Developments Towards a Satellite-Informed High-Resolution $PM_{2.5}$ Modeling System

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Goals …

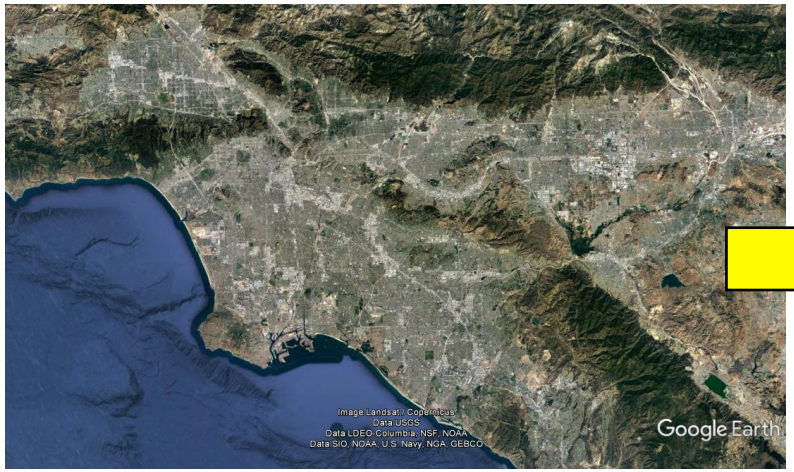
- PM2.5 @ sub-km resolution around a point of interest (POI)
- All scales (large -> neighborhood)
- Full physics (primary, secondary)
- Flexible & computationally efficient
- Wide applicability
  - AQ management, Health Effects & Forecasting
- Satellite key component
  - Linkage to large scale
  - Provide constraints due to emission uncertainty

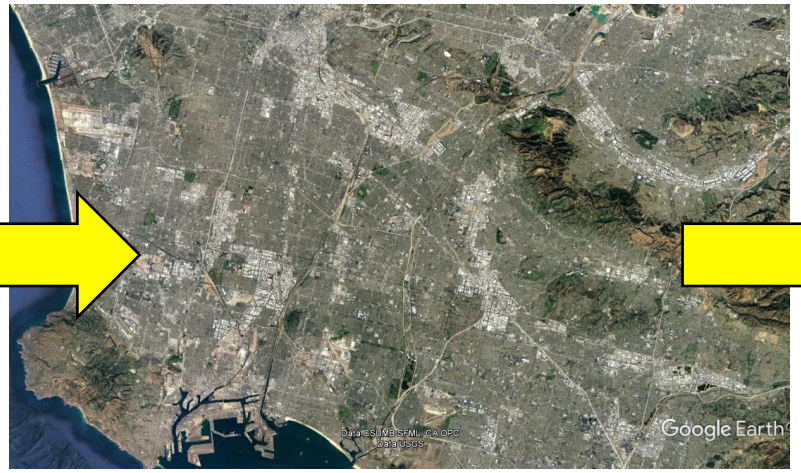
Basis: Downscaling satellite AQ fields to sub-km …

Large Scale / Regional
(satellite-informed)
(e.g. MODIS AOD -> PM2.5)
(~ 10 km)

Local
(~ 1 km)
(HYSPLIT + LBM)

Near-Source
(~ 100 m)
AERMOD





Primary + Secondary Background PM2.5

Near-Source PM2.5

Total PM2.5

HYSPLIT Stilt Emulation Mode

- Lagrangian Particle Model
- Backwards in integration
- Map out influence functions (I)
- Spatial maps: Influence of upwind regions on concentrations @ point of interest

Term 1: Couple to Surface Emissions

$$C(\mathbf{x}_r, t_r) = \int_{t_0}^{t_r} dt \int_V d^3x I(\mathbf{x}_r, t_r \mid \mathbf{x}, t) S(\mathbf{x}, t)$$

Concentration @ point of interest

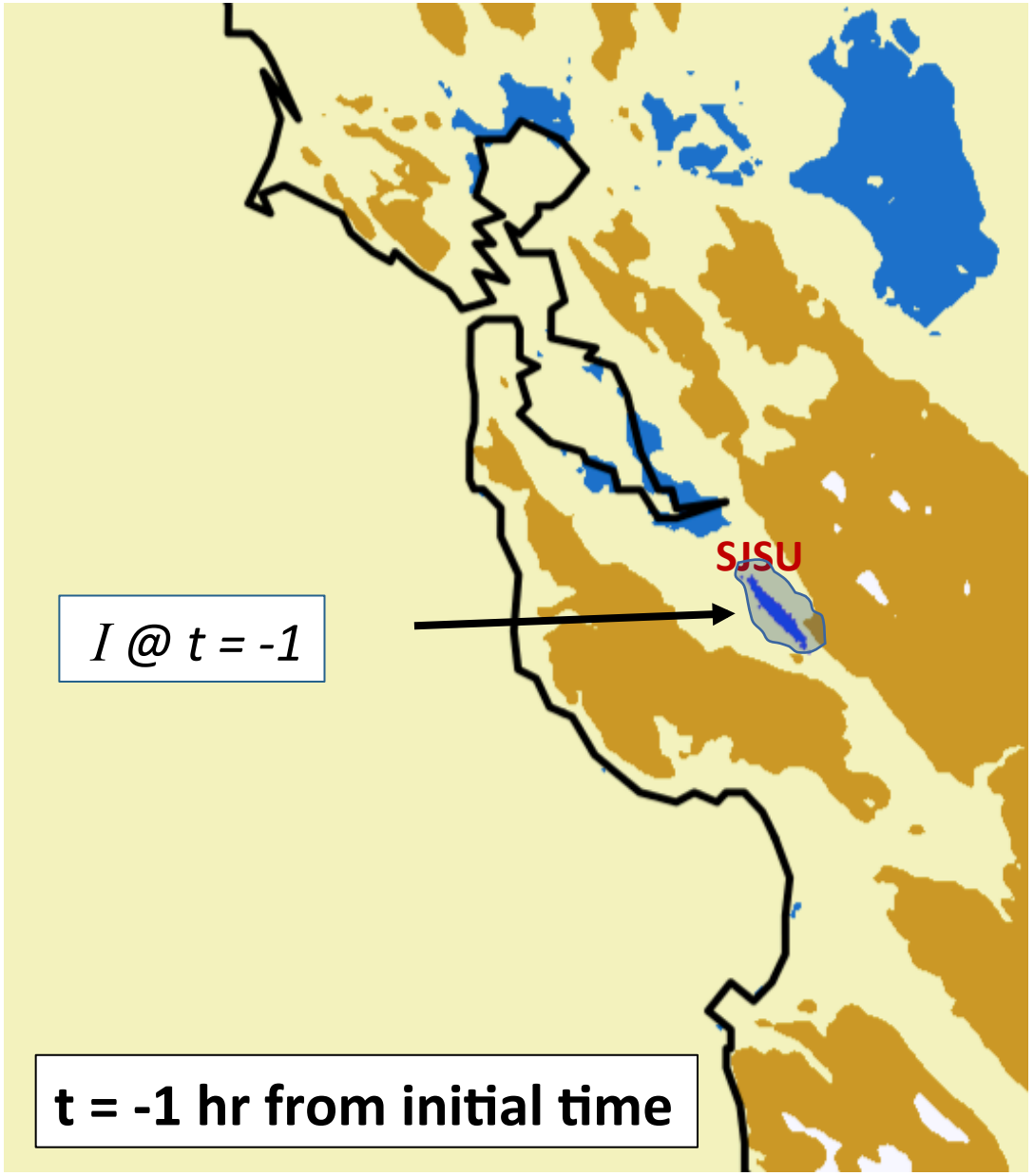
$$+ \int_V d^3x I(\mathbf{x}_r, t_r \mid \mathbf{x}, t_0) C(\mathbf{x}, t_0).$$

