Air Quality Data Fusion with Sensors, Satellites, and Models

Carl Malings

Morgan State University & GESTAR-II cooperative agreement

NASA Global Modeling and Assimilation Office

GESTAR II

GMAO

GODDARD EARTH SCIENCES

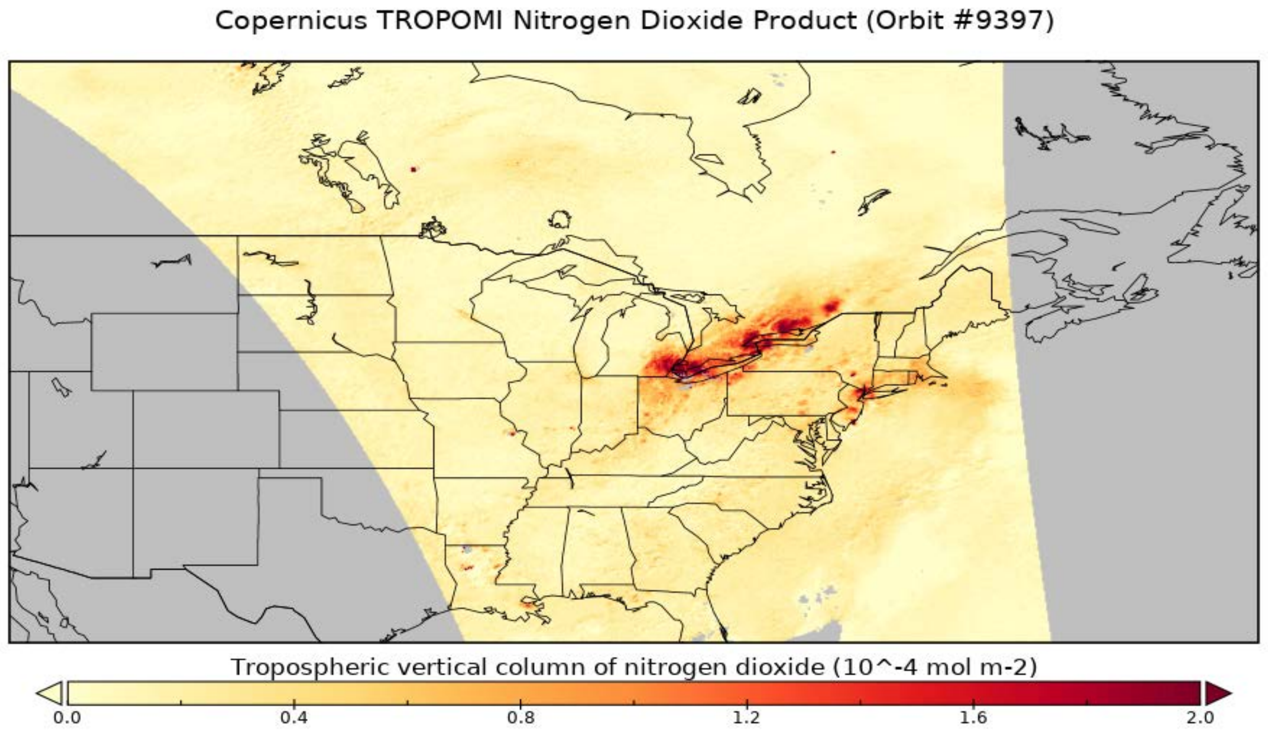
NASA Partner

- Motivation
  - Combining multiple sources of air quality data
  - NASA-funded project to support air quality managers
  - The advantages of uncertainty quantification
- Data Fusion Approach
  - Phase 1: model only
  - Phase 2: bring in satellite data
  - Phase 3: bring in historical ground monitor data
  - Phase 4: bring in near-real-time ground monitor data
  - Quantifying uncertainty and defining confidence intervals
- Case Study Results
  - Impacts of site-to-site differences
  - Impacts of different confidence intervals
  - Impacts of forecasting lead times
- Conclusions & Ongoing Work

regulatory monitoring

+ accurate
- expensive
? representativity

form the “backbone” of the monitoring system, but insufficient alone



satellite retrievals

+ global coverage
- low time resolution
- column-integrated

good coverage and frequency, but need ground validation

low-cost monitoring

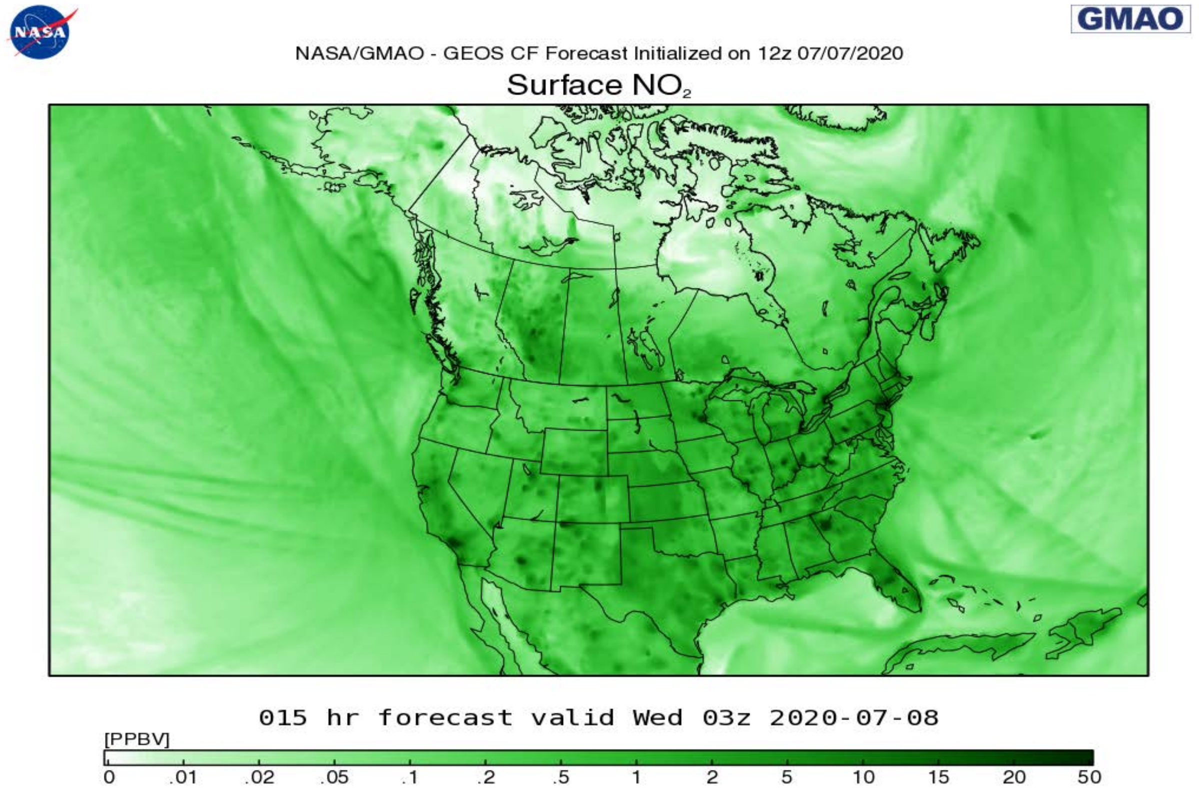
+ relatively inexpensive
+ dense/remote deployment
- greater noise and bias

calibration is an open issue, but network density might offset these shortcomings

simulation models

+ global coverage
+ forecasting
- limited resolution

provide complete maps and forecasts, but need validation

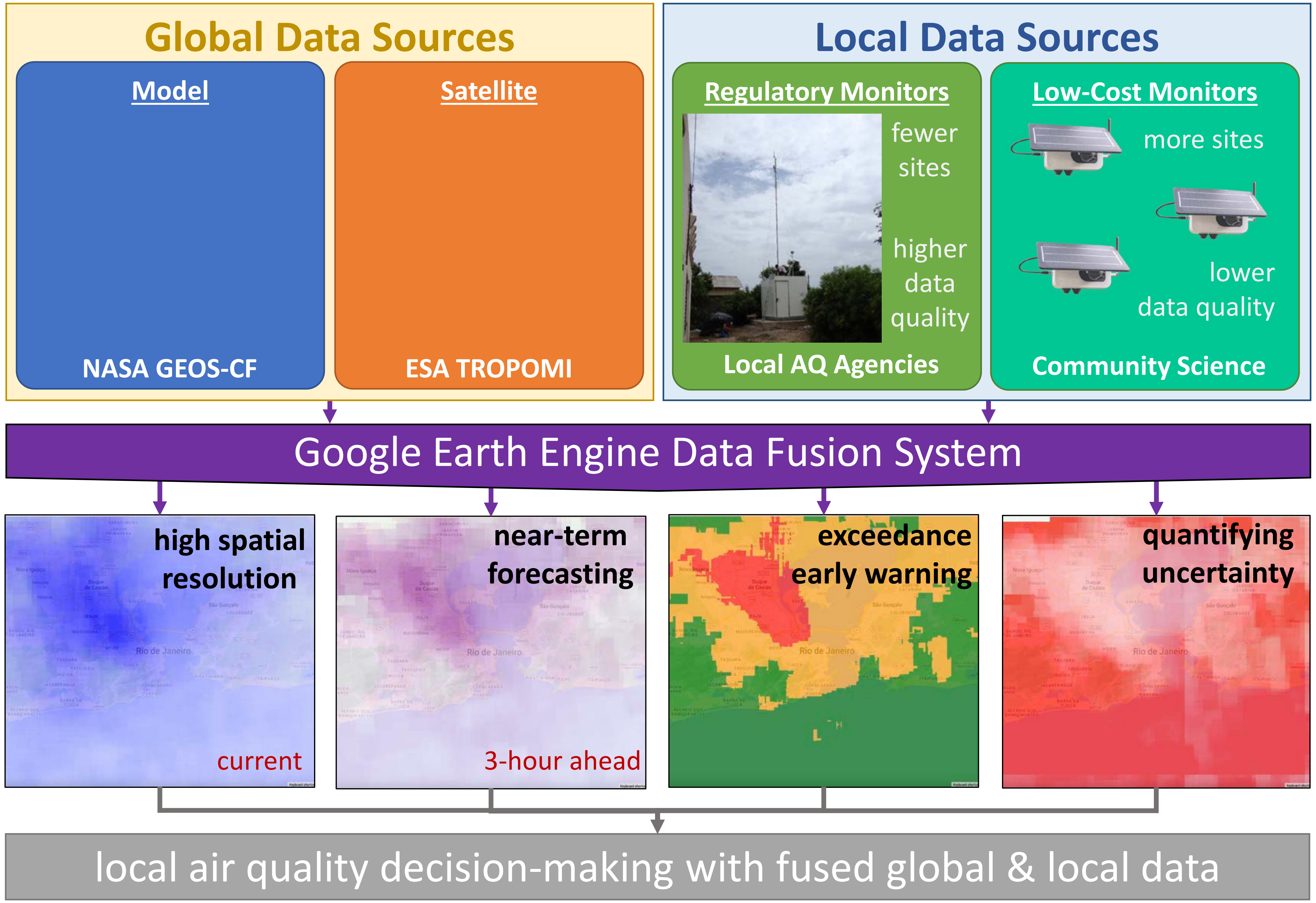


…integrate diverse **global** and **local** air quality data sources…

…using the cloud computing platform of **Google Earth Engine**…

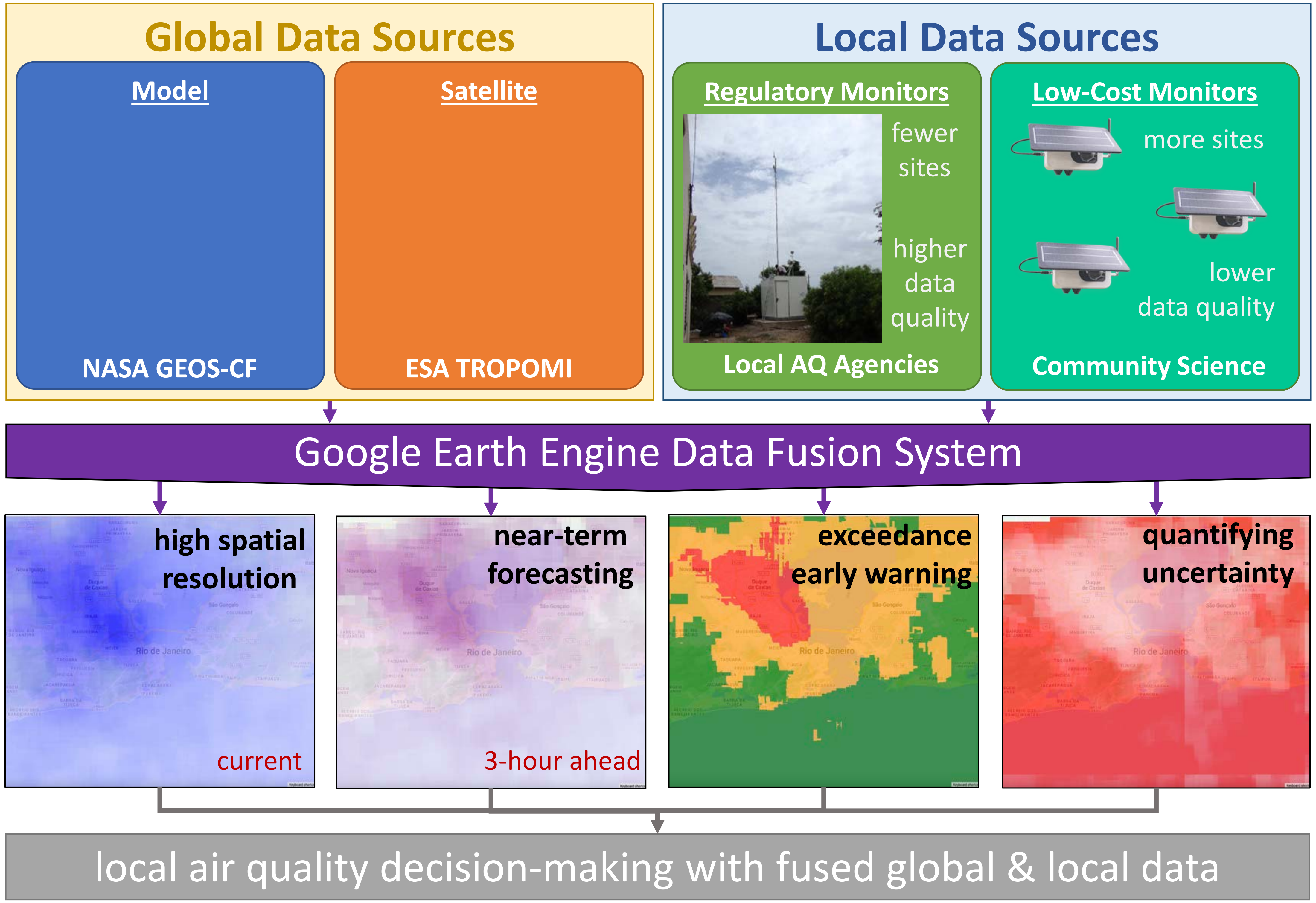
…to provide synthesized **estimates** and **forecasts** of air quality at a **local scale** but with a **global scope**…

…freely accessible by air quality managers worldwide, facilitating their **decision-making** processes.



