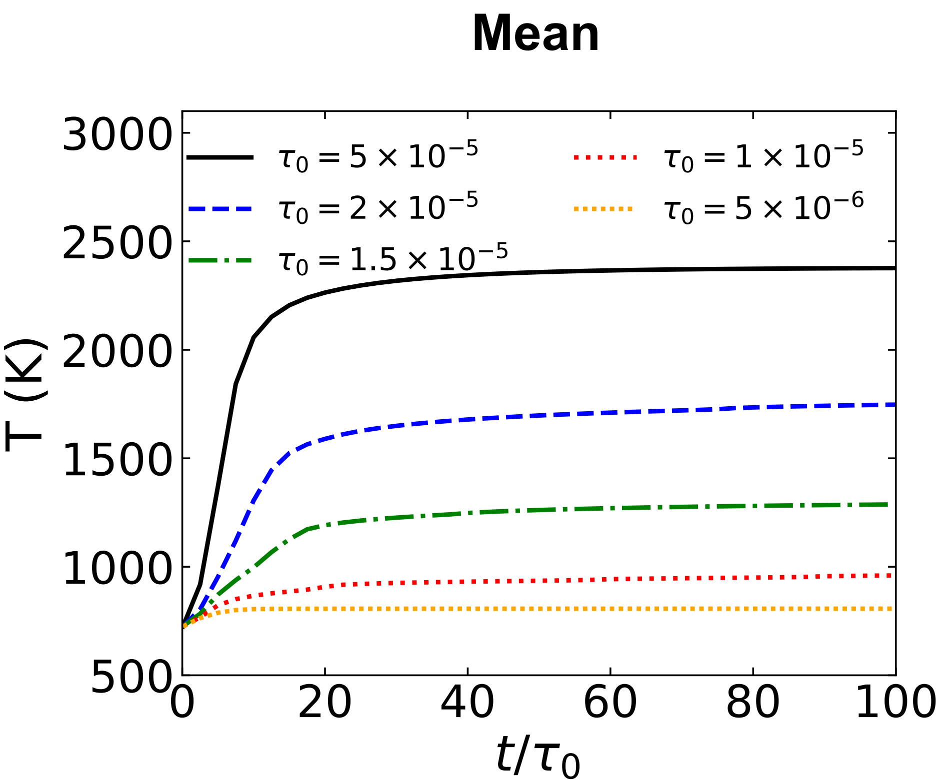

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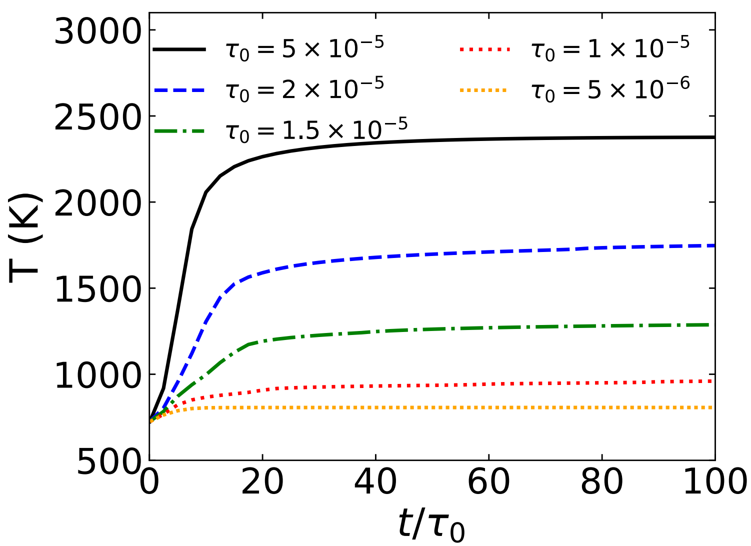
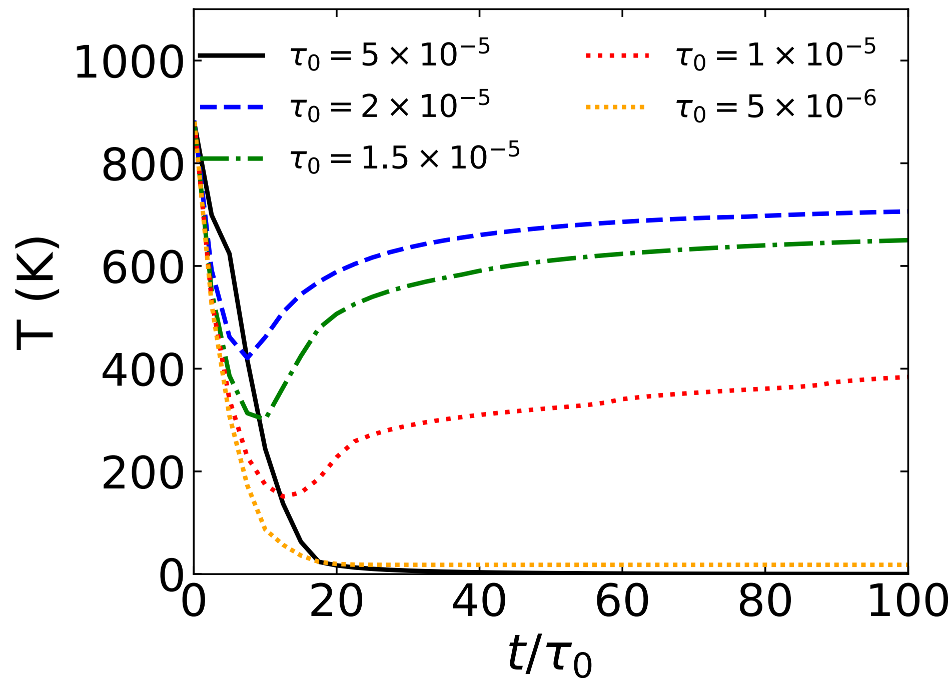


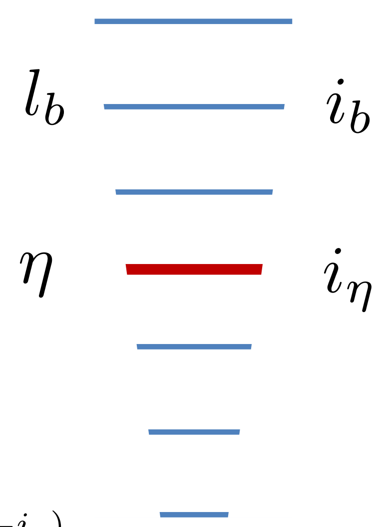
RMS



Differential Diffusion (nonunity Sc)

2 Cases

- High D: Sc < 1
- Low D: Sc > 1



High D: Sc < 1

- Scalar diffusion timescale = inertial timescale

$$\tau_b = \tau_i$$

$$\frac{l_b^2 Sc}{\nu} = \tau_\eta \left(\frac{l_b}{\eta}\right)^{2/3} = \frac{\eta^2}{\nu}\left(\frac{l_b}{\eta}\right)^{2/3}$$

$$Sc = \left(\frac{\eta}{l_b}\right)^{4/3}$$

$$\left.\begin{aligned} \eta &= \frac{L_0}{2^{i_\eta}} \\ l_b &= \frac{L_0}{2^{i_b}} \end{aligned}\right\} Sc = 4^{\frac{2}{3}(i_b - i_\eta)}$$

- Mix all parcels across the given level i_b

Differential Diffusion (nonunity Sc)

2 Cases

- High D: Sc < 1
- Low D: Sc > 1

Low D: Sc > 1

- Levels between i_η and i_b have timescale τ_η
- Scalar diffusion timescale = Kolmogorov timescale