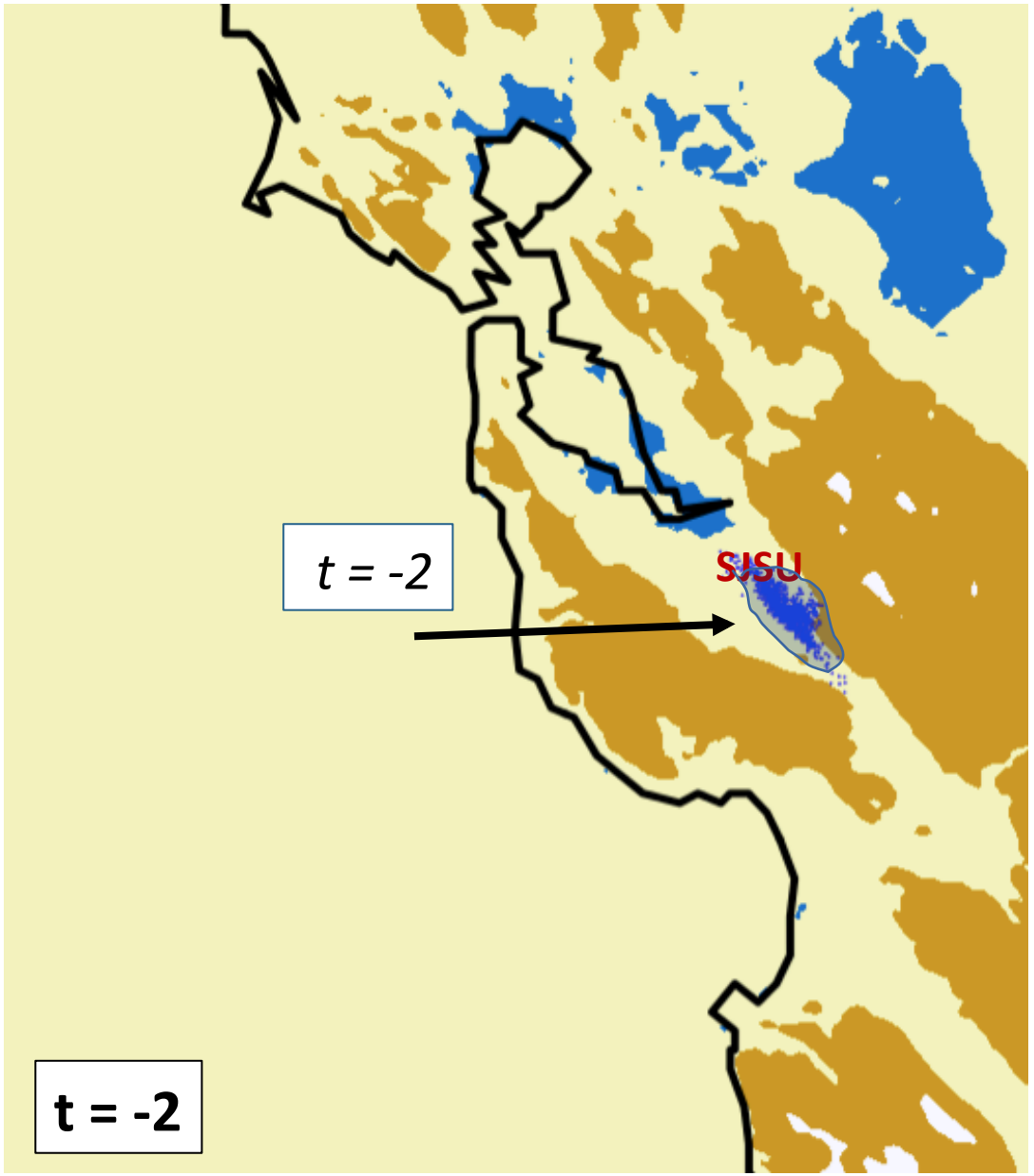
Term 2: Couple to initial conditions

Ref: Lin et al. 2003 (JGR)

Illustrative example …

- HYSPLIT
- Backwards-in-time nine hours
- Point of Interest: SJSU
- Driven by WRF wind field