Source: NASA GMAO Science Snapshot "Google Earth Engine Data Fusion Tool to support Air Quality Managers"

- **NASA GMAO:** basic algorithm development & refinement
- **Clarity:** low-cost sensor integration
- **Sonoma Technologies:** data fusion system implementation & user interface
- **WUSTL:** air quality data integration expertise (monthly/annual timescales)
- **Columbia LDEO:** experience training end-users in AQ data interpretation
- **UNEP:** integration with global users
  - Dakar, Senegal
  - Rio de Janeiro, Brazil
- **US EPA:** integration with US end-users
  - Oregon, Colorado, Idaho, Louisiana



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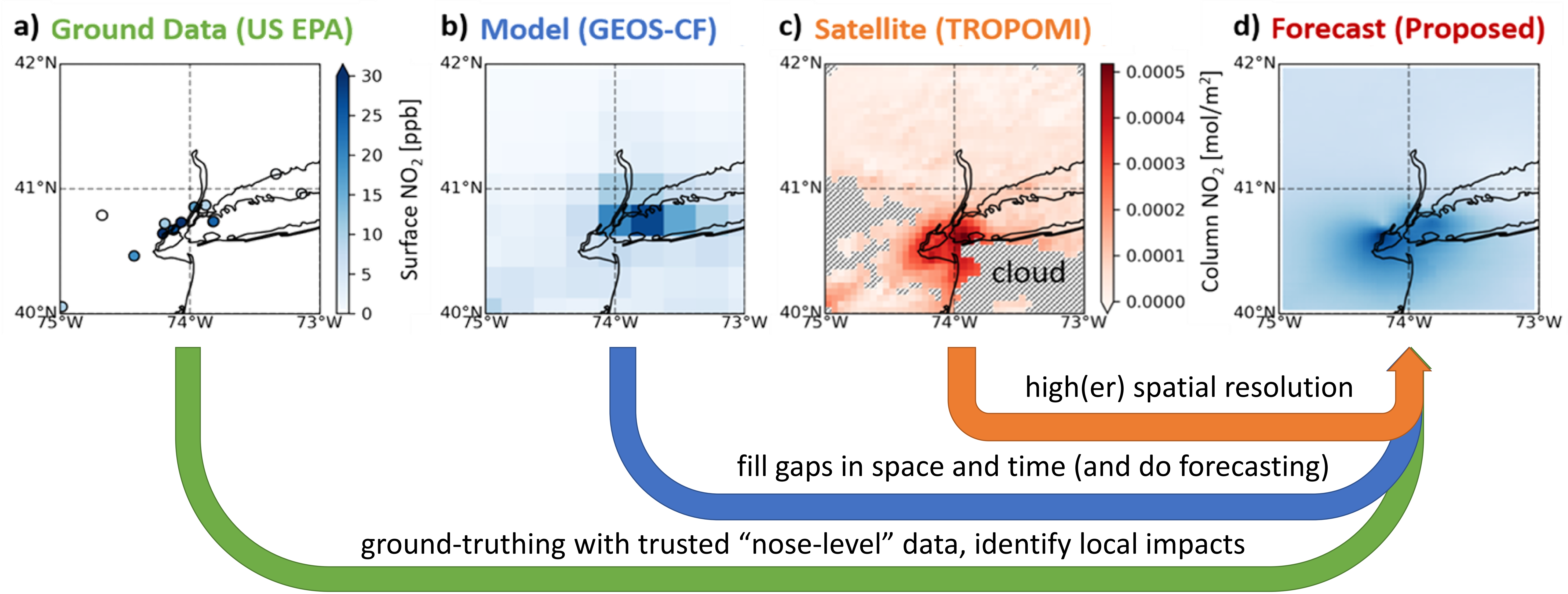


Source: Malings et al. (2021), “Sub-City Scale Hourly Air Quality Forecasting by Combining Models, Satellite Observations, and Ground Measurements” *Earth & Space Science.* DOI: 10.1029/2021EA001743

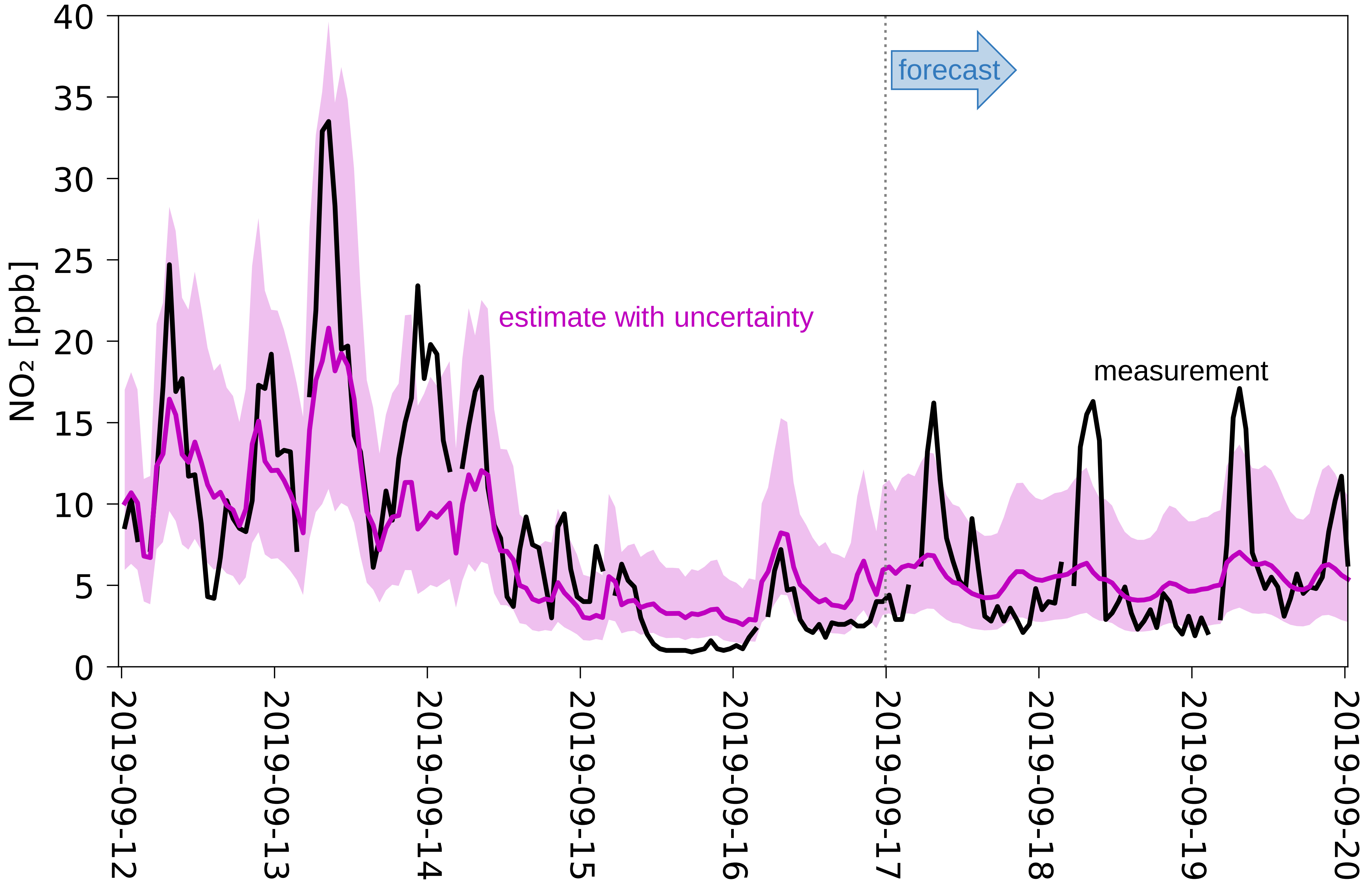
Provide a prior estimate of the relative confidence in a forecast

Convey probabilities of specific events, e.g., exceedance of standards

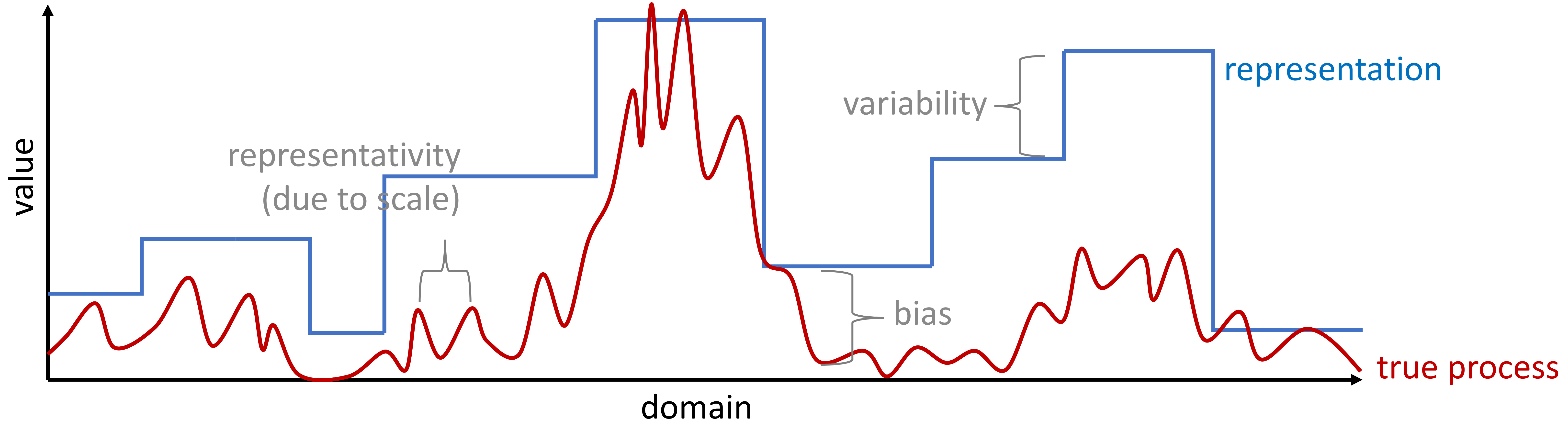
Identify a range of likely outcomes

Quantify the impacts of different data sources in reducing uncertainties

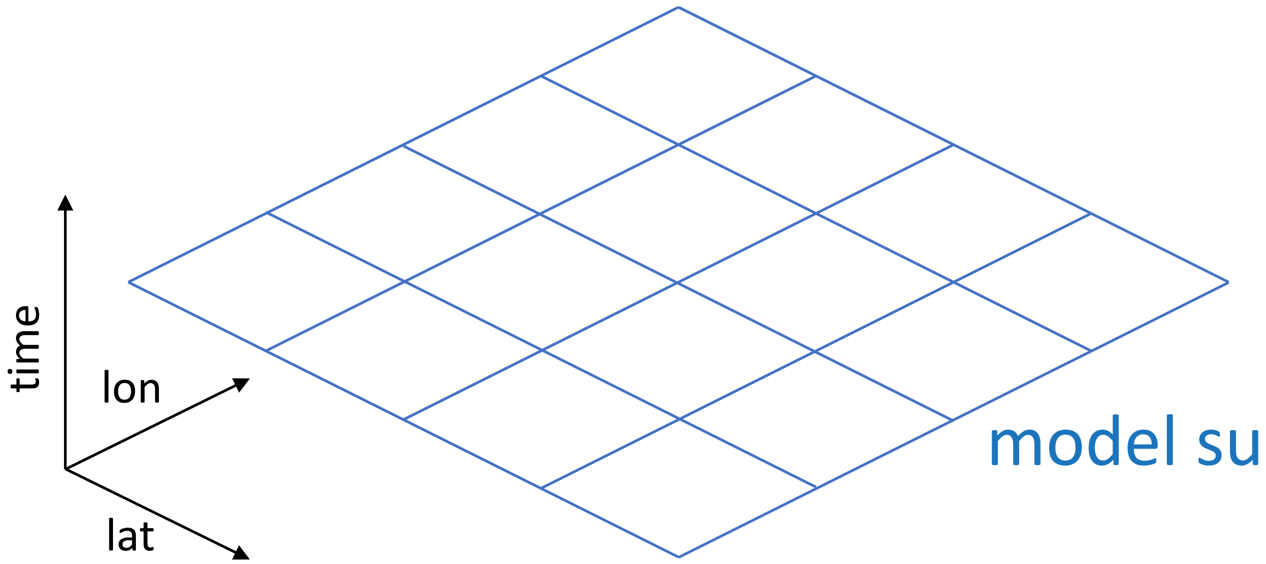
Identify the potential to reduce uncertainties through additional data collection



- Uncertainty – Overall characterization of potential errors in reproducing a process
  - Bias – Systematic errors in reproducing a process
  - Variability – Random errors in reproducing a process
  - Representativity – Errors in representing a process due to mismatched resolution



Phase	Estimate
1	forecast model (GEOS-CF)



model surface concentration $M(x,t)$

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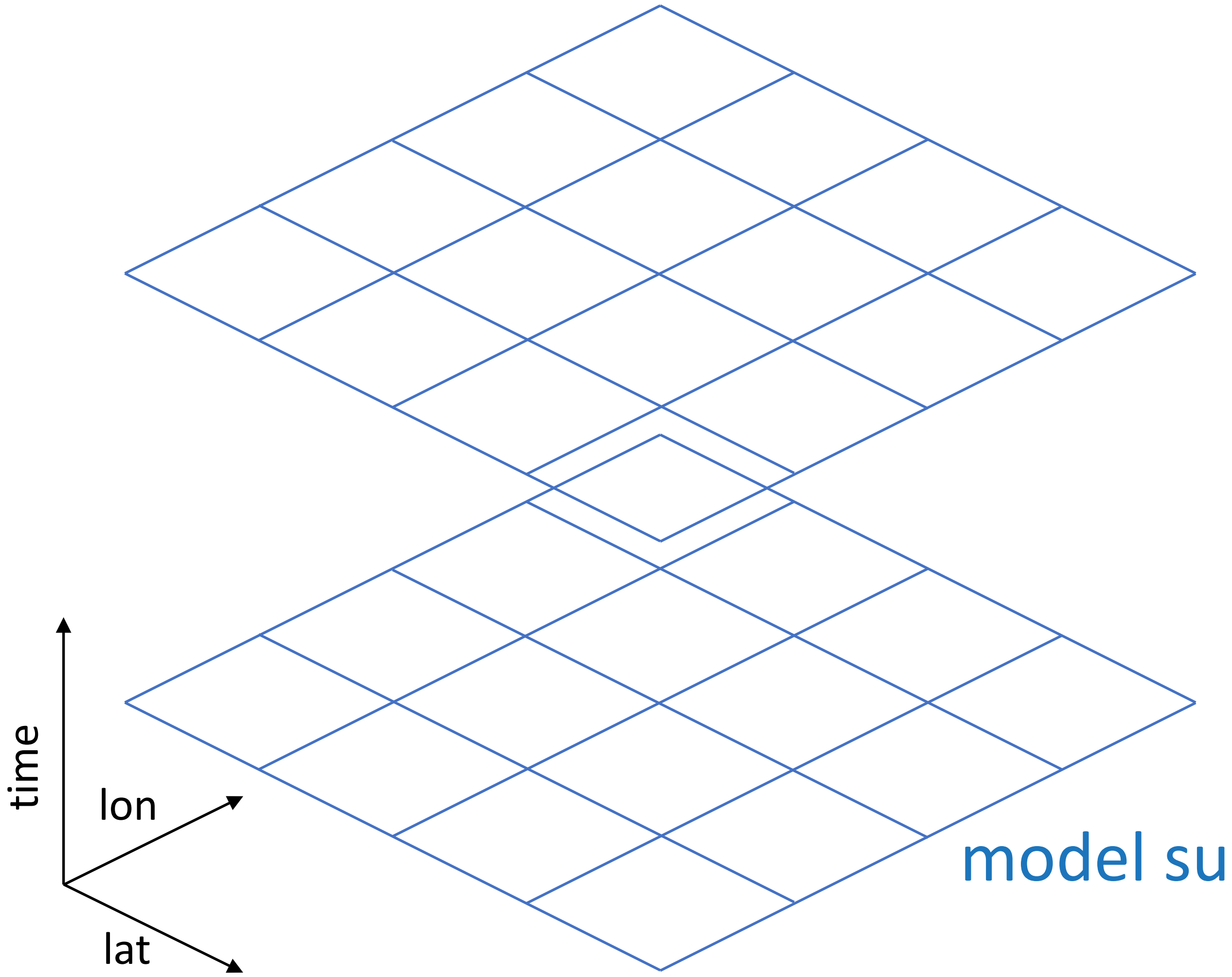