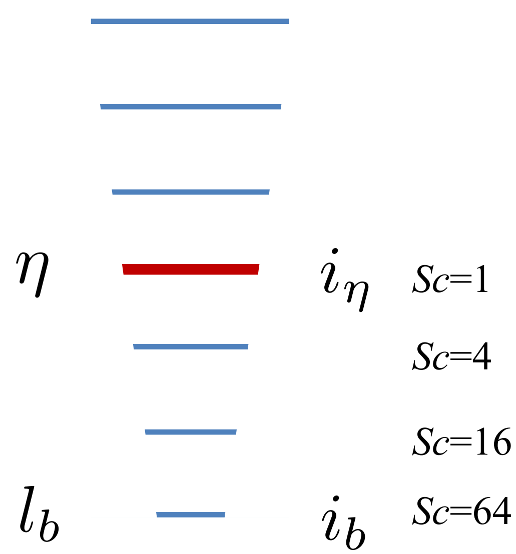
$$\tau_b = \tau_\eta$$

$$\frac{l_b^2 Sc}{\nu} = \frac{\eta^2}{\nu}$$

$$Sc = \left(\frac{\eta}{l_b}\right)^2$$

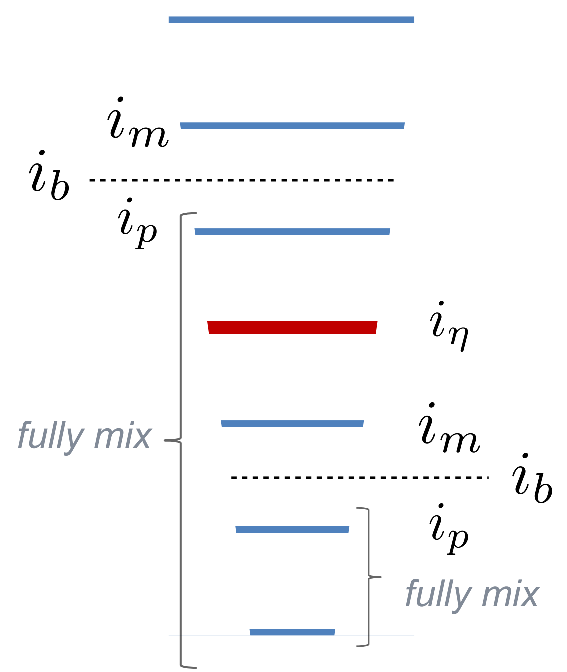
$$\left.\begin{aligned} \eta &= \frac{L_0}{2^{i_\eta}} \\ l_b &= \frac{L_0}{2^{i_b}} \end{aligned}\right\} Sc = 4^{(i_b - i_\eta)}$$

- Mix all parcels across the given level i_b



Arbitrary Sc

Low D: Sc > 1 **High D: Sc < 1**



- Eddy events at levels greater or equal to i_p result in full mixing of the scalar across the relevant subtree.
- With $i_m<i_b<i_p$ mixing events at level i_m homogenize the scalar across the subtree with probability p_m.

$$p_m = 1 \text{ for } i_b = i_m$$
$$p_m = 0 \text{ for } i_b = i_p$$

- Linear profile for p_m

$$p_m = \frac{i_p - i_b}{i_p - i_m} = i_p - i_b$$

$$p_m = \frac{\log(l_b/l_{i_p})}{\log(l_{i_m}/l_{i_p})} = \frac{\log(\lambda_b/\lambda_{i_p})}{\log(\lambda_{i_m}/\lambda_{i_p})}$$

$$i_p = \text{ceil}(i_b)$$

$$i_b = i_\eta + \frac{3}{2}\log_4(Sc) \qquad Sc < 1$$

$$i_b = i_\eta + \log_4(Sc) \qquad Sc > 1$$

Conclusions

- HiPS is a promising mixing model for turbulent flows.
- Can include reactions and variable Sc number effects.
- Captures a range of time and length scales.
- Highly efficient mixing process that follows turbulent scaling laws.
- Formulations as both a mixing model, and as a flow model are possible. These follow LEM and ODT analogs.
- Can be used as a SGS mixing model for PDF transport methods.
- Initial results demonstrate capabilities for reacting flows and variable Sc number.

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