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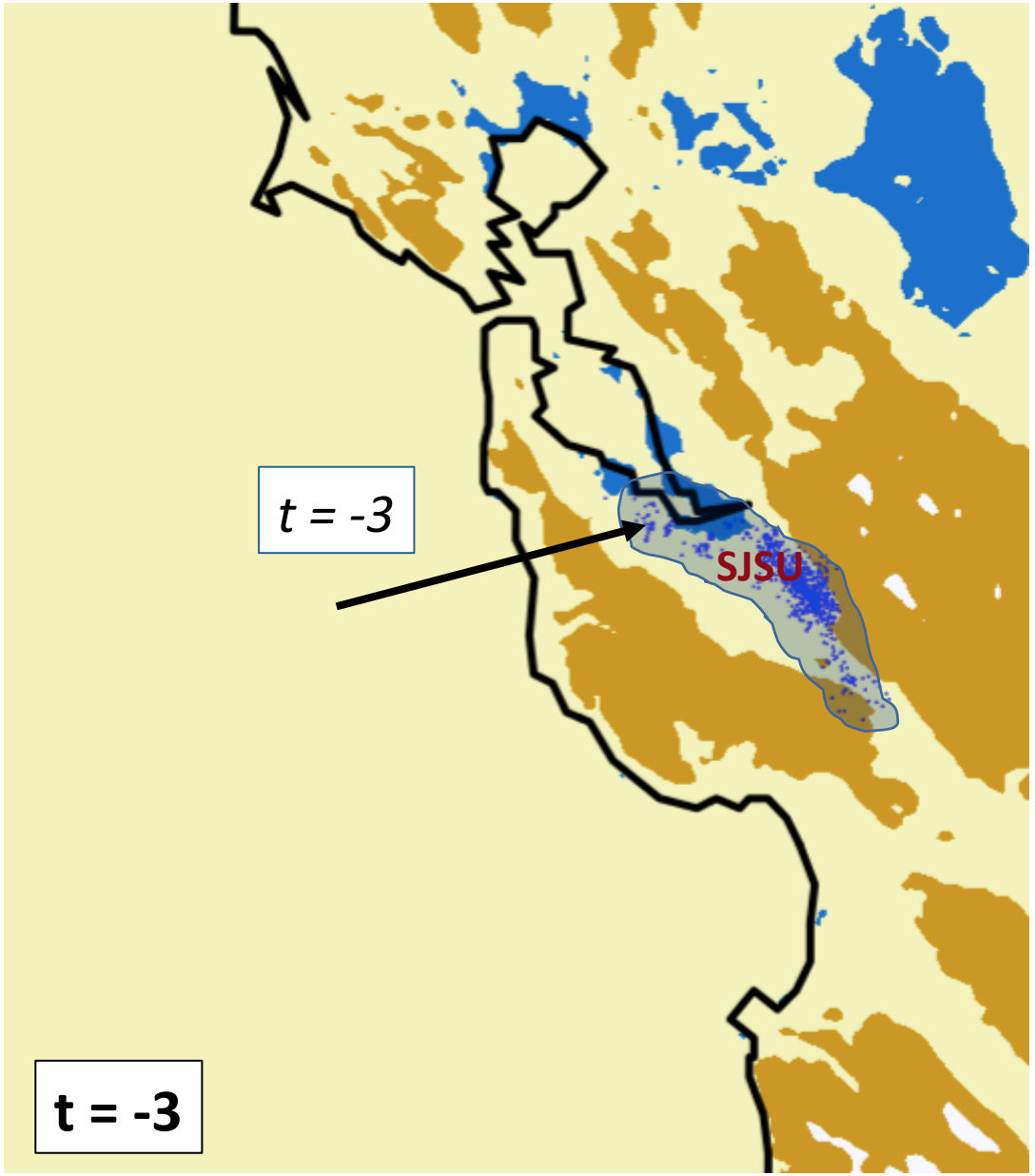
SJSU
t = -2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