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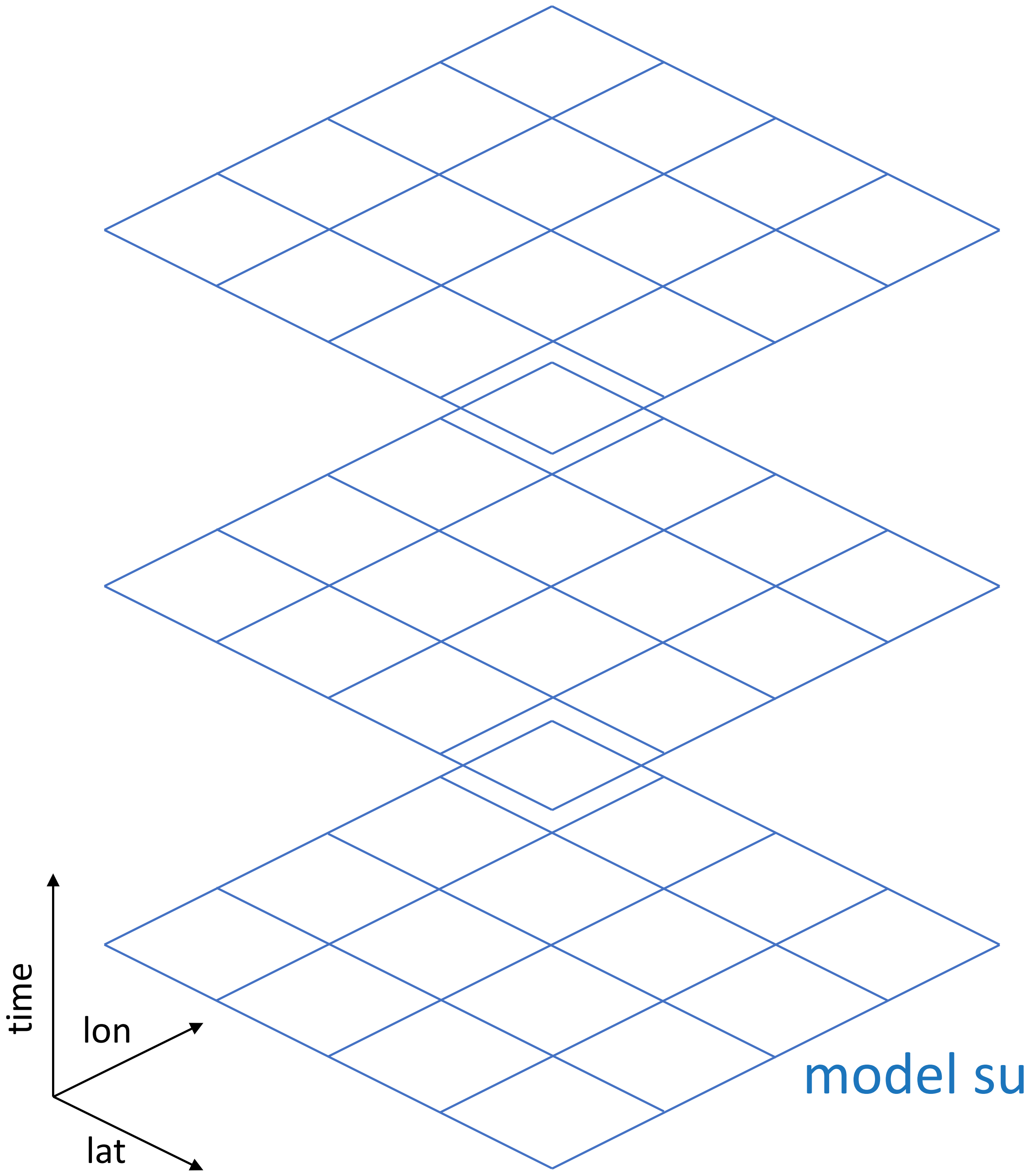
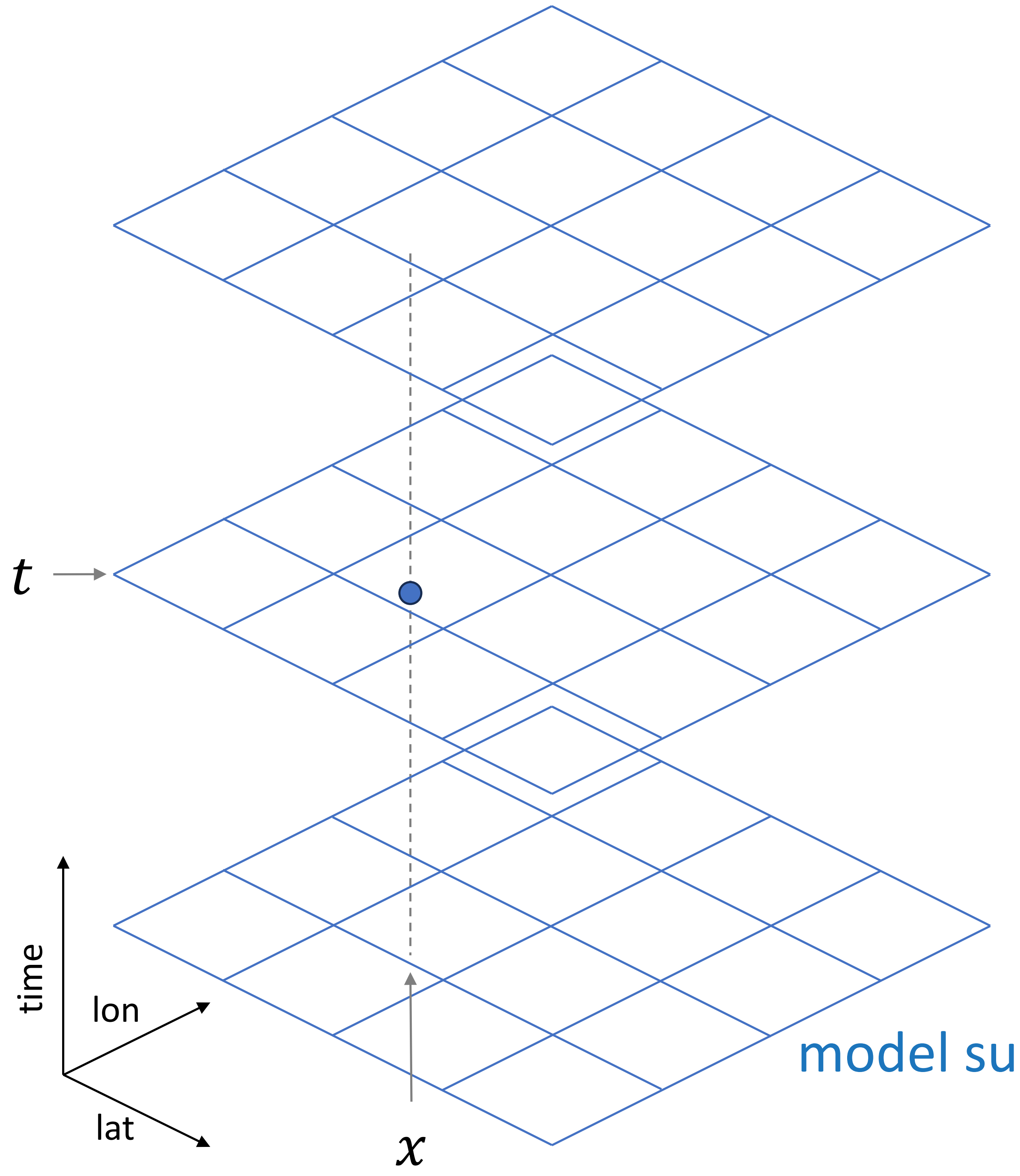
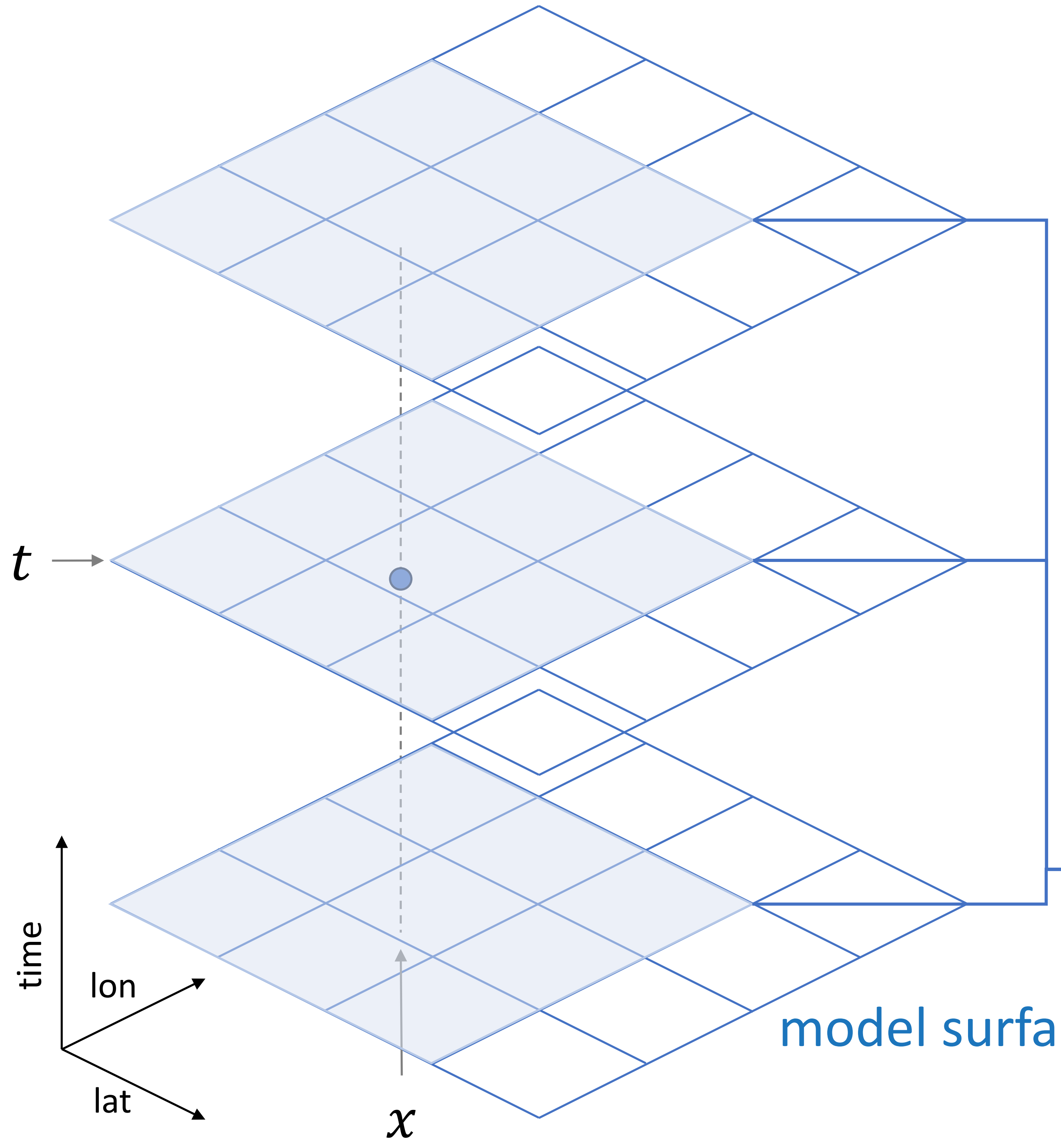


model surface concentration $M(x,t)$

Phase	Estimate
1	forecast model (GEOS-CF)

$$F_1(x,t) = M(x,t)$$





Phase	Estimate	Uncertainty
1	forecast model (GEOS-CF)	cell-to-cell variability of model

$$F_1(x,t) = M(x,t)$$

data fusion uncertainty (variance) at phase 1

$$V_1(x,t) = V_{F1}(x,t,\tau)$$

uncertainty due to forecasting by τ ahead (ignore this for now…)

$$+V_M(x,t)$$

uncertainty due to model internal variability

$$+V_{B1}(x,t)$$

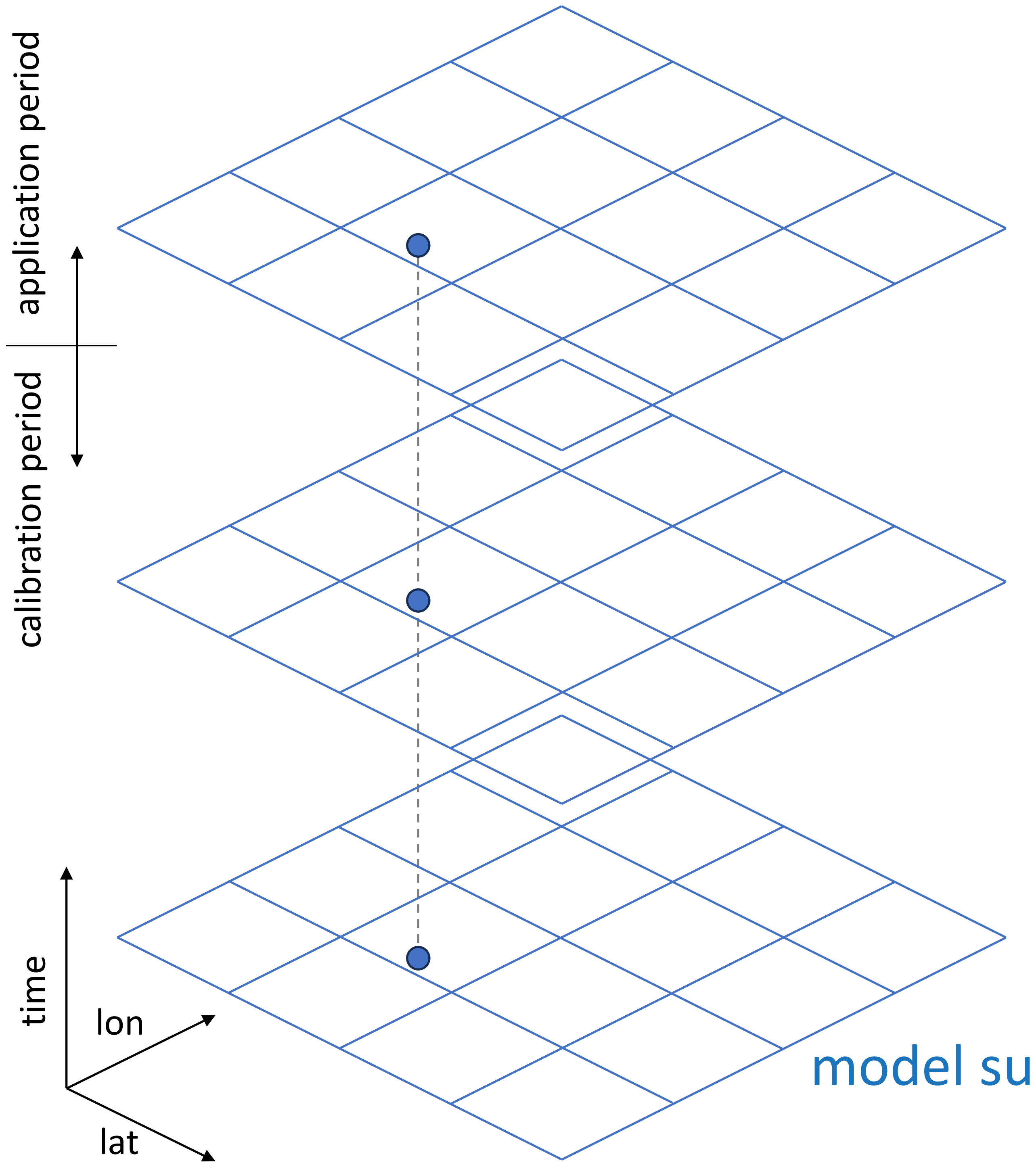
uncertainty due to model bias

$$+\,V_{R1}(x,t)$$

uncertainty due to spatial representativity (model scale)

$$V_M(x,t) \approx \mathbb{E}_{x' \in X_n(x), t' \in T_n(t)} \left[\left(M(x',t') - M(x,t) \right)^2 \right]$$

model surface concentration $M(x,t)$



Phase	Estimate	Uncertainty
1	forecast model (GEOS-CF)	cell-to-cell variability of model
2		

model surface concentration $M(x, t)$

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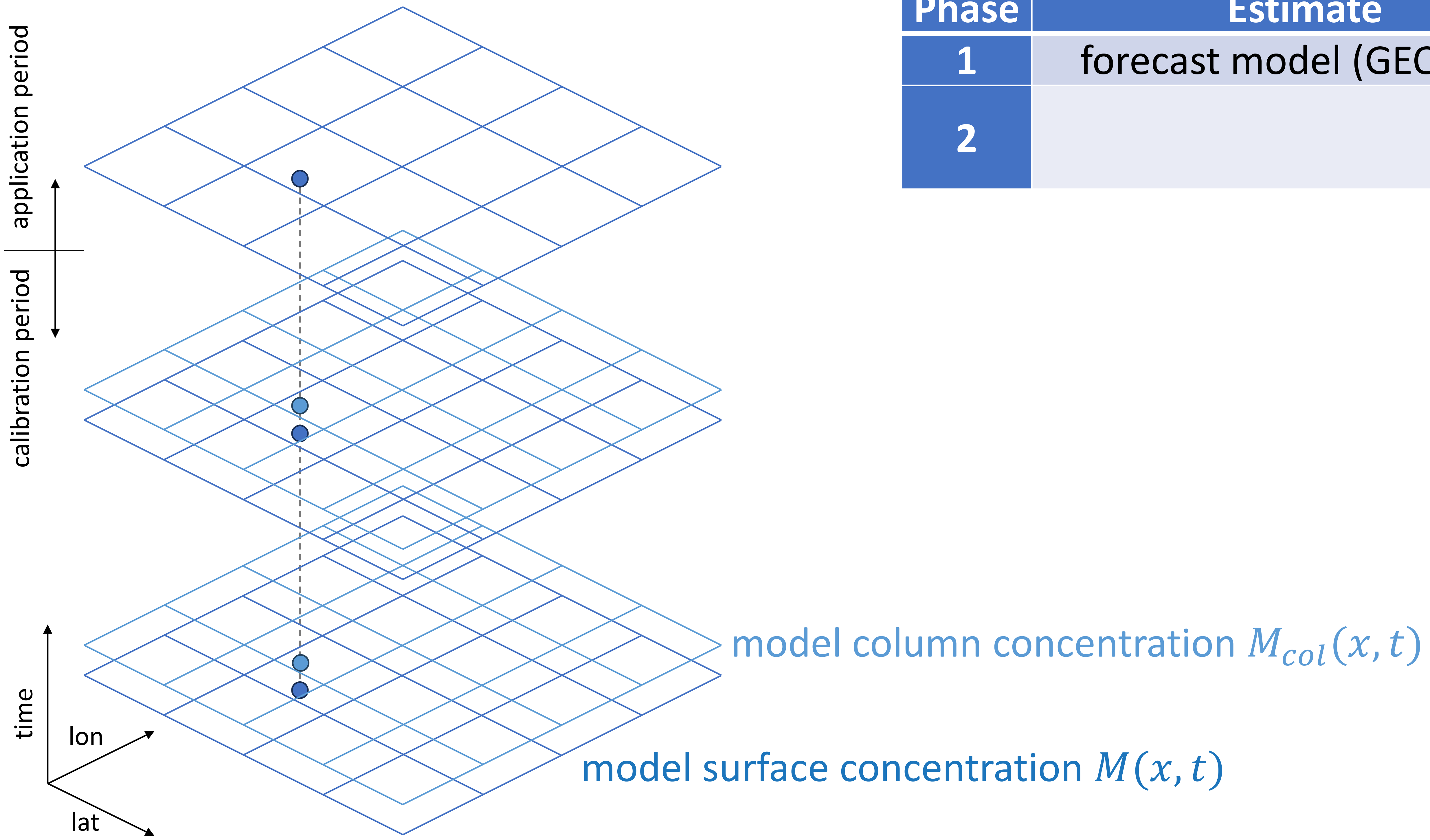