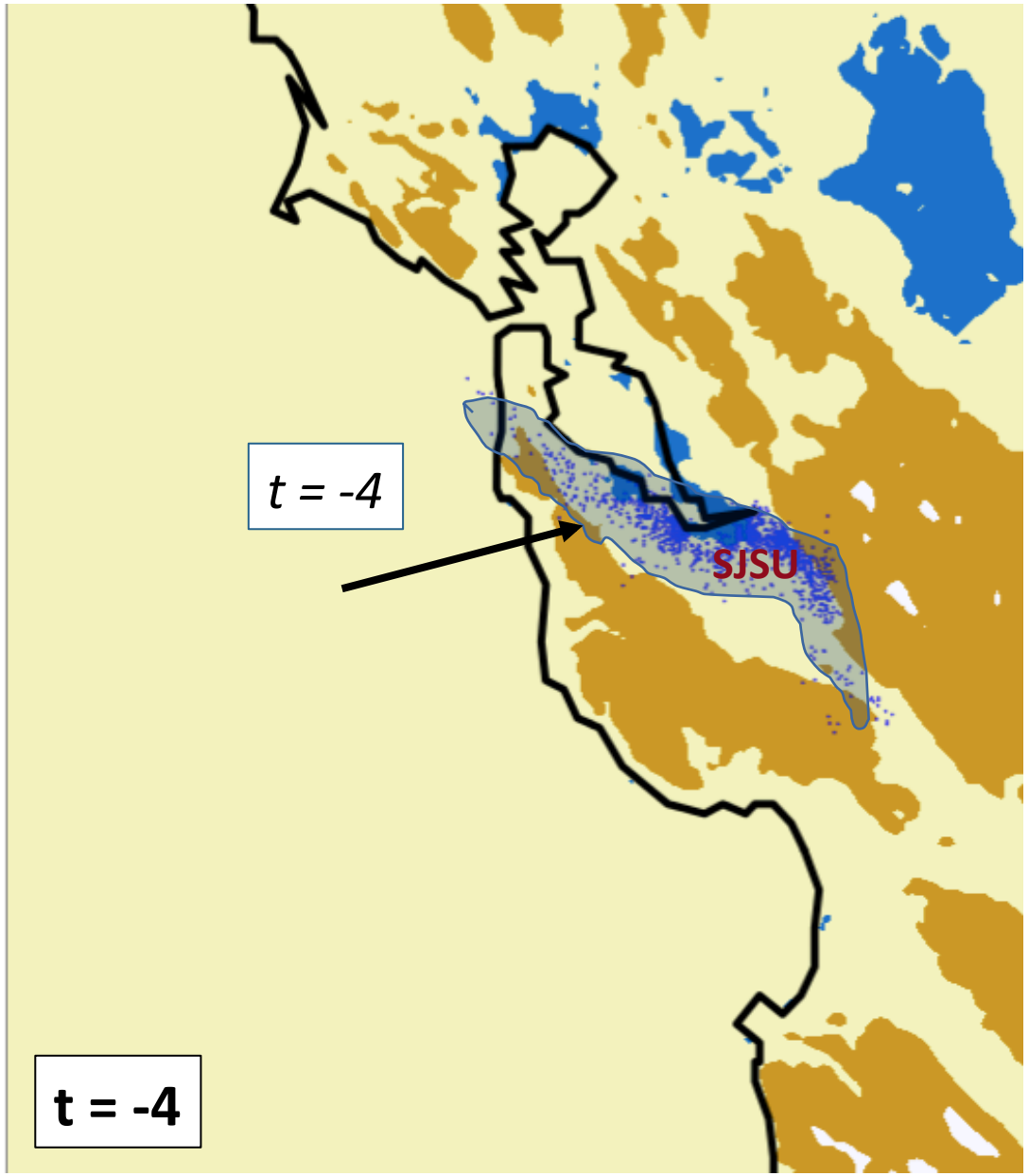
SJSU
t = -3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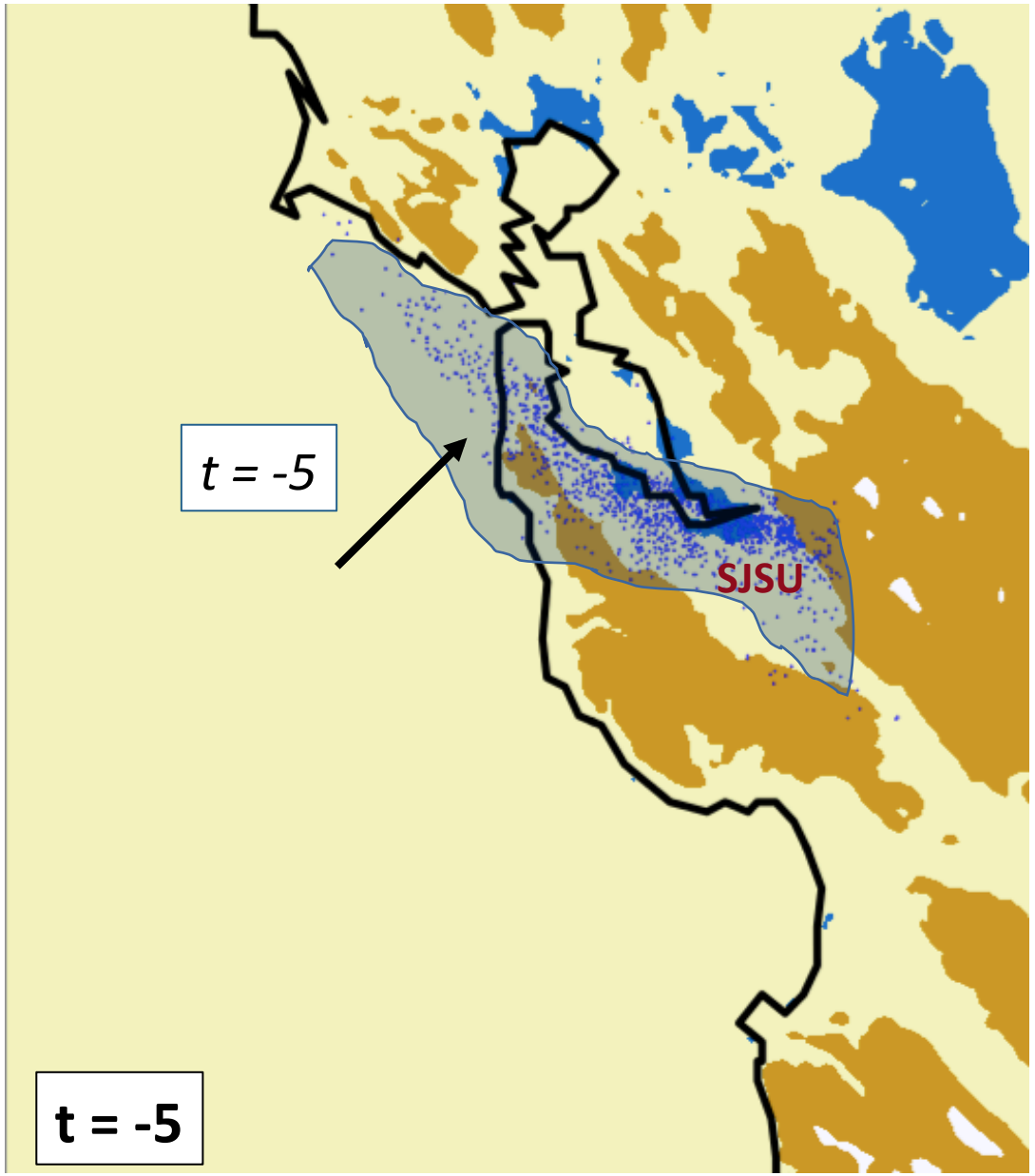
SJSU
t = -4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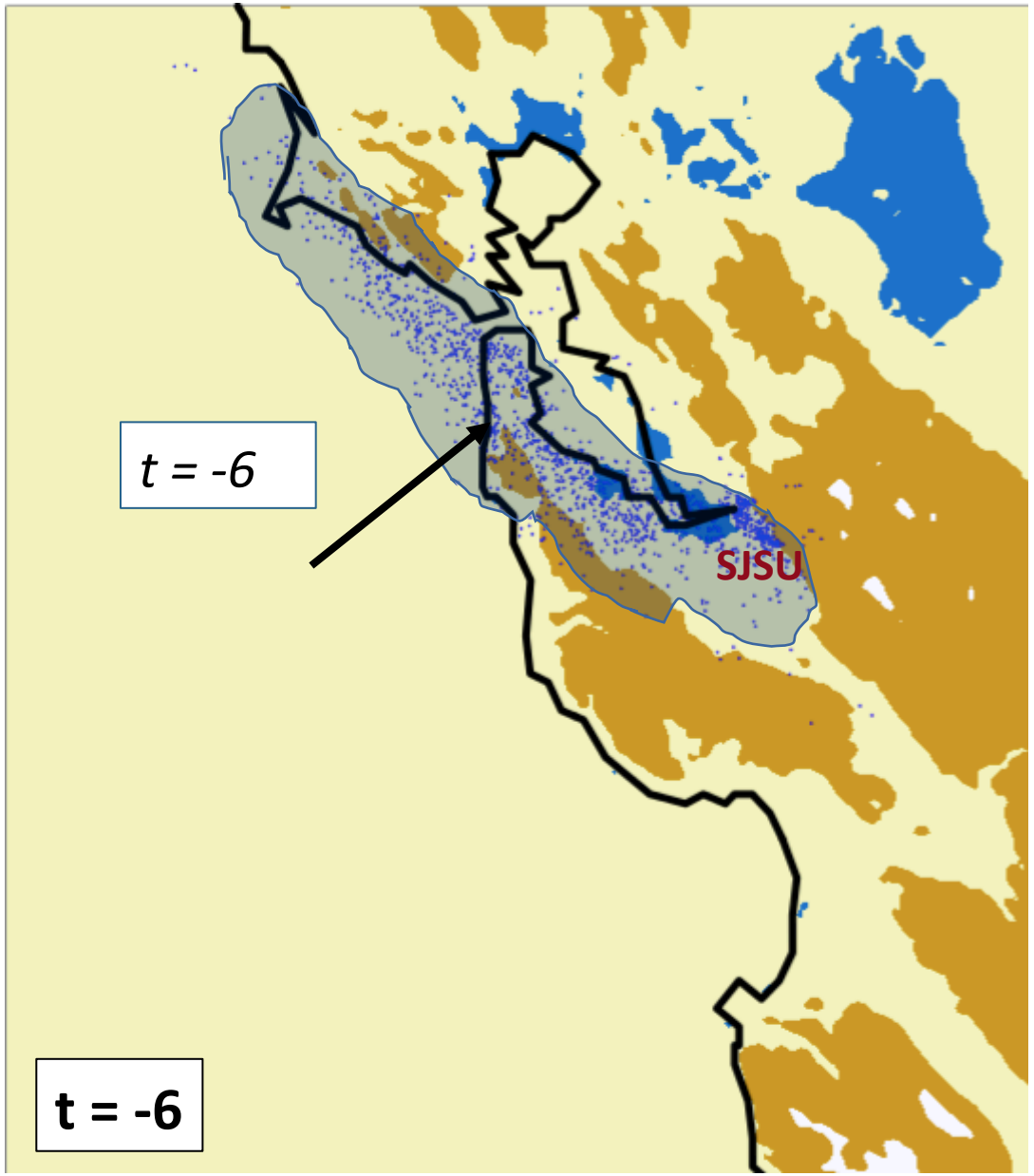