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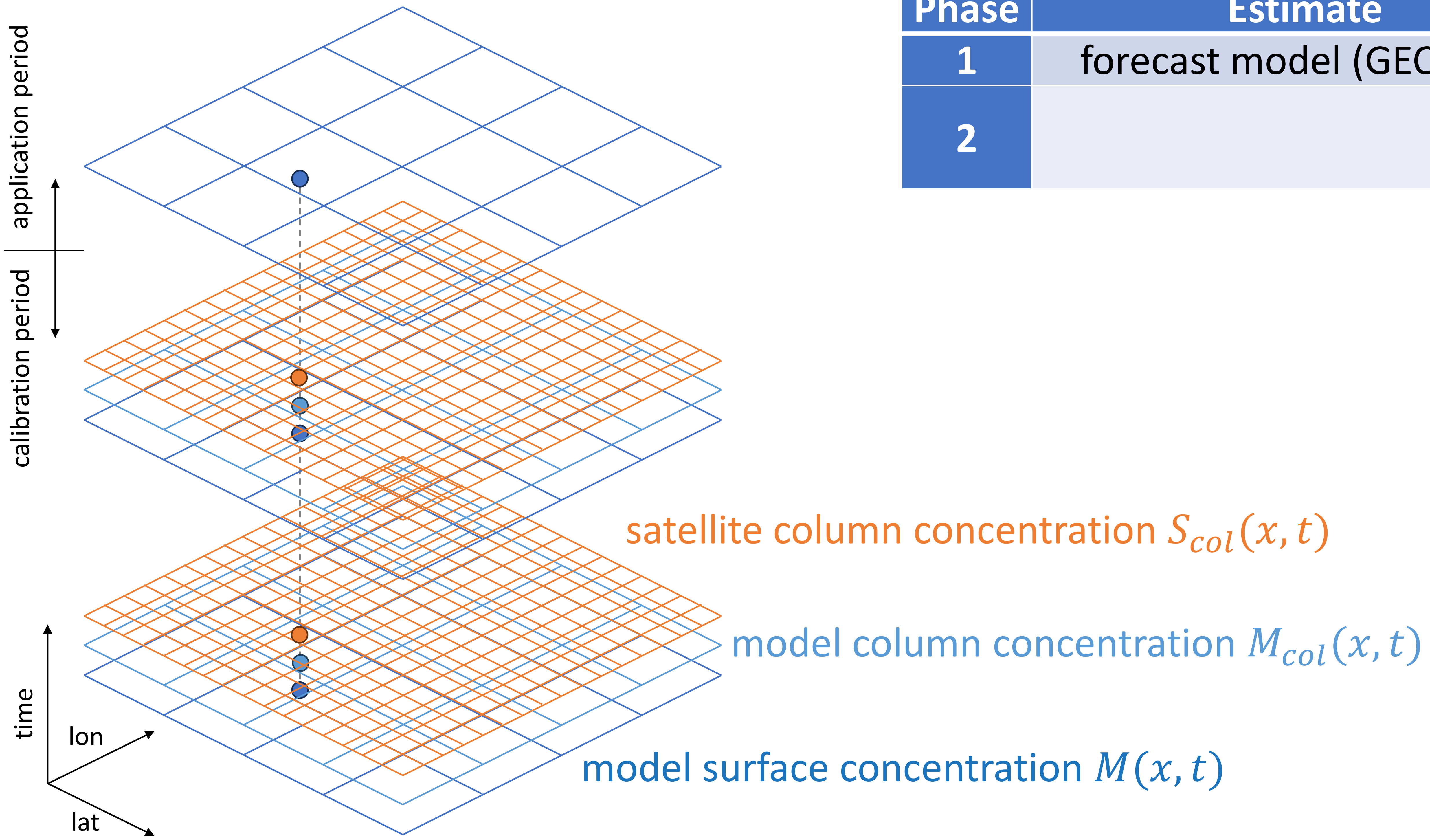
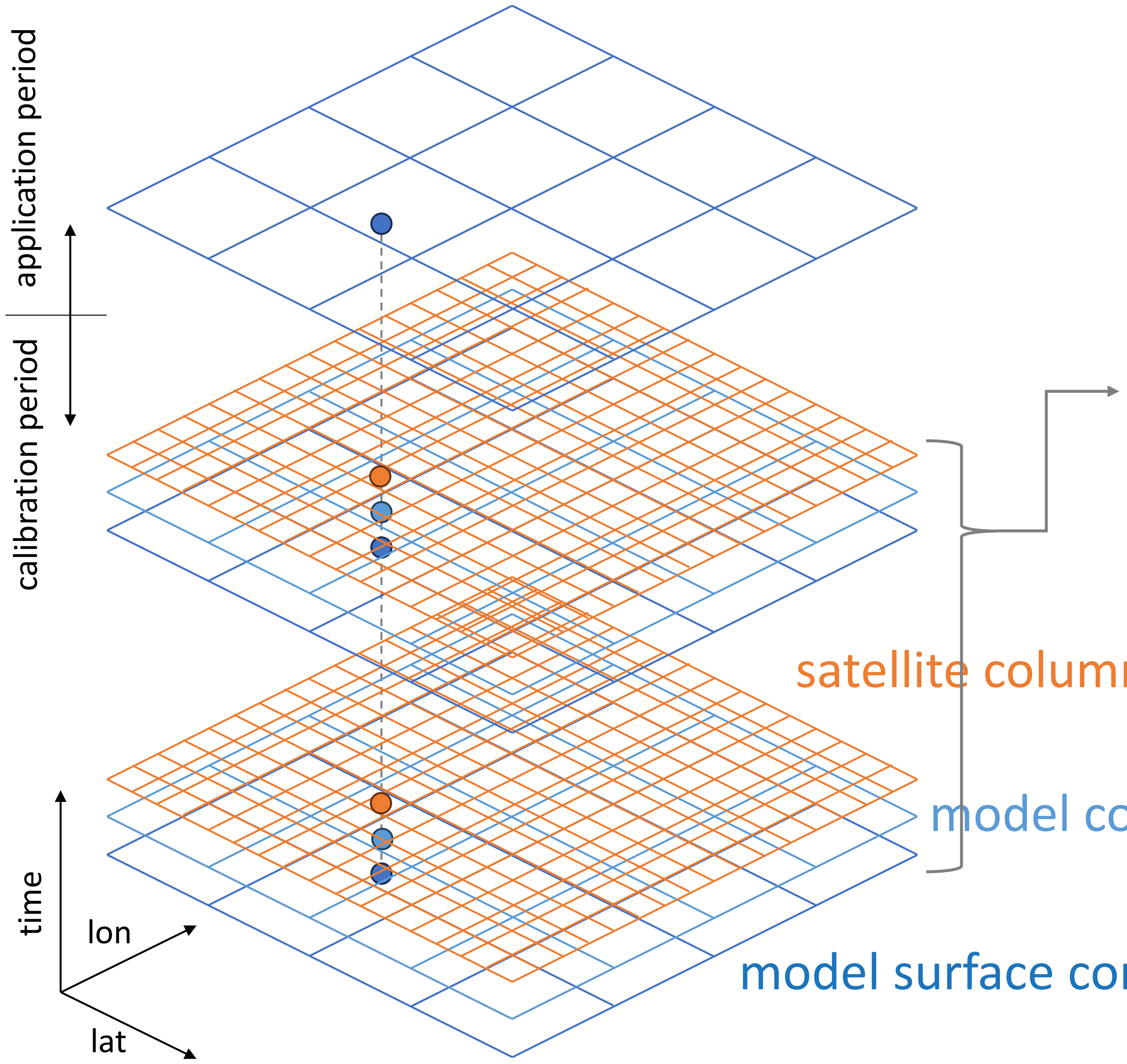


Phase	Estimate	Uncertainty
1	forecast model (GEOS-CF)	cell-to-cell variability of model
2	satellite (TROPOMI) informs sub-model-grid variability	



$$F_2(x,t) = F_1(x,t) + D(x,t)$$

$$D(x,t) = \mathbb{E}_{t' \in T_{c,overpass}(t)}\left[\left(S_{col}(x,t') - M_{col}(x,t')\right)\phi(x,t')\,\psi(x,t,t')\right]$$

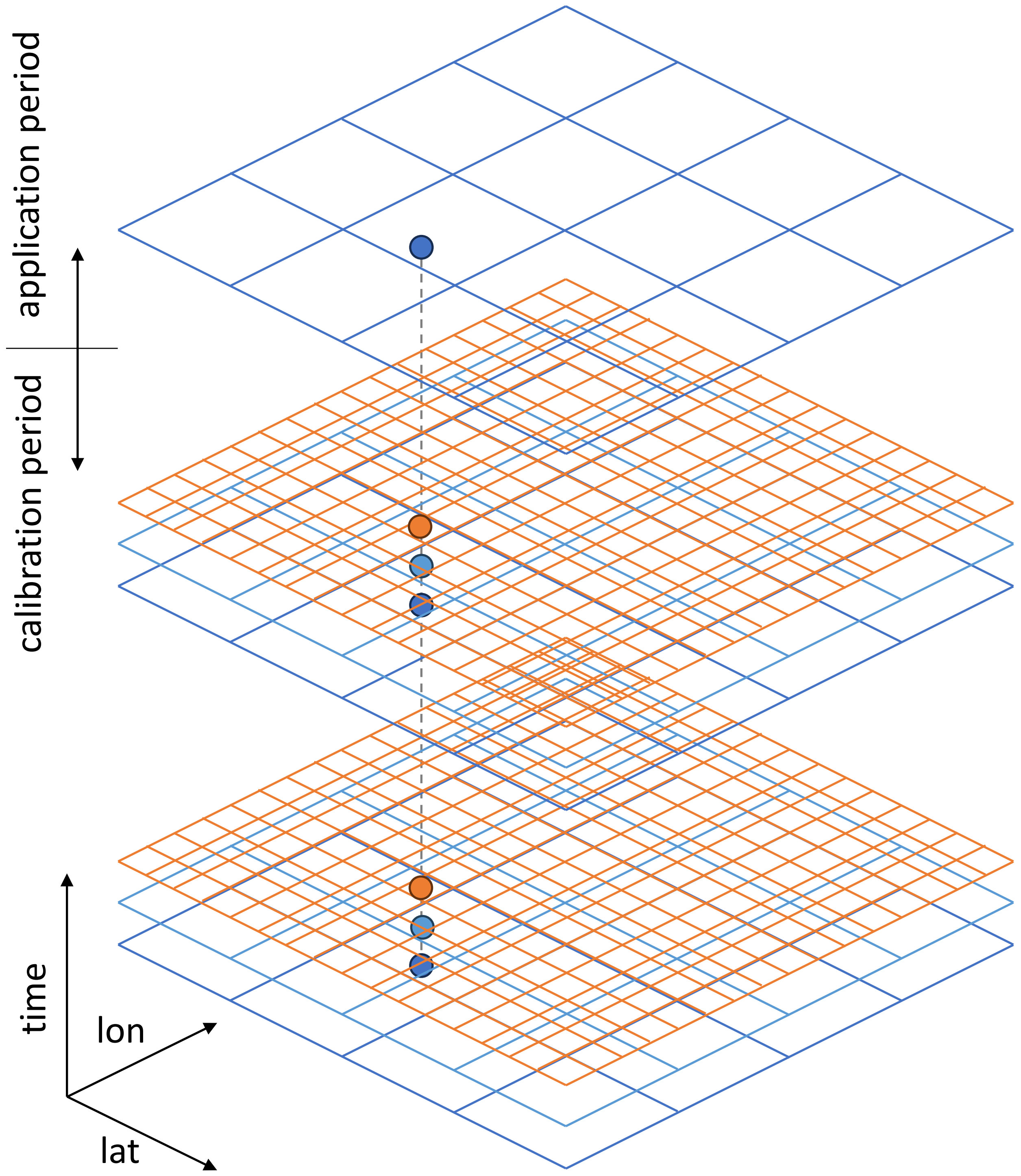
satellite column concentration $S_{col}(x,t)$

model column concentration $M_{col}(x,t)$

model surface concentration $M(x,t)$

$$\phi(x,t') \approx \frac{M(x,t')}{M_{col}(x,t')}$$ surface-to-column relationship

$$\psi(x,t,t') \approx \frac{M(x,t)}{M(x,t')}$$ target-time-to-overpass-time relationship



Phase	Estimate	Uncertainty
1	forecast model (GEOS-CF)	cell-to-cell variability of model
2	satellite (TROPOMI) informs sub-model-grid variability	satellite-to-model and surface-to-column ratios vary over time

$V_2(x,t) = V_{F2}(x,t,\tau)$ ⟵ uncertainty due to forecasting by τ ahead

$+V_M(x,t)$ ⟵ uncertainty due to model internal variability

$+V_D(x,t)$ ⟵ uncertainty in satellite-to-model differences

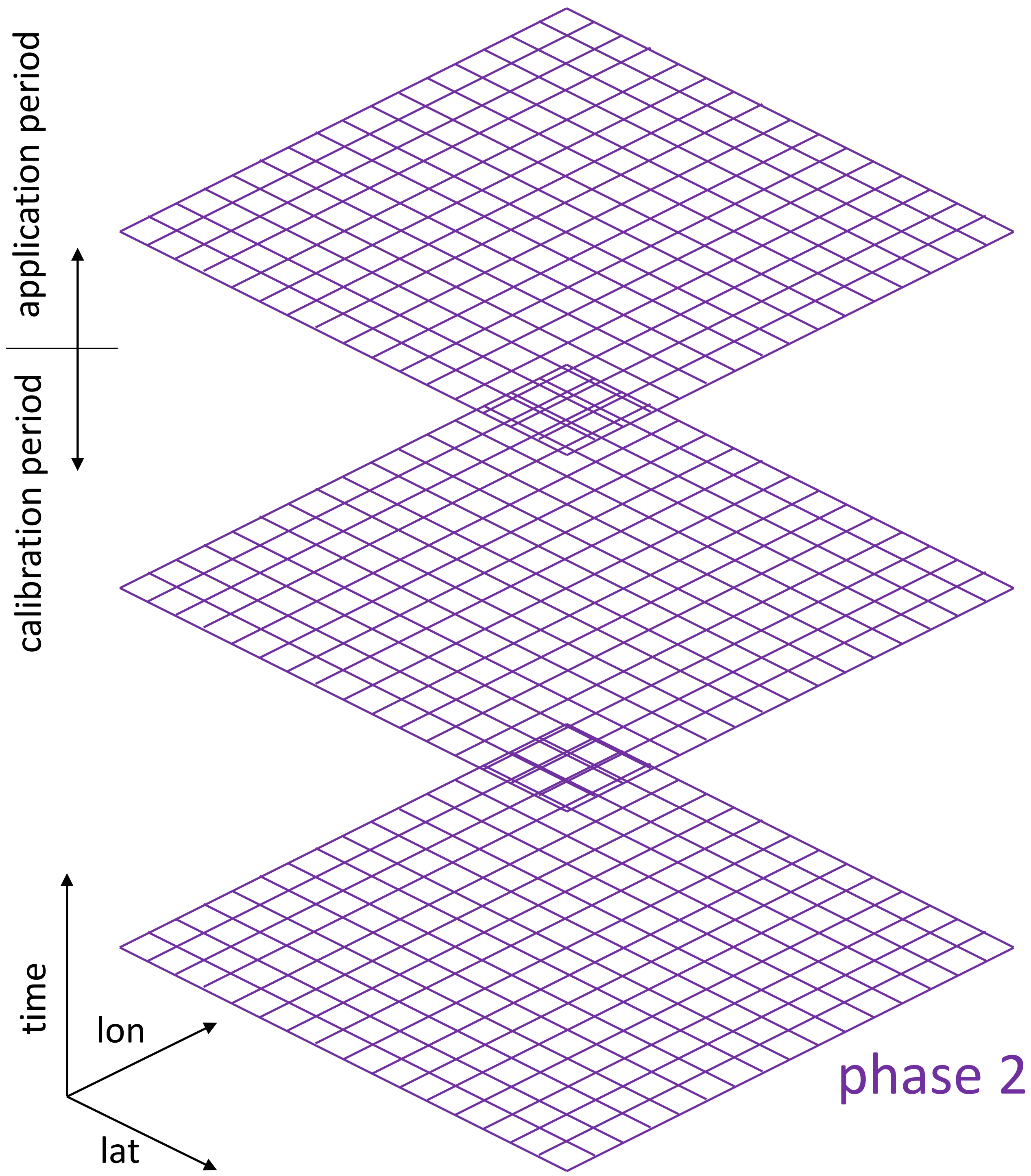
$+2V_{MD}(x,t)$ ⟵ co-variance of satellite-to-model differences with model outputs

$+V_{B2}(x,t)$ ⟵ uncertainty due to model & satellite bias

$+V_{R2}(x,t)$ ⟵ uncertainty due to spatial representativity (satellite scale)

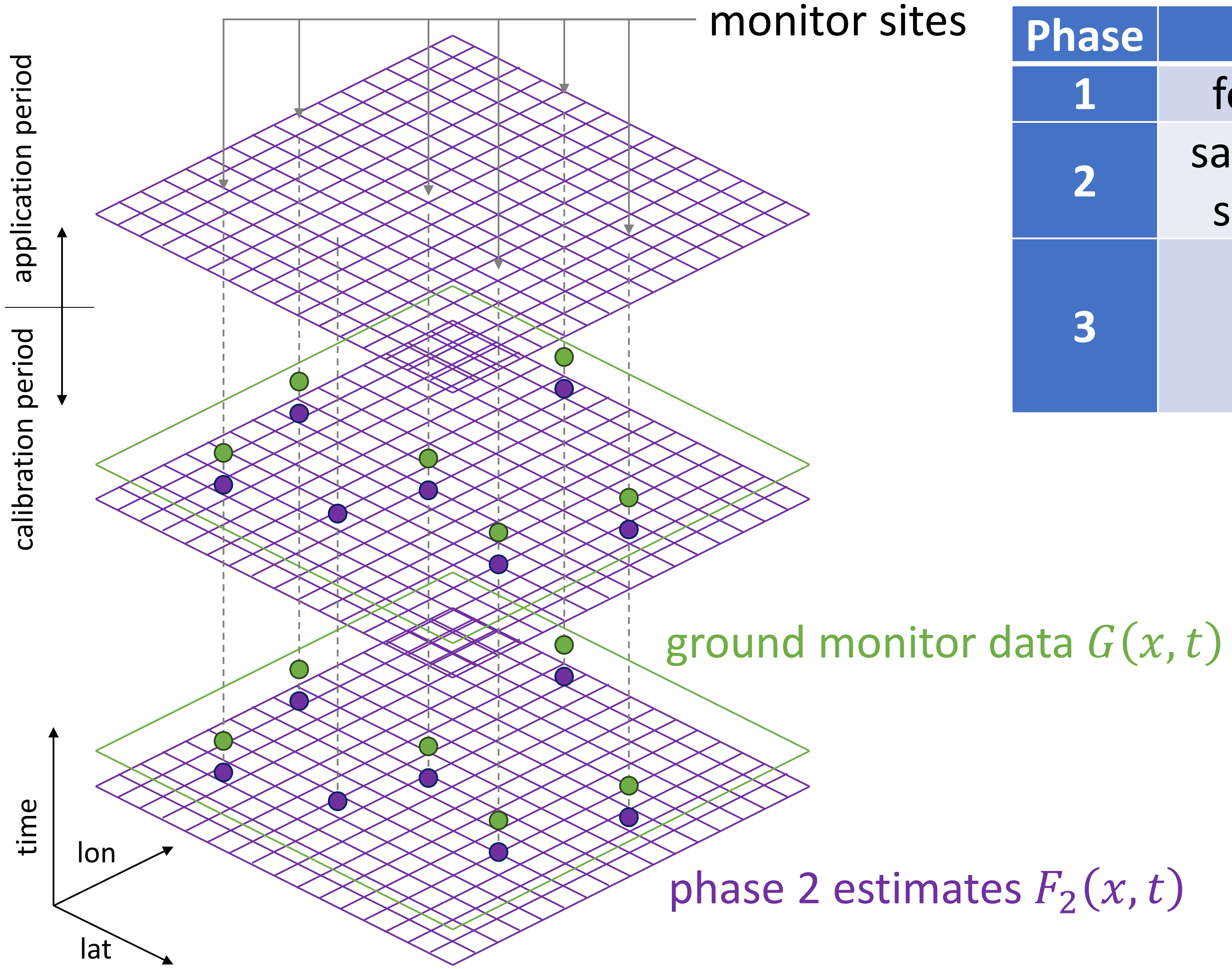
$$V_D(x,t) \approx \mathbb{V}_{t' \in T_{c,overpass}(t)}\left[\left(S_{col}(x,t') - M_{col}(x,t')\right)\phi(x,t')\,\psi(x,t,t')\right]$$

$$V_{MD}(x,t) \approx \mathbb{E}_{x' \in X_n(x), t' \in T_n(t)}\left[\left(M(x',t') - M(x,t)\right)\left(D(x',t') - D(x,t)\right)\right]$$