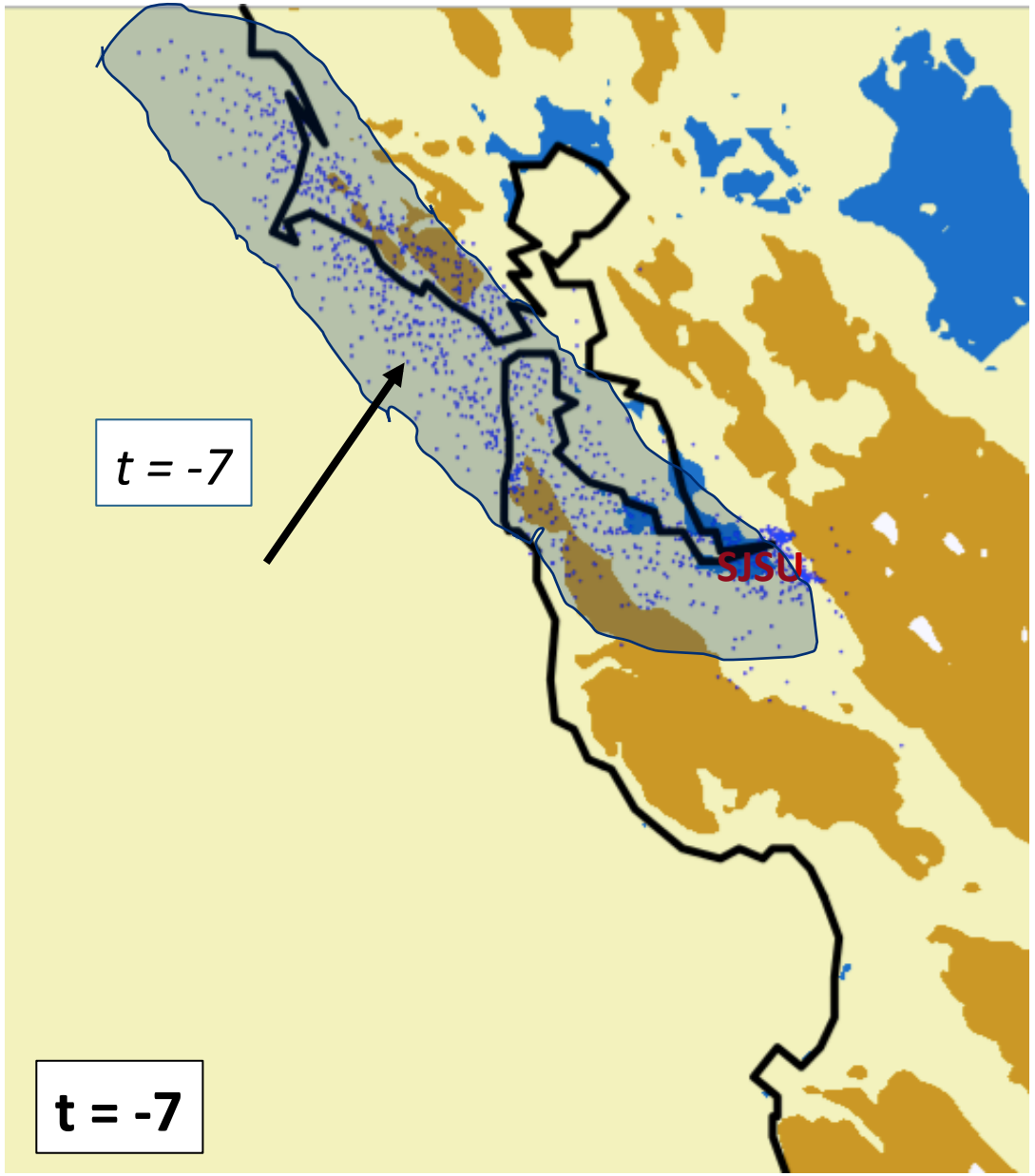
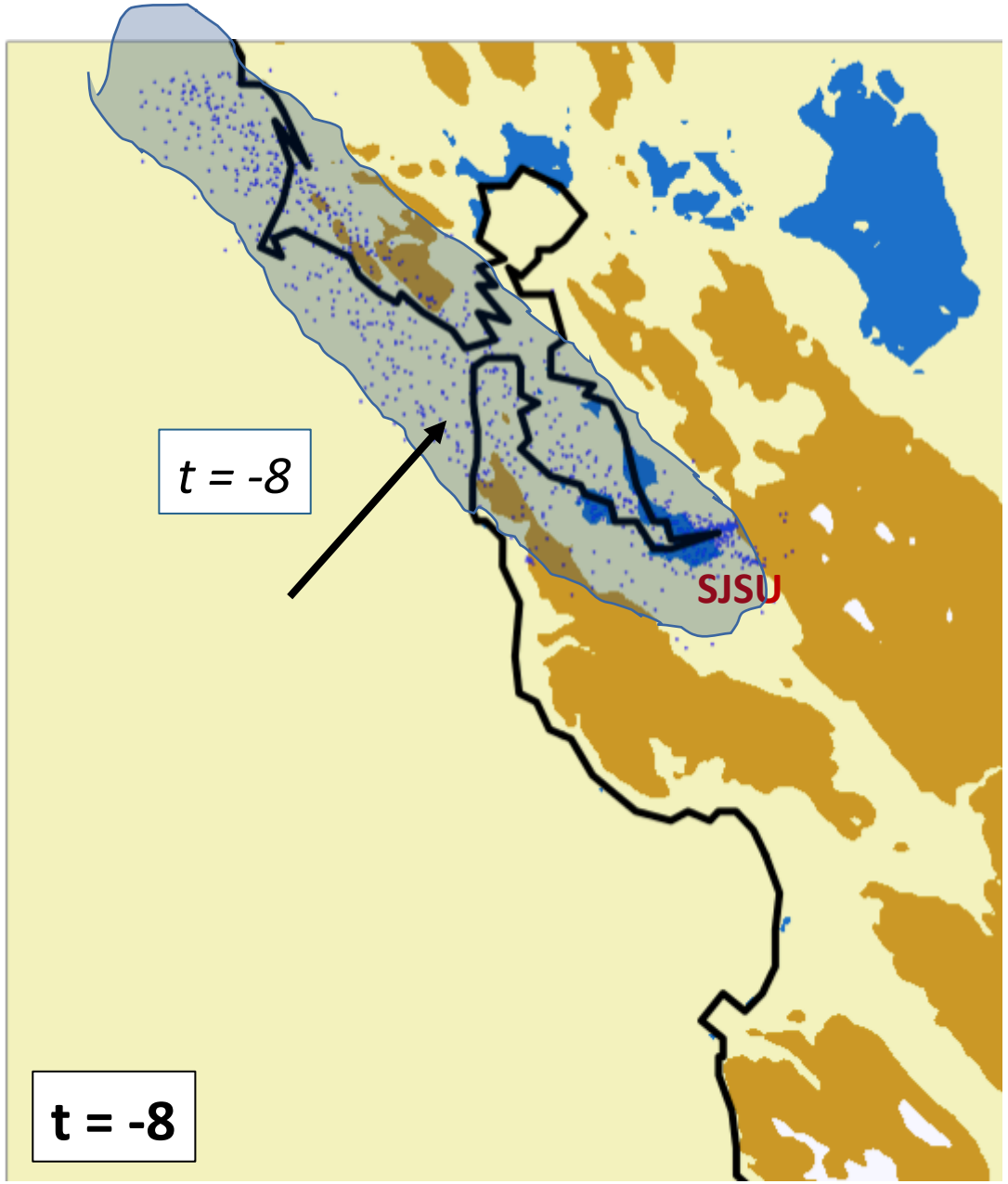
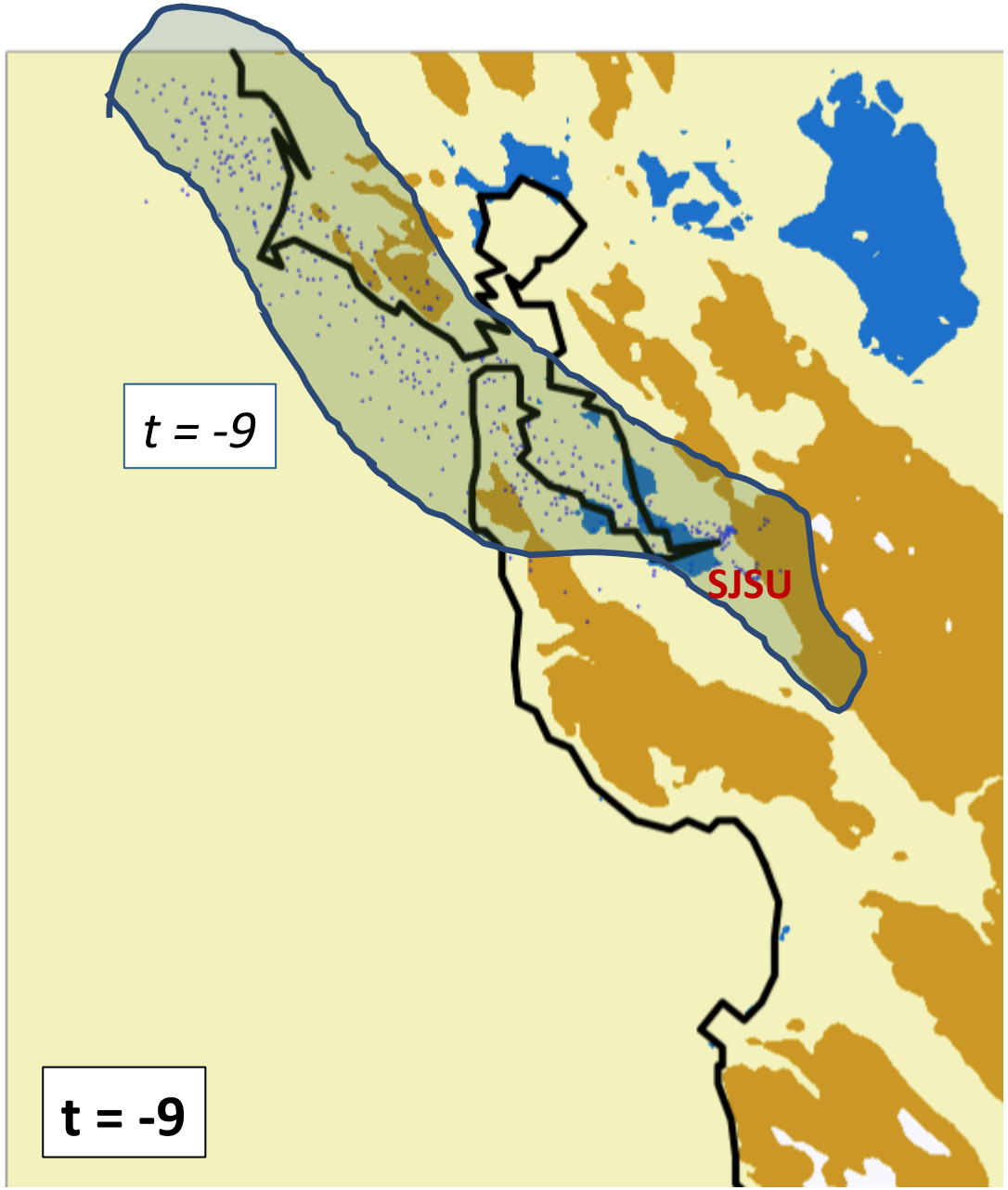
SJSU
t = -5


t = -6
SJSU
t = -6


t = -7
SJSU
t = -7


t = -8
SJSU
t = -8


t = -9
SJSU
t = -9

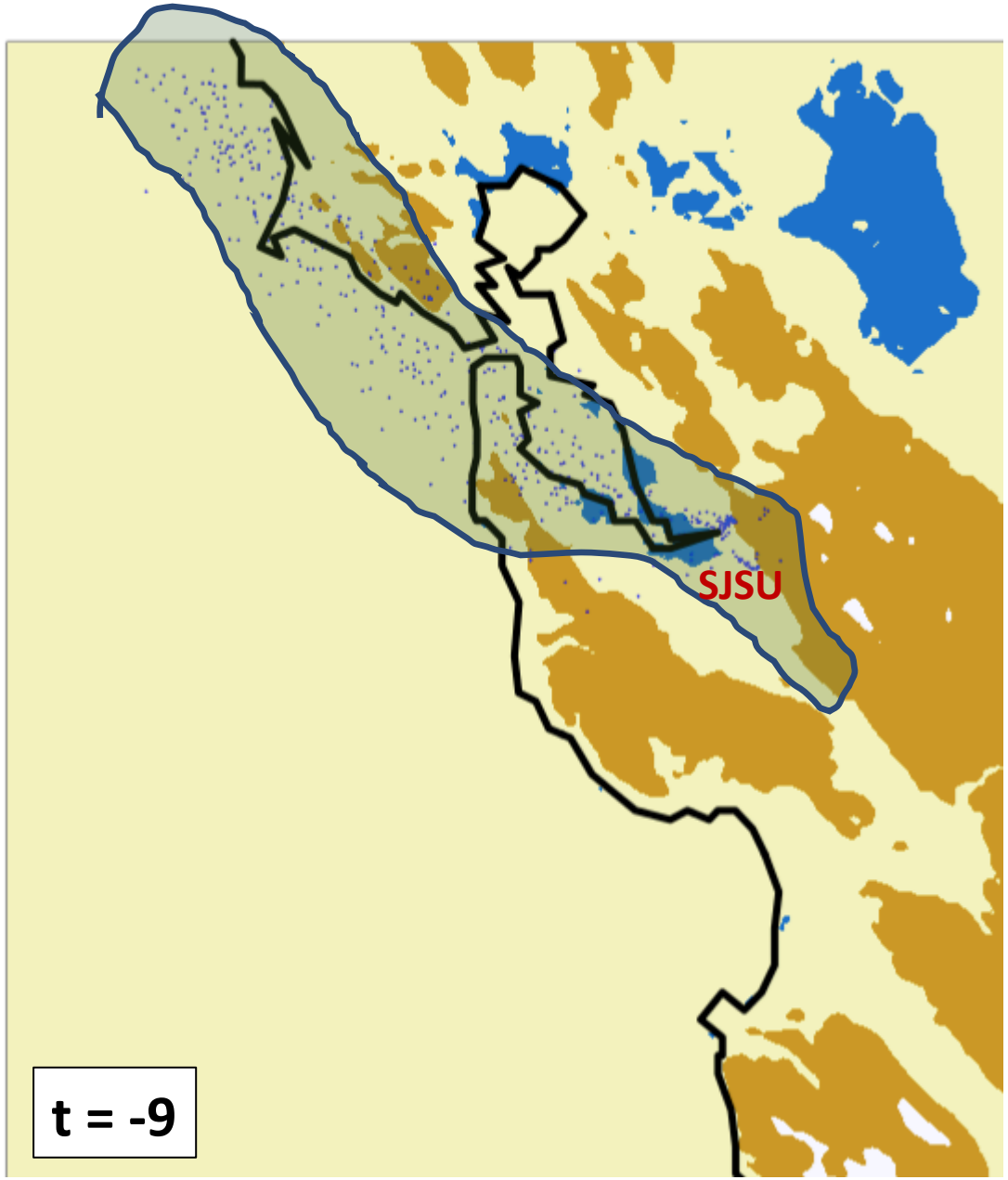
Apply to …

- *PM25 (primary local)*
- *NOx (precursors, secondary local)*
- *VOC (precursors, secondary local)*