Phase	Estimate	Uncertainty
1	forecast model (GEOS-CF)	cell-to-cell variability of model
2	satellite (TROPOMI) informs sub-model-grid variability	satellite-to-model and surface-to-column ratios vary over time
3		

phase 2 estimates $F_2(x, t)$



Phase	Estimate	Uncertainty
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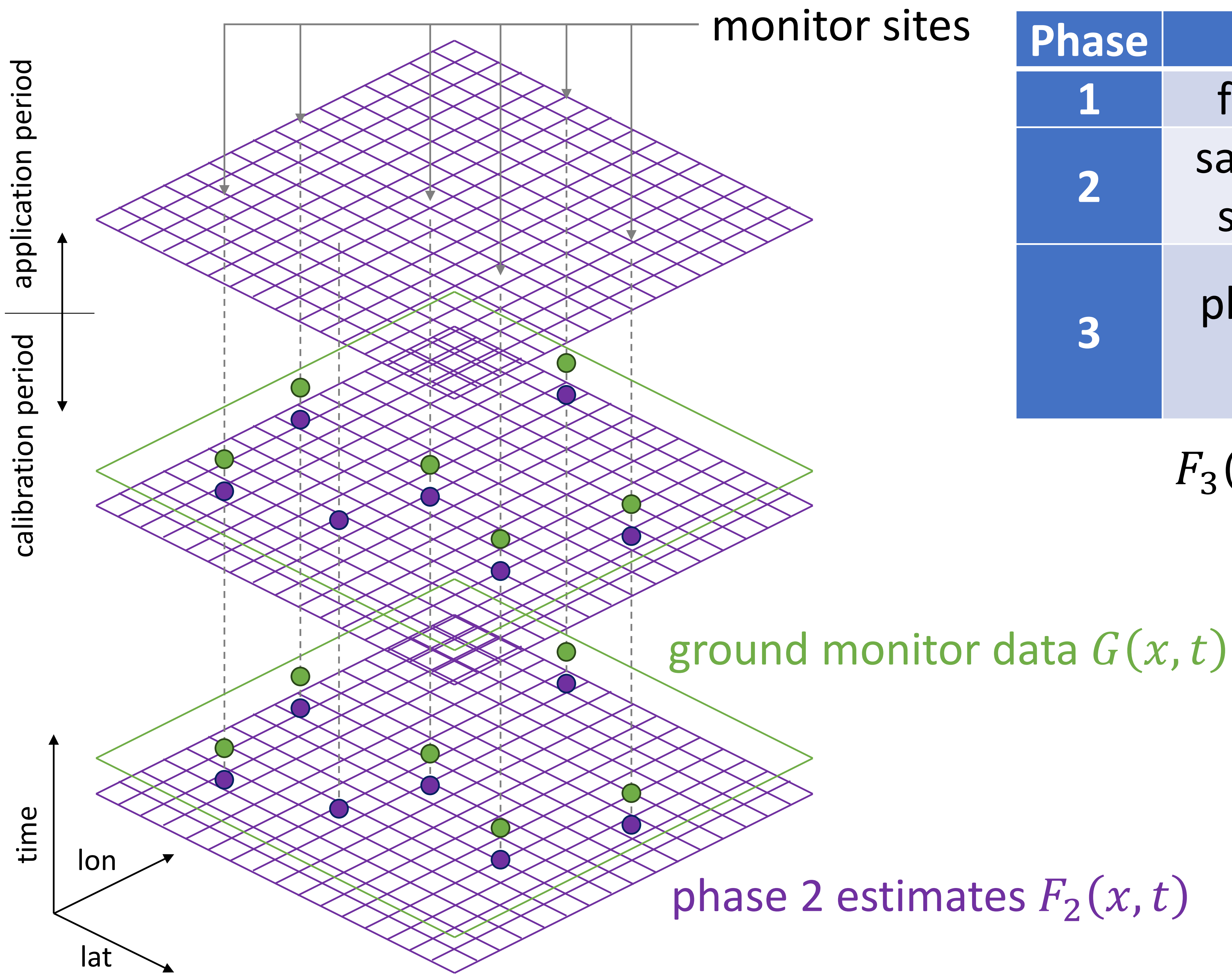
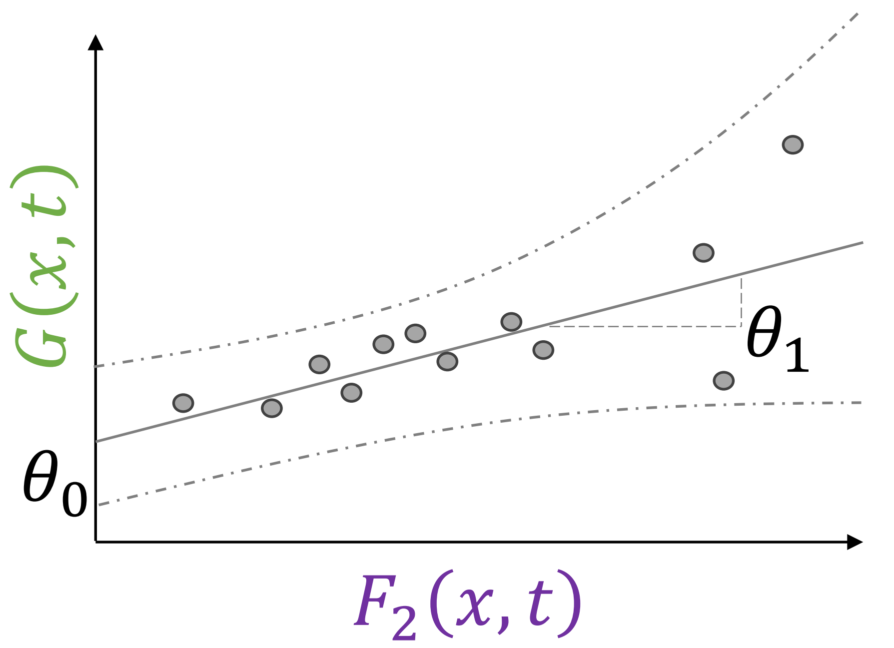
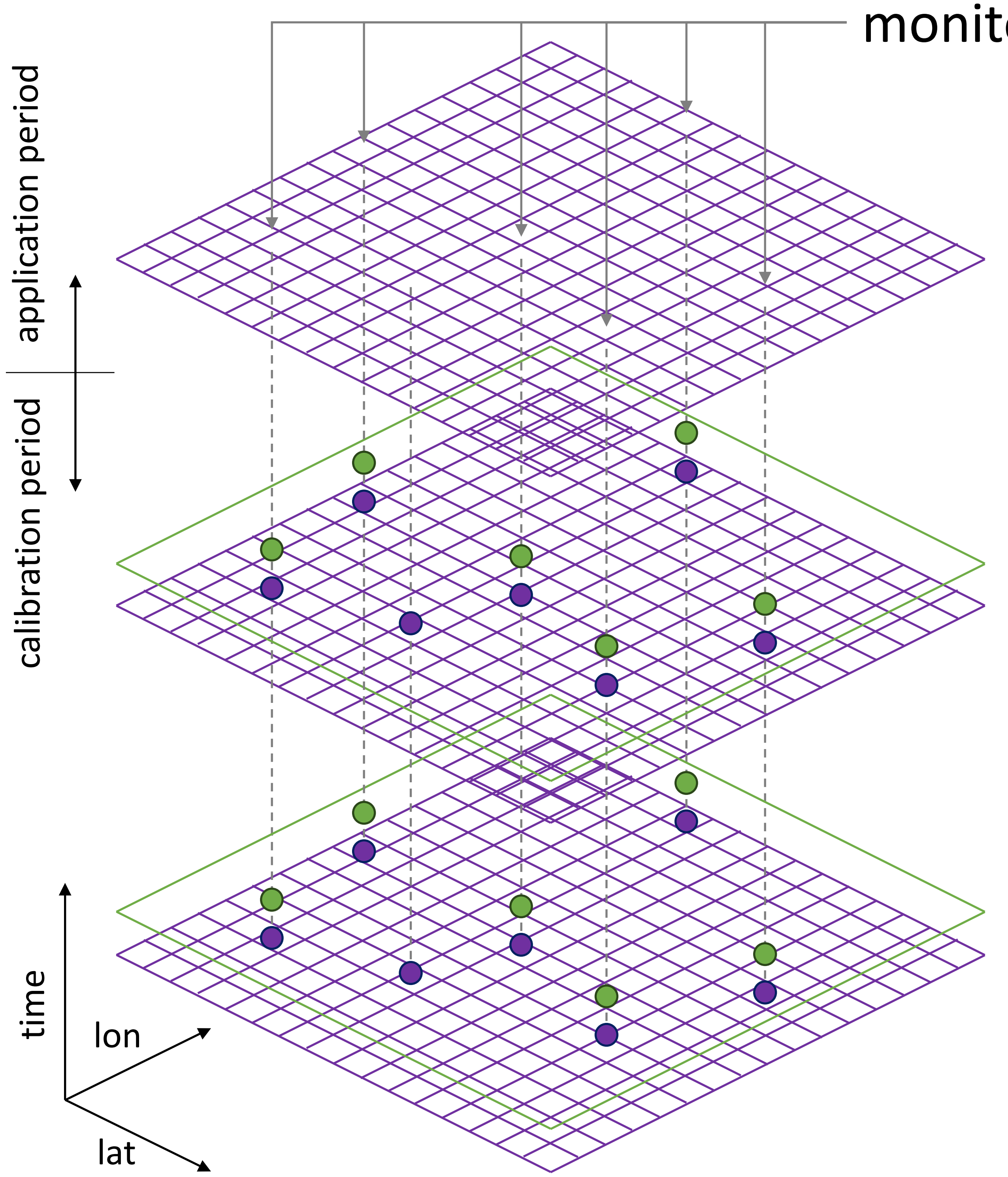


Phase	Estimate	Uncertainty
1	forecast model (GEOS-CF)	cell-to-cell variability of model
2	satellite (TROPOMI) informs sub-model-grid variability	satellite-to-model and surface-to-column ratios vary over time
3	phase 2 corrected to match surface monitor data	

$$F_3(x,t) = \theta_1 F_2(x,t) + \theta_0$$

$$\theta_0, \theta_1 = \mathbb{LR}_{t' \in T_c(t), x' \in X_c(x)}[G(x',t') \sim F_2(x',t')]$$





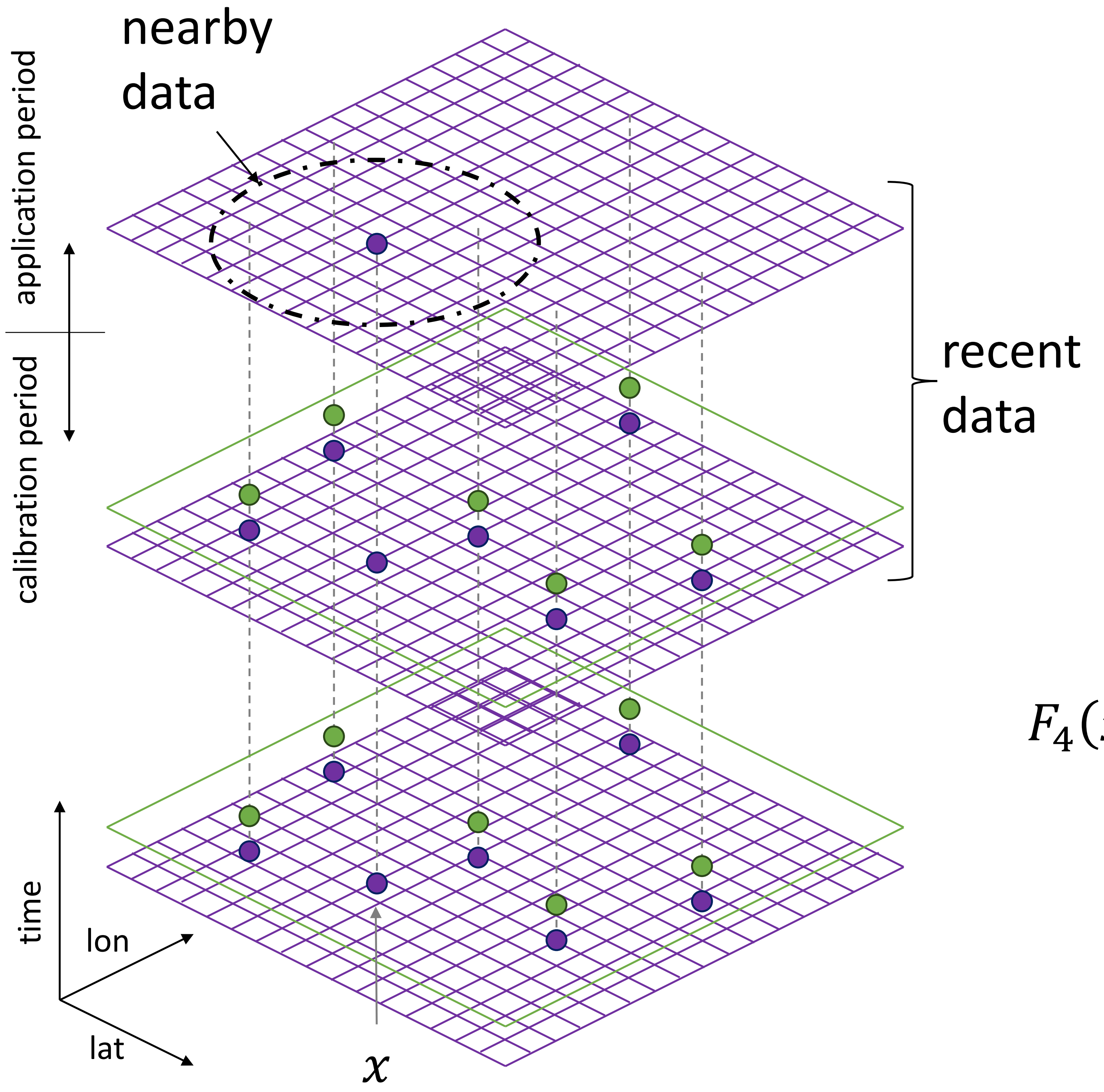
Phase	Estimate	Uncertainty
1	forecast model (GEOS-CF)	cell-to-cell variability of model
2	satellite (TROPOMI) informs sub-model-grid variability	satellite-to-model and surface-to-column ratios vary over time
3	phase 2 corrected to match surface monitor data	uncertain regression parameters between phase 2 output and surface monitor data

$V_3(x,t) = V_{F3}(x,t,\tau)$ ← uncertainty due to forecasting by τ ahead

$+\theta_1^2[V_M(x,t) + V_D(x,t) + 2V_{MD}(x,t)]$ ← rescaled from phase 2

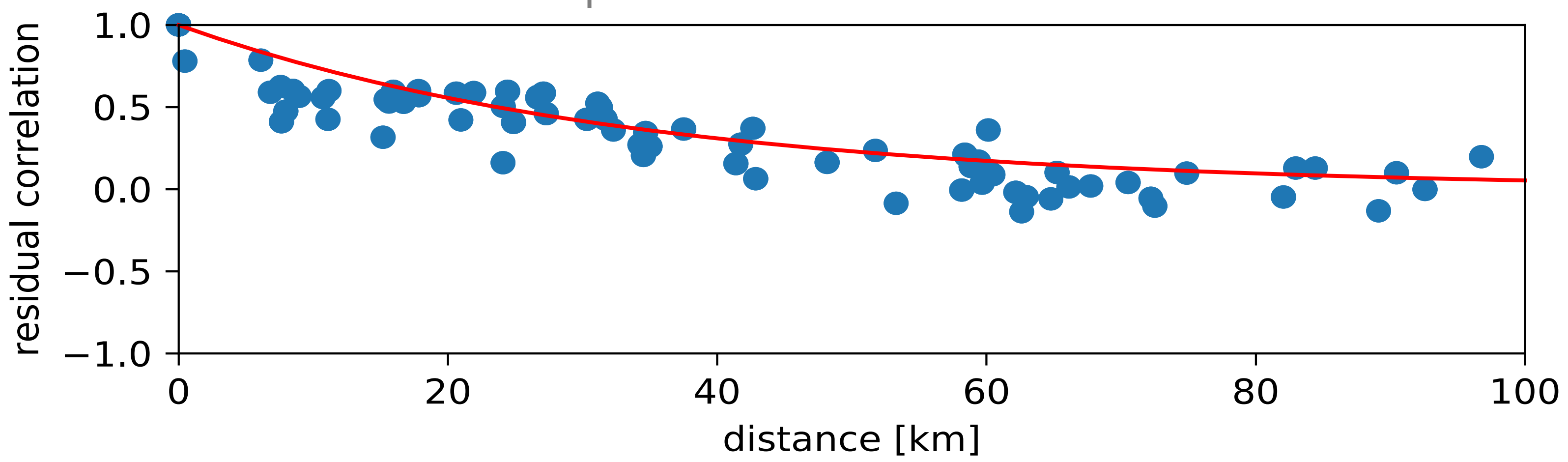
$$\left.\begin{aligned} &+\mathrm{var}[\theta_1]F_2(x,t)^2 \\ &+2\mathrm{cov}[\theta_0,\theta_1]F_2(x,t) \\ &+\mathrm{var}[\theta_0] \\ &+\sigma_{residual}^2 \end{aligned}\right\}$$