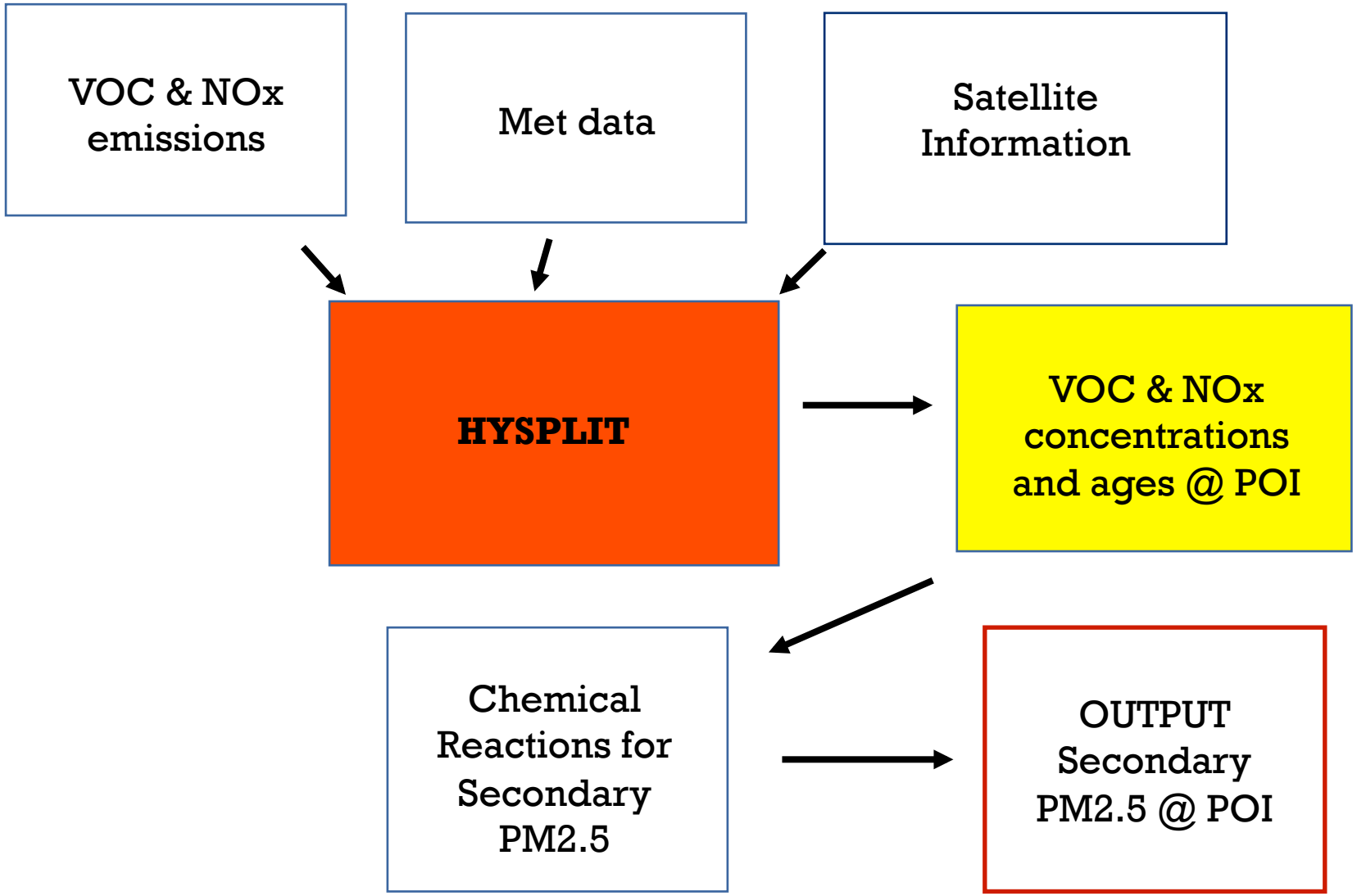
Role of Satellite Fields

Probe large-scale satellite field <u>within influence region</u> to provide …

- Initial conditions (t = -9)
- Constraints on model calculations (t = 0 to -9)



Local Secondary: Lagrangian Background Model (LBM)



Pournazeri et al. (2014)

LBM achieves computational efficiency by uncoupling transport and chemistry using the concept of species age (Venkatram et al. 1998; Pournazeri et al., 2014).

We can reduce computing time using time using parameterized chemistry to compute PM2.5 concentrations (Venkatram et al, 2011).

$$\mathrm{ROC1} + h\nu \xrightarrow{O_2} \mathrm{RP} + \mathrm{ROC1}$$

$$\mathrm{AROM} + h\nu \xrightarrow{O_2} \mathrm{RP} + \mathrm{AROM}$$

$$\mathrm{TERP} + h\nu \xrightarrow{O_2} \mathrm{RP} + \mathrm{TERP}$$

$$\mathrm{RP} + \mathrm{NO} \rightarrow \mathrm{NO_2}$$

$$\mathrm{NO_2} + h\nu \xrightarrow{O_2} \mathrm{NO} + \mathrm{O_3}$$

$$\mathrm{NO} + \mathrm{O_3} \rightarrow \mathrm{NO_2}$$

$$\mathrm{RP} + \mathrm{RP} \rightarrow \mathrm{RP} + \alpha\mathrm{H_2O_2}$$

$$\mathrm{RP} + \mathrm{NO_2} \rightarrow \mathrm{RNO3}$$

$$\mathrm{OH} + \mathrm{SO_2} \rightarrow \mathrm{SO4}$$

$$\mathrm{OH} + \mathrm{NO_2} \rightarrow \mathrm{HNO3}$$

$$\mathrm{OH} + \mathrm{AROM} \rightarrow \mathrm{y_1OC}$$

$$\mathrm{OH} + \mathrm{TERP} \rightarrow \mathrm{y_2OC}$$

$$[OH] = 2.2 \times 10^{-6}[O_3] - 4.81 \times 10^{-9}$$

RP: “Radical pool”

Secondary PM2.5

- Sulfate
- Nitrate
- Secondary Organic

Ongoing Work …

- **Fuse Components**
  - MODIS AOD -> PM2.5: large-scale, regional
  - HYSPLIT: primary local
  - LBM: secondary local
  - AERMOD: near-source
- **Details of Satellite Linkage**
  - Suggestions from HAQAST & others
- **Applications & first use cases**
- **Evaluation**
  - EPA AQS
  - Low cost sensors

References & further details …

Pournazeri, S., Tan, S., Schulte, N., Jing, Q., & Venkatram, A. (2014). A computationally efficient model for estimating background concentrations of NO x, NO 2, and O 3. *Environmental Modelling & Software*, *52*, 19-37.

Venkatram, A., & Horst, T. W. (2006). Approximating dispersion from a finite line source. *Atmospheric Environment*, *40*(13), 2401-2408.

Venkatram et al. (1998). The Concept of Species Age in Photochemical Modeling, *Atmospheric Environment, 32, 3403-3413.*

Venkatram et al. (1997). The Development of a Model to Examine Source-Receptor Relationships for Visibility on the Colorado Plateau, *J. Air Waste Manage. Assoc., 47, 286 – 301.*

See https://sites.google.com/a/sjsu.edu/met-haqast/home for more details.