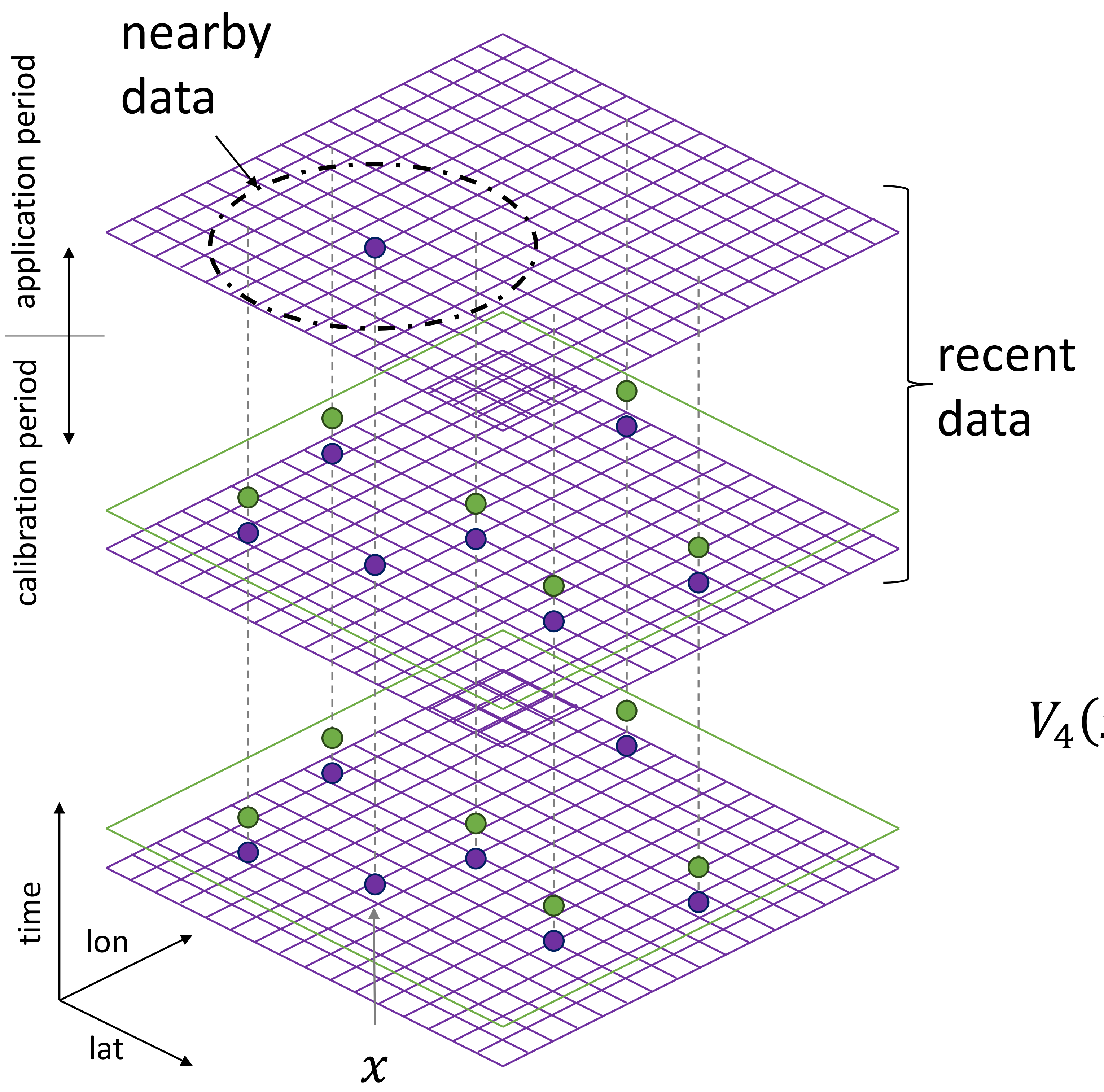
variance and co-variance of regression parameters as well as regression residual are known



Phase	Estimate	Uncertainty
1	forecast model (GEOS-CF)	cell-to-cell variability of model
2	satellite (TROPOMI) informs sub-model-grid variability	satellite-to-model and surface-to-column ratios vary over time
3	phase 2 corrected to match surface monitor data	uncertain regression parameters between phase 2 output and surface monitor data
4	update phase 3 based on recent surface monitor data	

$$F_4(x,t) = F_3(x,t) + \sum_{x' \in X_n(x), t' \in T_n(t)} K(x,x',t,t') \left[G(x',t') - F_3(x',t')\right]$$



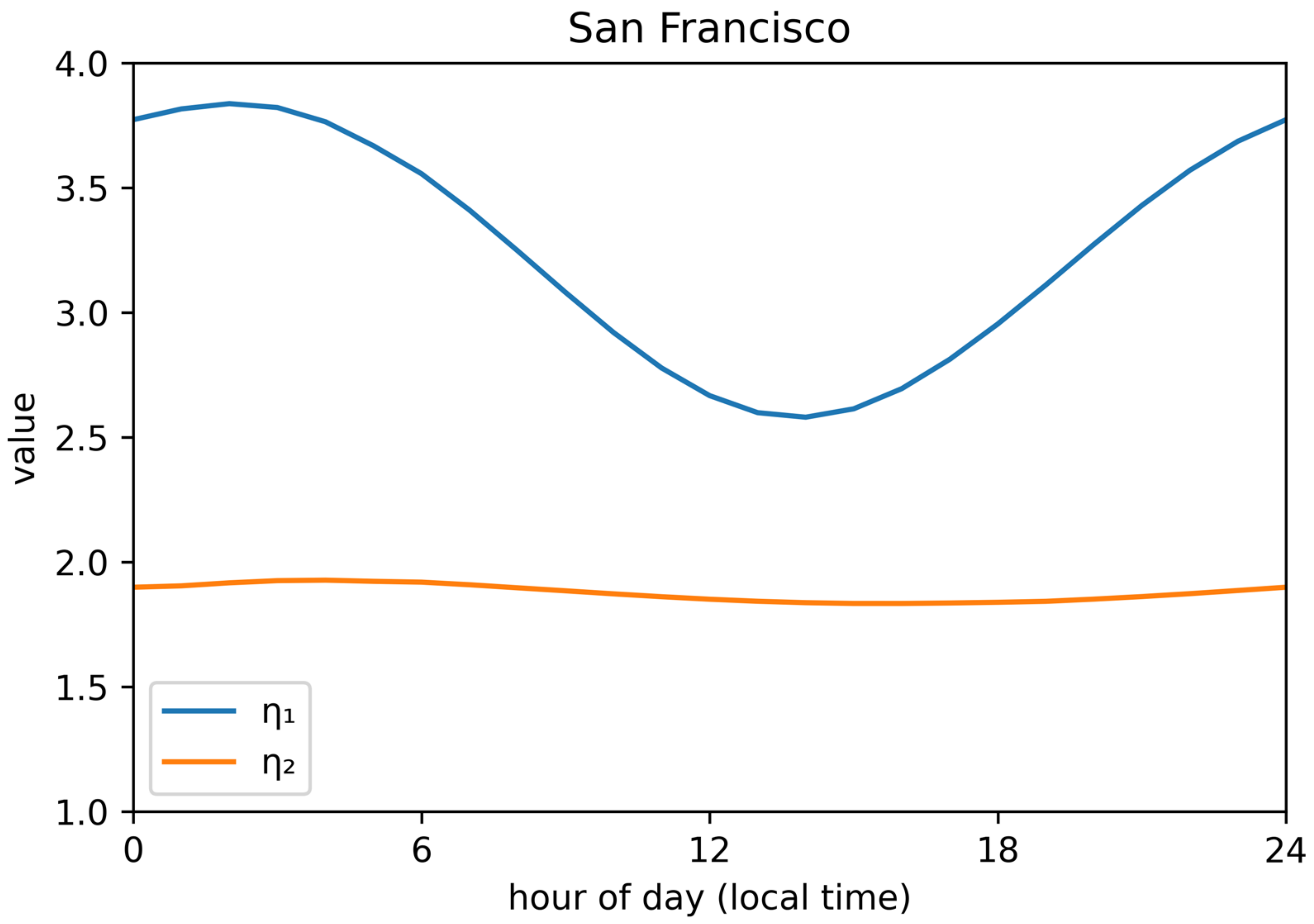


Phase	Estimate	Uncertainty
1	forecast model (GEOS-CF)	cell-to-cell variability of model
2	satellite (TROPOMI) informs sub-model-grid variability	satellite-to-model and surface-to-column ratios vary over time
3	phase 2 corrected to match surface monitor data	uncertain regression parameters between phase 2 output and surface monitor data
4	update phase 3 based on recent surface monitor data	uncertainty reduction via updating with nearby & recent data (kriging)

$$V_4(x,t) = V_3(x,t) - \sum_{x' \in X_n(x), t' \in T_n(t)} K(x,x',t,t') \operatorname{cov}[G(x',t'), F_3(x',t')]$$

<table>
<tr><th rowspan="2" colspan="2">Phase</th><th rowspan="2">Estimate</th><th colspan="4">Uncertainty</th></tr>
<tr><th>Bias</th><th>Model Variability</th><th>Model Scale Spatial Representativity</th><th>Satellite Scale Spatial Representativity</th></tr>
<tr><td>1</td><td>Model</td><td>$F_1(x,t) = M(x,t)$</td><td>$V_{B1}(x,t)$</td><td>$V_M(x,t)$</td><td colspan="2">$V_{R1}(x,t)$</td></tr>
<tr><td>2</td><td>Model & Satellite</td><td>$F_2(x,t) = \mathrm{avg}_{t'\in T_c(t)}\left[\left(S_{col}(x,t') - M_{col}(x,t')\right)\phi(x,t')\,\psi(x,t,t')\right] + F_1(x,t) = D(x,t) + F_1(x,t)$</td><td>$V_{B2}(x,t)$</td><td>$V_M(x,t)$</td><td>$V_D(x,t) + 2V_{MD}(x,t)$</td><td>$V_{R2}(x,t)$</td></tr>
<tr><td>3</td><td>Model & Satellite & Ground</td><td>$F_3(x,t) = \theta_1 F_2(x,t) + \theta_0$
$with\ \ \theta_0,\theta_1 = \mathbb{LR}_{t'\in T_c(t),x'\in X_c(x)}[G(x',t') \sim F_2(x',t')]$</td><td>0*</td><td>$\theta_1^2 V_M(x,t)$</td><td>$\theta_1^2[V_D(x,t) + 2V_{MD}(x,t)]$</td><td>$\mathrm{var}[\theta_1]F_2(x,t)^2 + 2\mathrm{cov}[\theta_0,\theta_1]F_2(x,t) + \mathrm{var}[\theta_0] + \sigma^2_{residual}$</td></tr>
<tr><td rowspan="2">4</td><td rowspan="2">Model & Satellite & Ground & Kriging</td><td rowspan="2">$F_4(x,t) = \mathrm{F}_3(x,t) + \sum_{x'\in X_n(x),t'\in T_n(t)} K(x,x',t,t')\,[G(x',t') - F_3(x',t')]$</td><td>0*</td><td>$\theta_1^2 V_M(x,t)$</td><td>$\theta_1^2[V_D(x,t) + 2V_{MD}(x,t)]$</td><td>$\mathrm{var}[\theta_1]F_2(x,t)^2 + 2\mathrm{cov}[\theta_0,\theta_1]F_2(x,t) + \mathrm{var}[\theta_0] + \sigma^2_{residual}$</td></tr>
<tr><td colspan="4">$-\sum_{x'\in X_n(x),t'\in T_n(t)} K(x,x',t,t')\,\mathrm{cov}[G(x',t'),F_3(x,t)]$</td></tr>
</table>

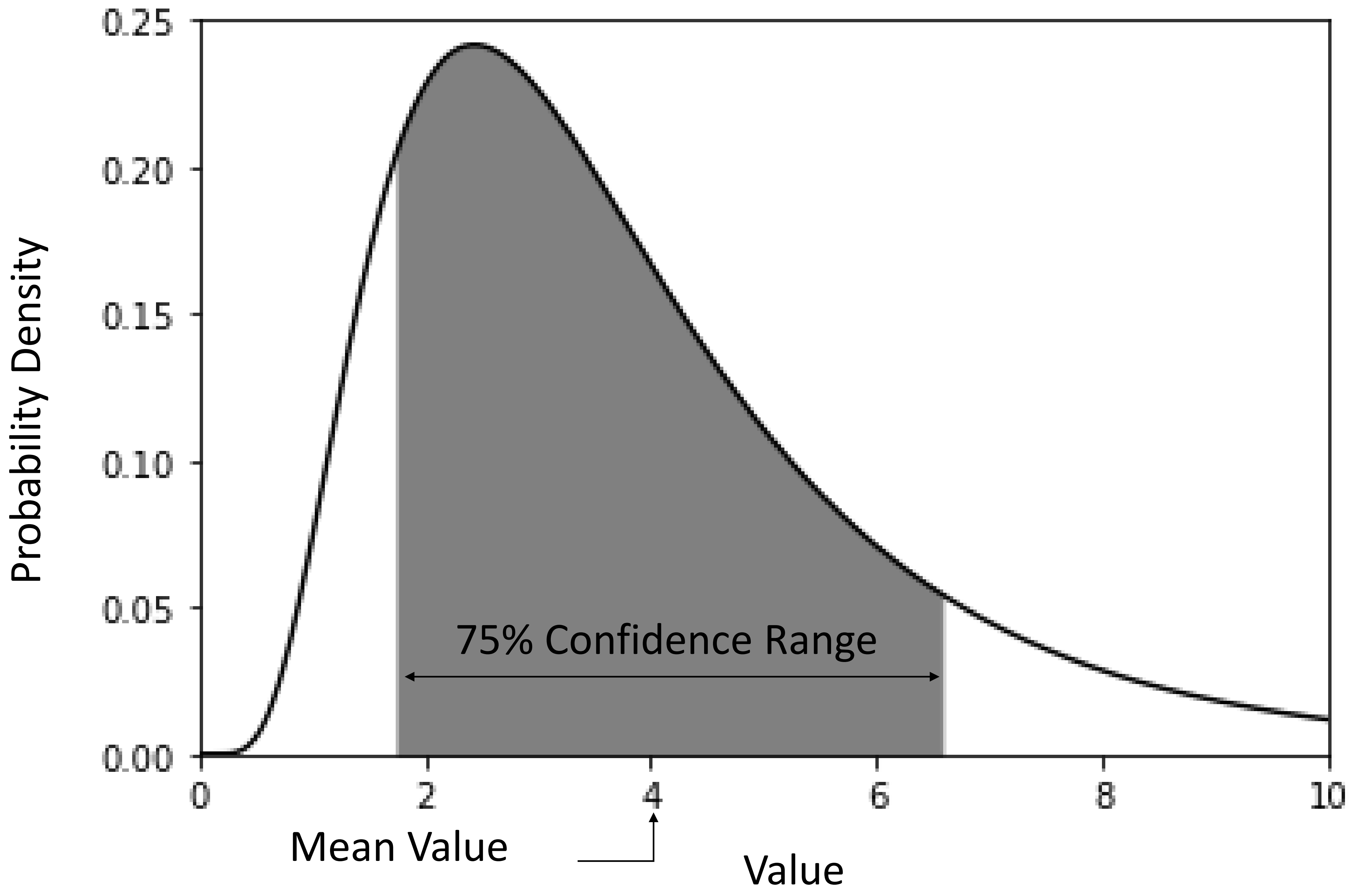
Phase		Estimate	Uncertainty			
			Bias	Model Variability	Model Scale Spatial Representativity	Satellite Scale Spatial Representativity
1	Model	$F_1(x,t) = M(x,t)$	$V_{B1}(x,t)$	$V_M(x,t)$	$V_{R1}(x,t)$	
2	Model & Satellite	$F_2(x,t)$ $= \text{avg}_{t' \in T_c(t)}\left[\left(S_{col}(x,t') - M_{col}(x,t')\right) \phi(x,t')\, \psi(x,t,t')\right]$ $+ F_1(x,t) = D(x,t) + F_1(x,t)$	$V_{B2}(x,t)$	$V_M(x,t)$	$V_D(x,t)$ $+ 2V_{MD}(x,t)$	$V_{R2}(x,t)$
3	Model & Satellite & Ground	$F_3(x,t) = \theta_1 F_2(x,t) + \theta_0$ $with \quad \theta_0, \theta_1 = \mathbb{LR}_{t' \in T_c(t), x' \in X_c(x)}[G(x',t') \sim F_2(x',t')]$	0*	$\theta_1^2 V_M(x,t)$	$\theta_1^2[V_D(x,t)$ $+ 2V_{MD}(x,t)]$	$\text{var}[\theta_1]F_2(x,t)^2$ $+ 2\text{cov}[\theta_0,\theta_1]F_2(x,t)$ $+ \text{var}[\theta_0]$ $+ \sigma^2_{residual}$
4	Model & Satellite & Ground & Kriging	$F_4(x,t)$ $= \text{F}_3(x,t)$ $+ \sum_{x' \in X_n(x), t' \in T_n(t)} K(x,x',t,t')\,[G(x',t') - F_3(x',t')]$	0*	$\theta_1^2 V_M(x,t)$	$\theta_1^2[V_D(x,t)$ $+ 2V_{MD}(x,t)]$	$\text{var}[\theta_1]F_2(x,t)^2$ $+ 2\text{cov}[\theta_0,\theta_1]F_2(x,t)$ $+ \text{var}[\theta_0]$ $+ \sigma^2_{residual}$
			$-\sum_{x' \in X_n(x), t' \in T_n(t)} K(x,x',t,t')\, \text{cov}[G(x',t'), F_3(x,t)]$			



Assume an empirical relationship between bias and representation errors and the quantifiable component of the uncertainty in phases 1 and 2.

$$V_{B1}(x,t) + V_{R1}(x,t) \approx \eta_1^2\, V_M(x,t)$$

$$V_{B2}(x,t) + V_{R2}(x,t) \approx \eta_2^2\left(V_M(x,t) + V_D(x,t) + 2V_{MD}(x,t)\right)$$



Assuming a distribution for the values being estimated (a lognormal distribution is assumed in this case), confidence intervals can be estimated.

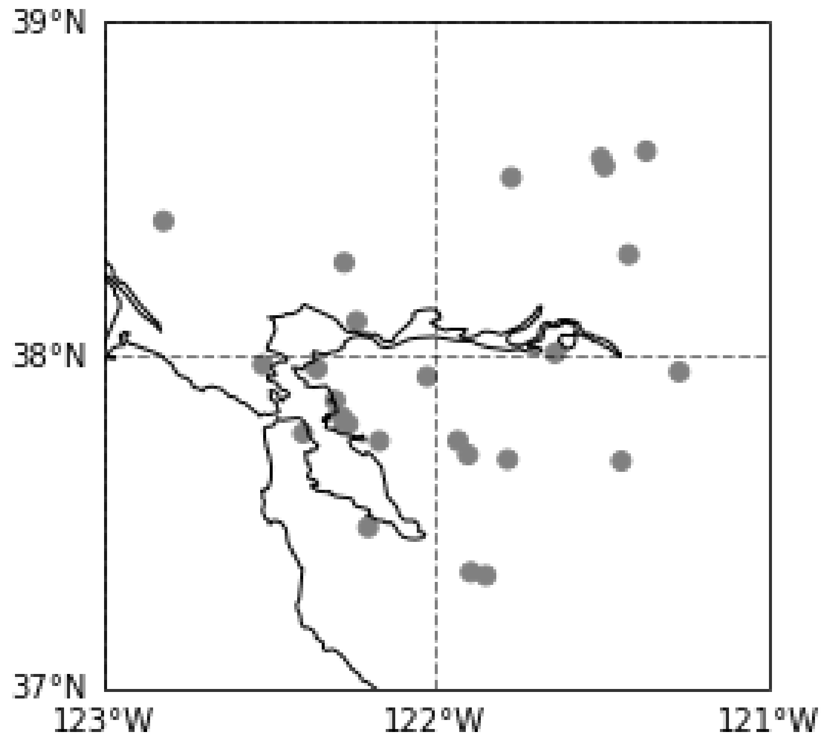
$$\mu(x,t) = \log\left[\frac{F(x,t)}{\sqrt{1+\frac{V(x,t)}{F(x,t)^2}}}\right]$$

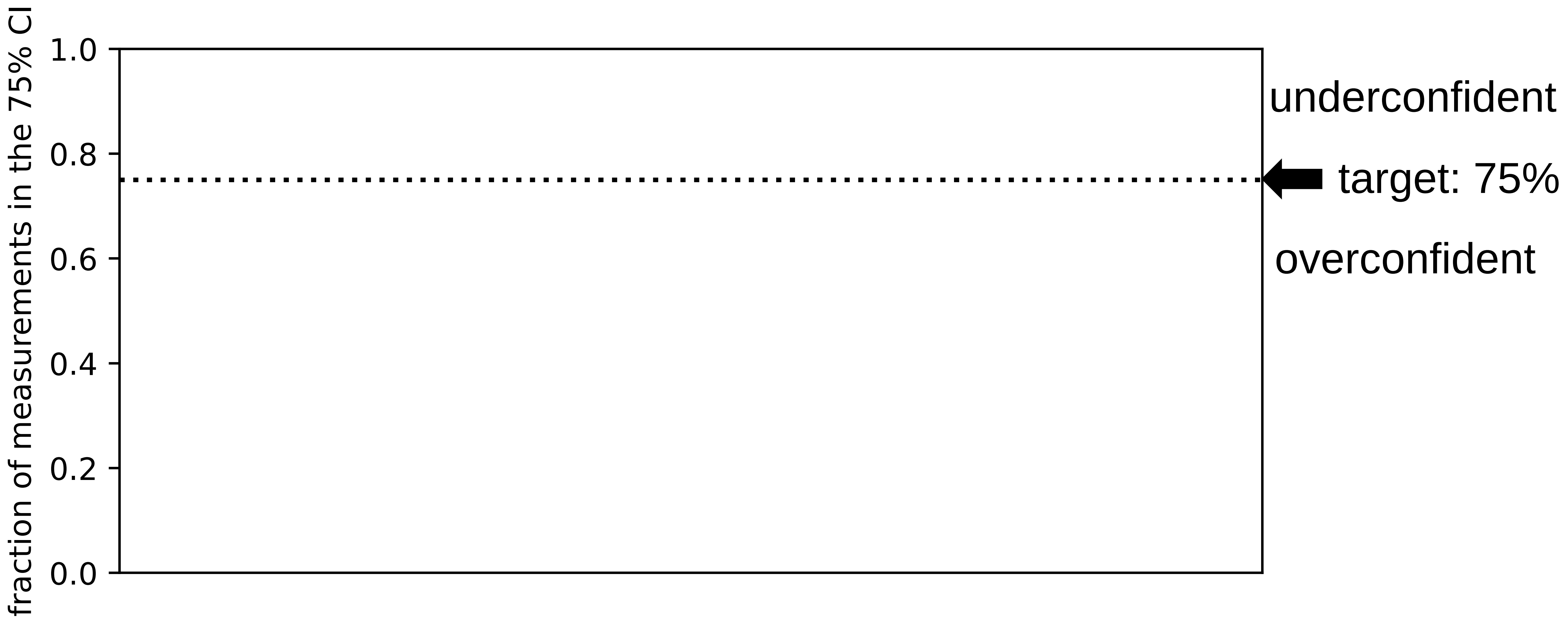
$$\sigma(x,t) = \sqrt{\log\left[1+\frac{V(x,t)}{F(x,t)^2}\right]}$$

$$f(x,t) \sim LN\big(\mu(x,t), \sigma(x,t)\big)$$

Case Study Details
San Francisco
September 2019
Surface NO_2
Lognormal distribution
Cross-validation test
25 ground monitors

Ground Sites





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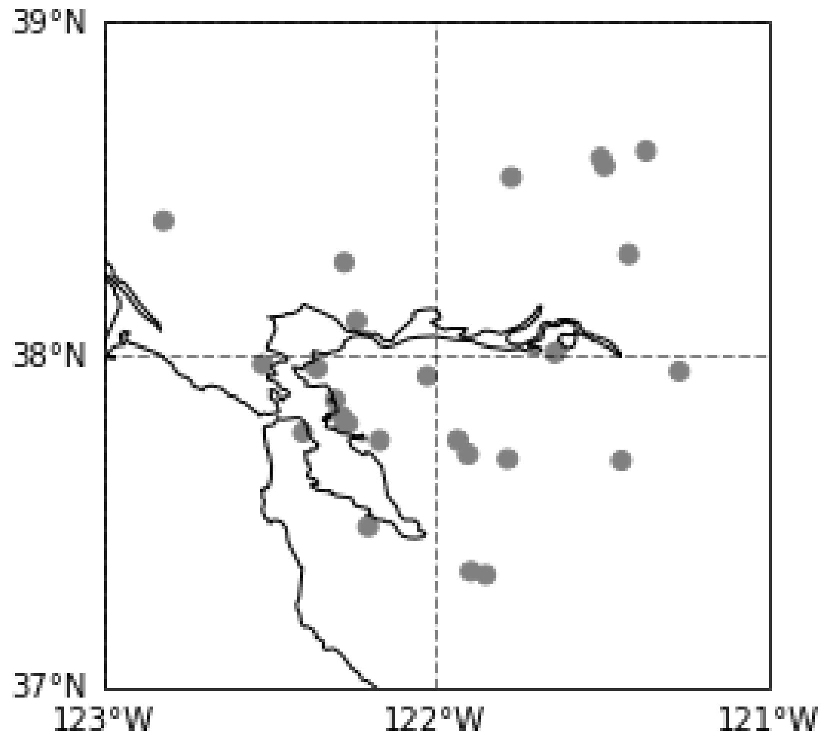

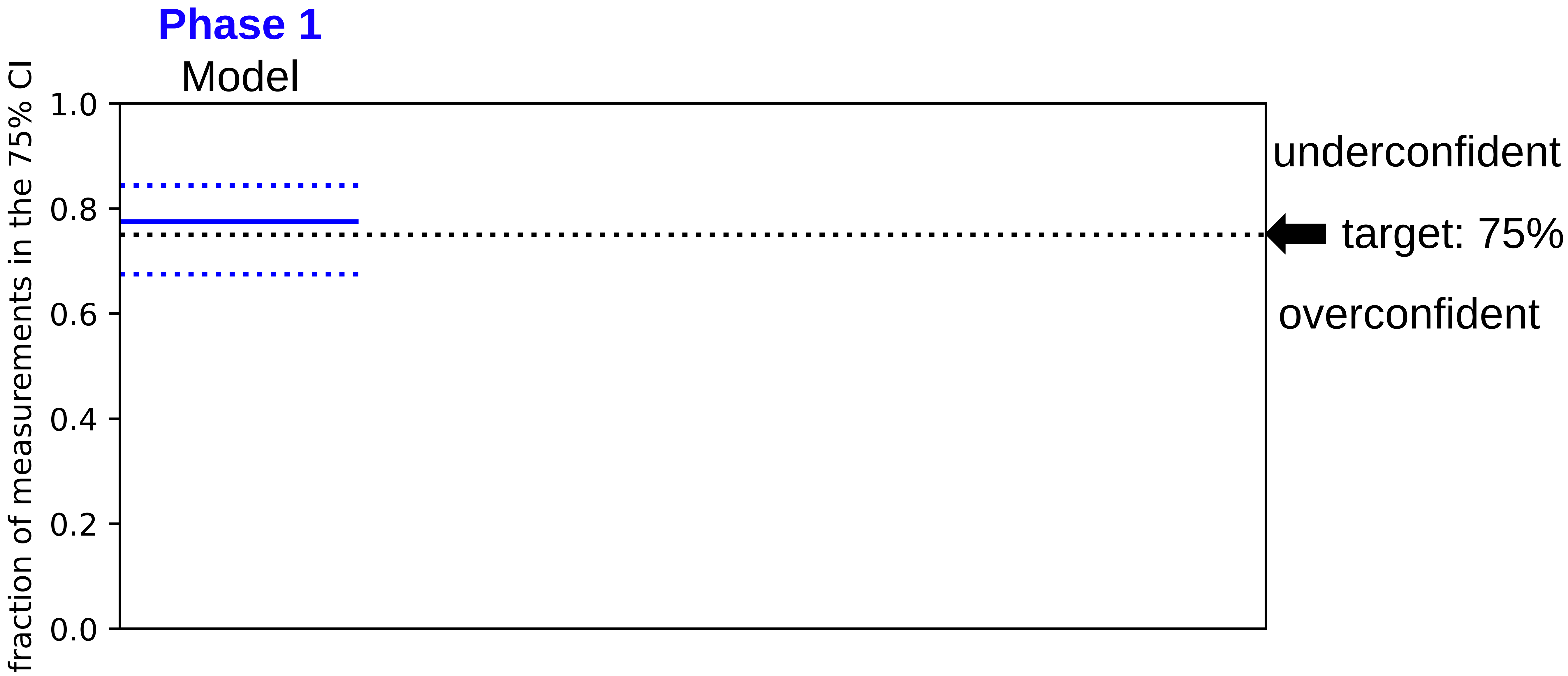

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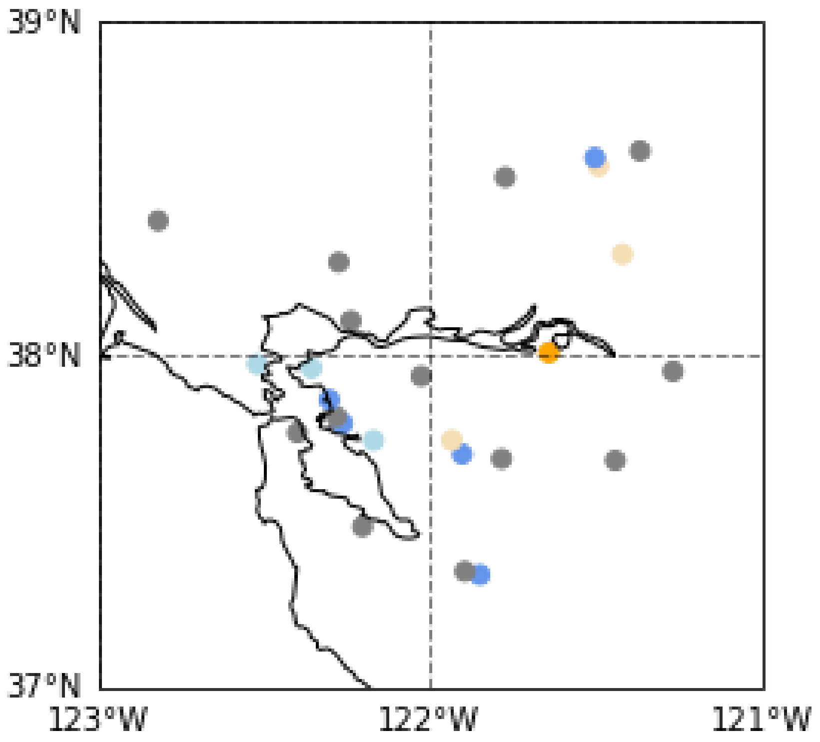
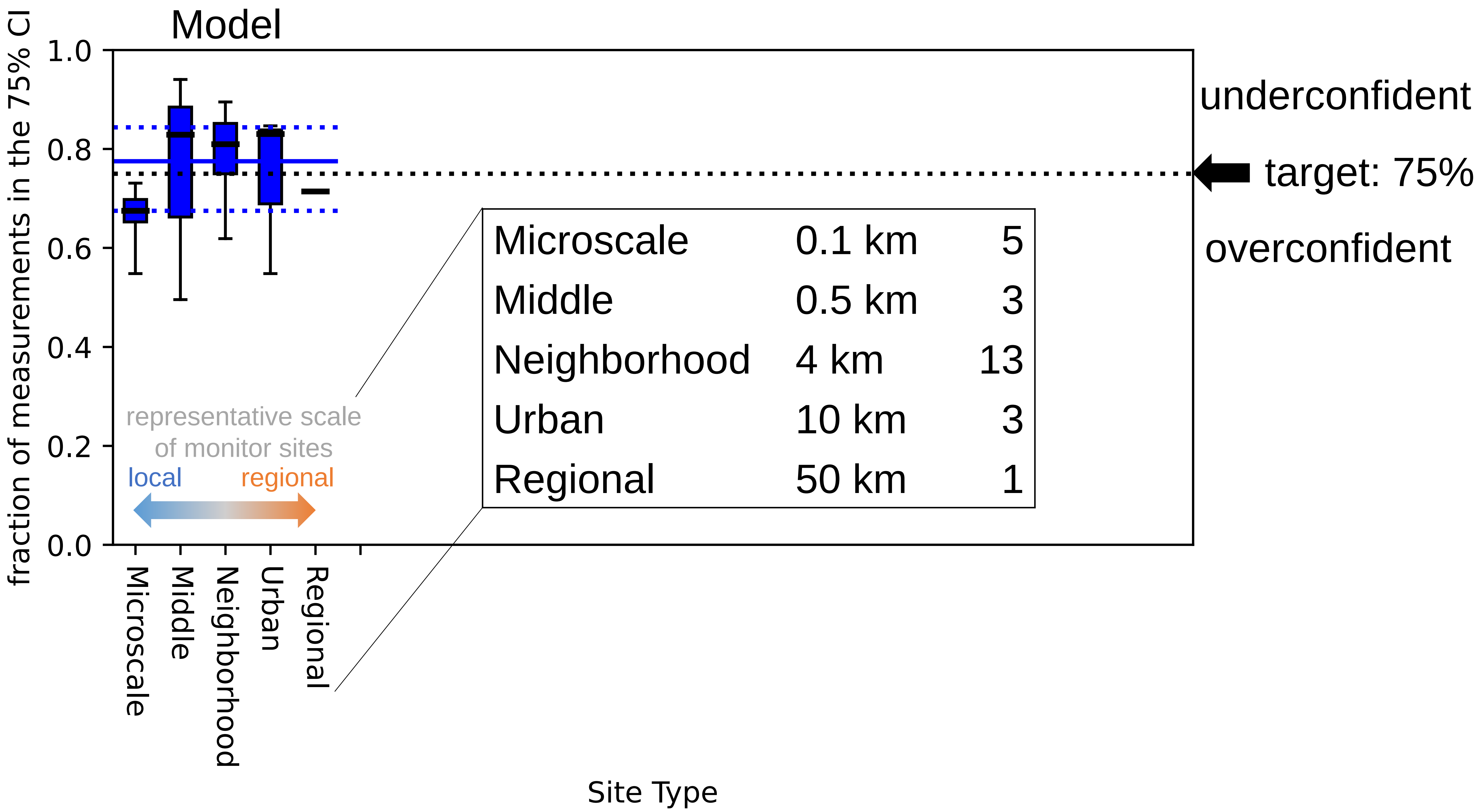
25 ground monitors

Ground Sites

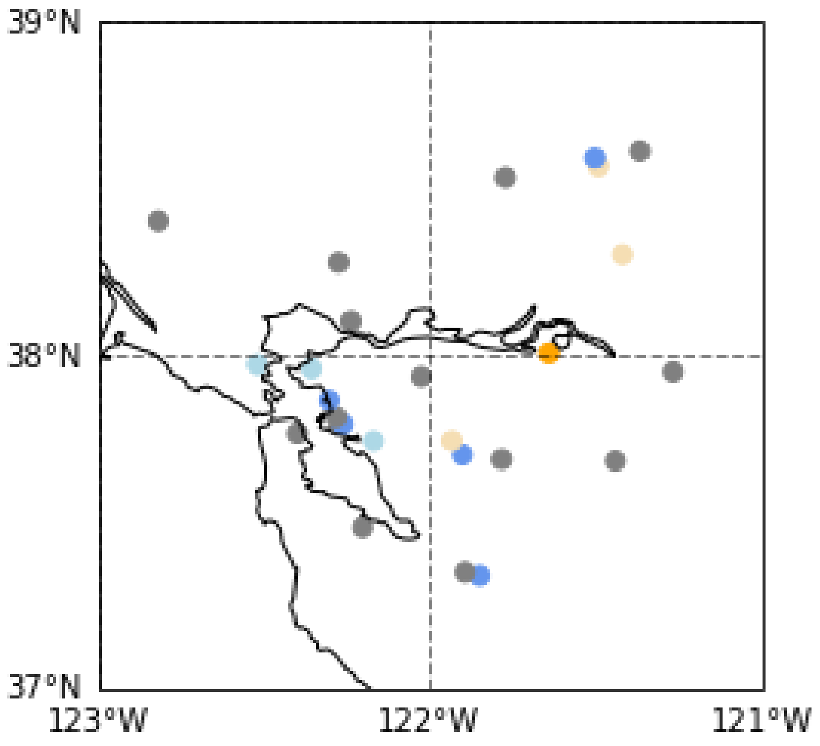


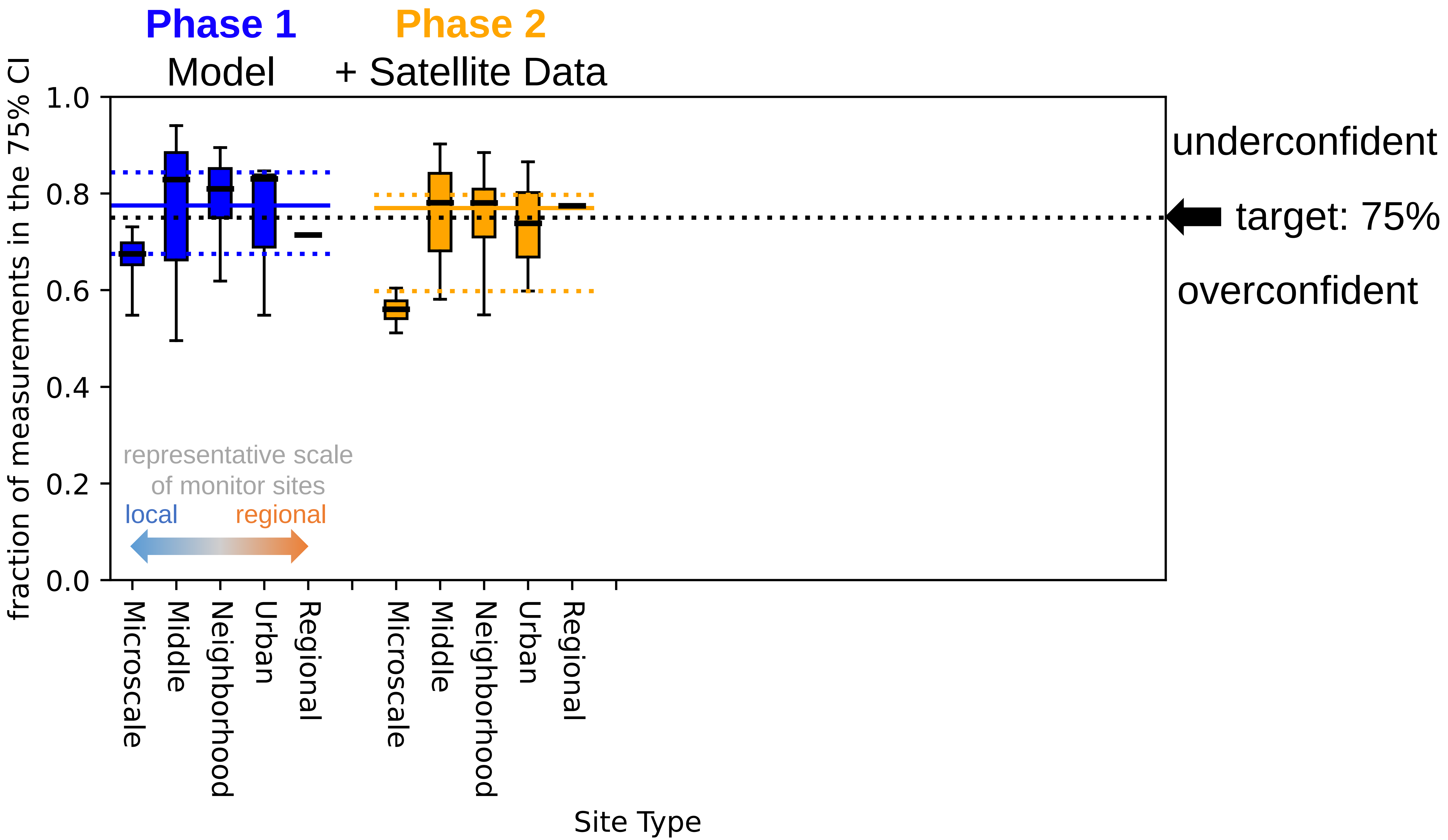
Phase 1



Case Study Details
San Francisco
September 2019
Surface NO_2
Lognormal distribution
Cross-validation test
25 ground monitors

Ground Sites





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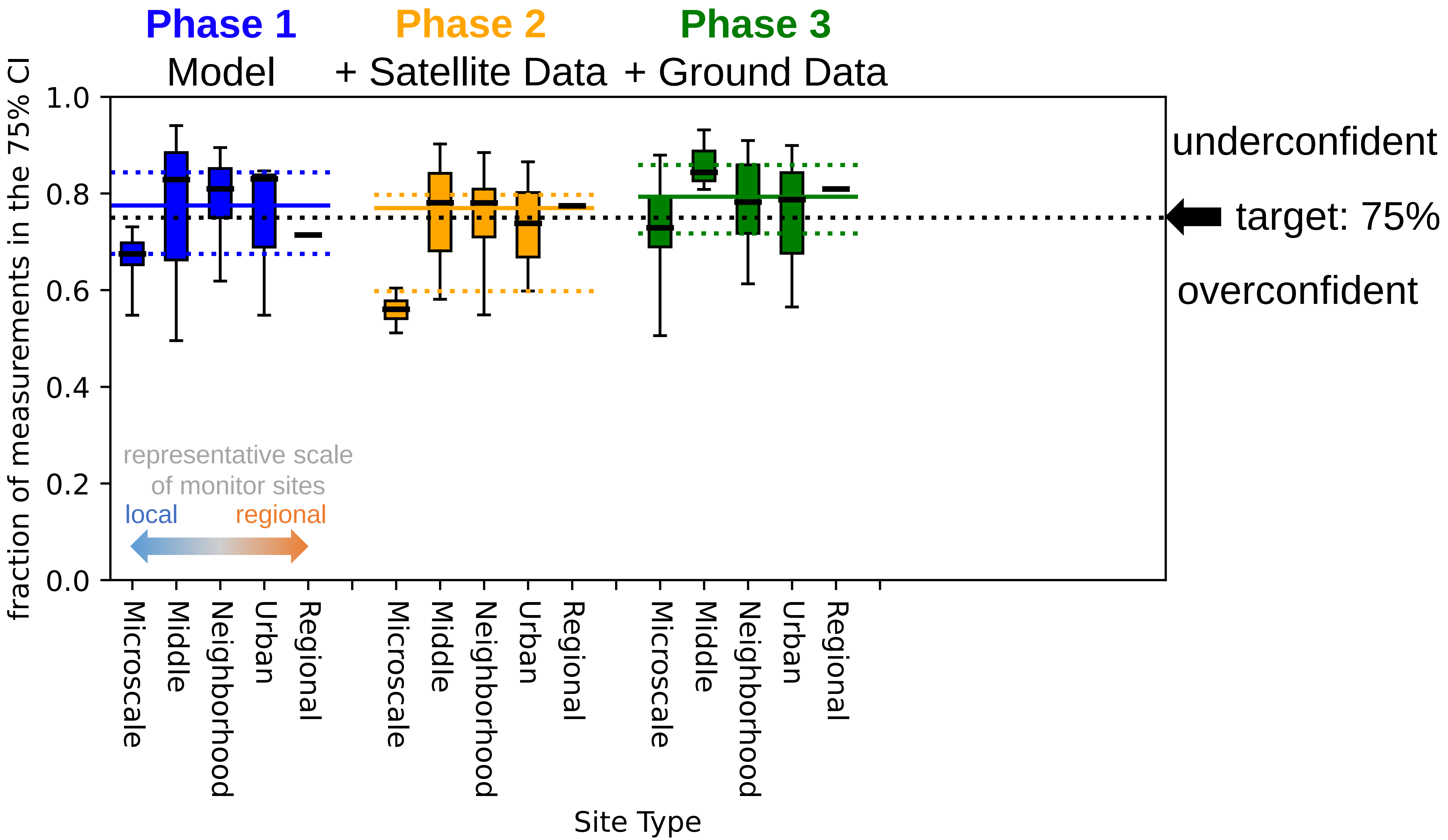
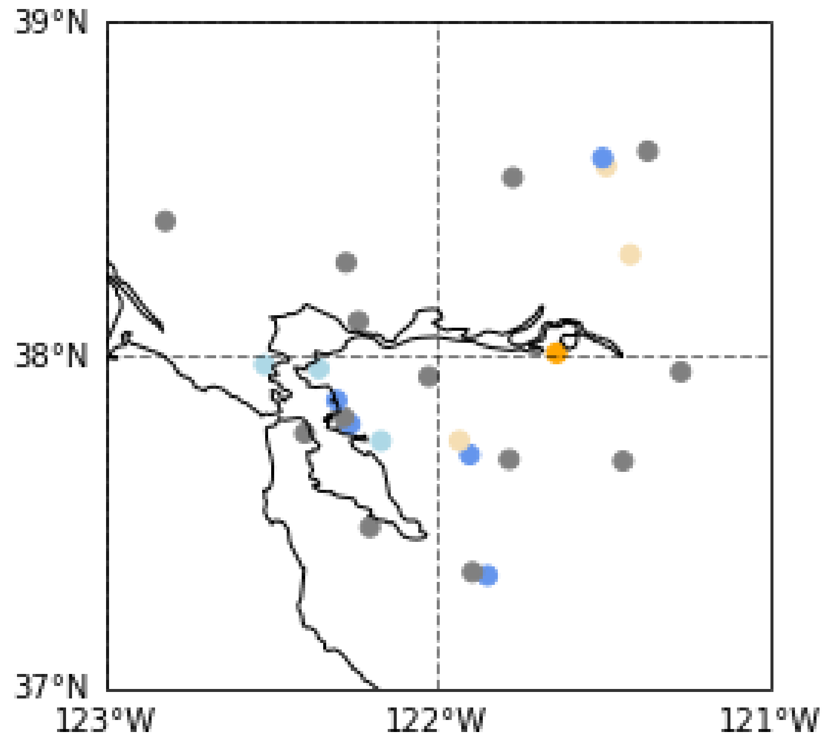


Ground Sites



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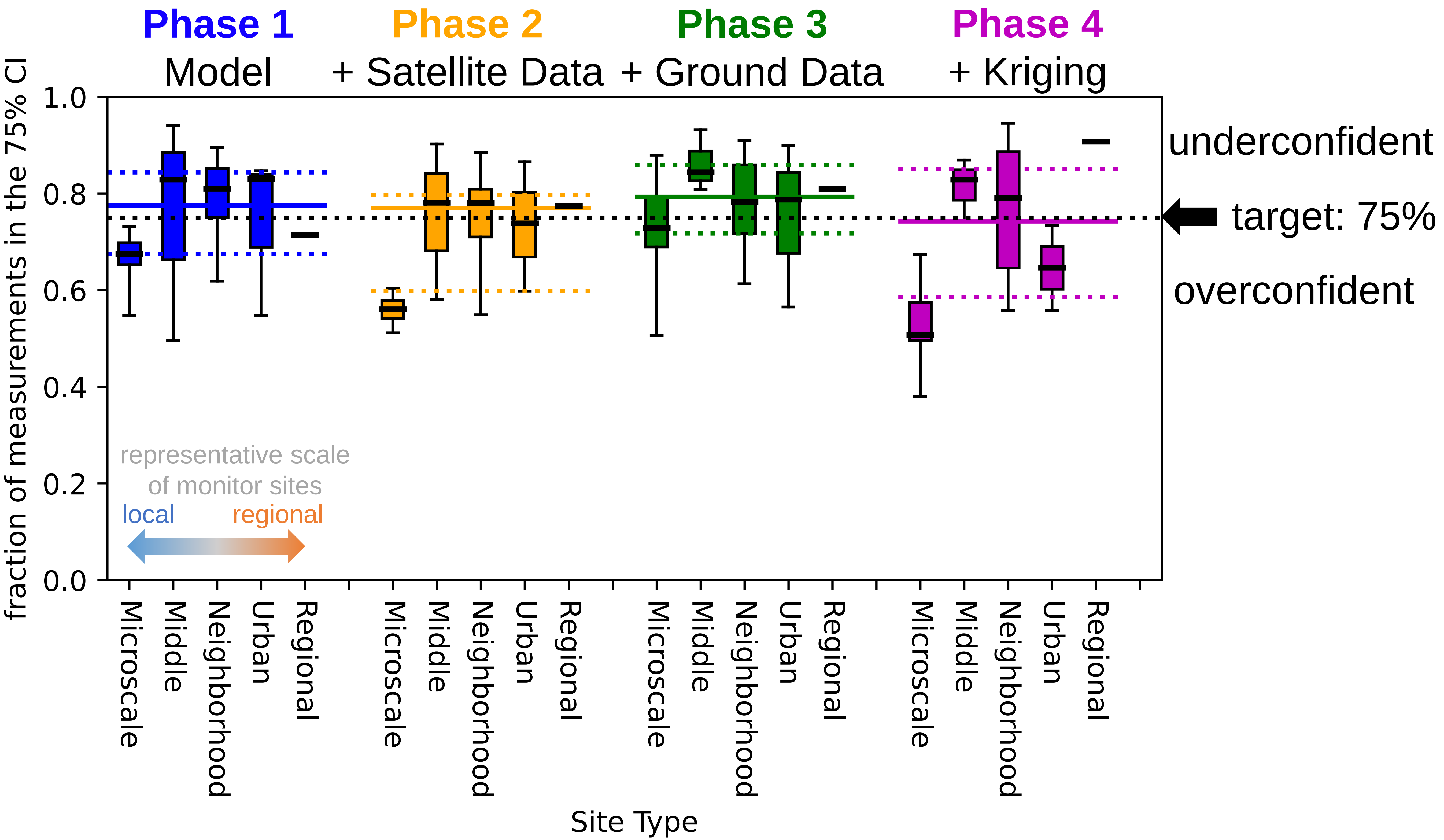
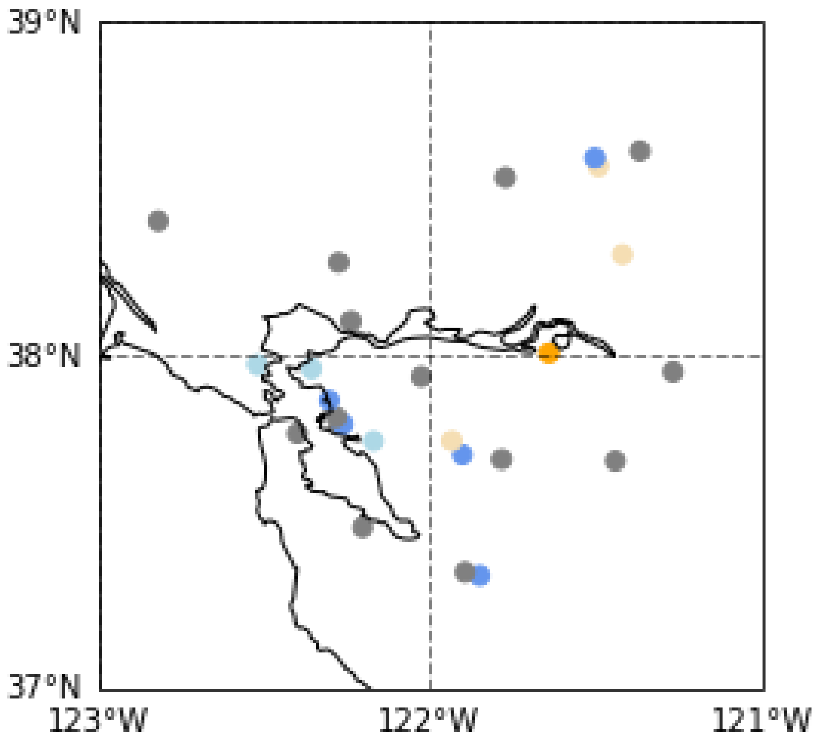
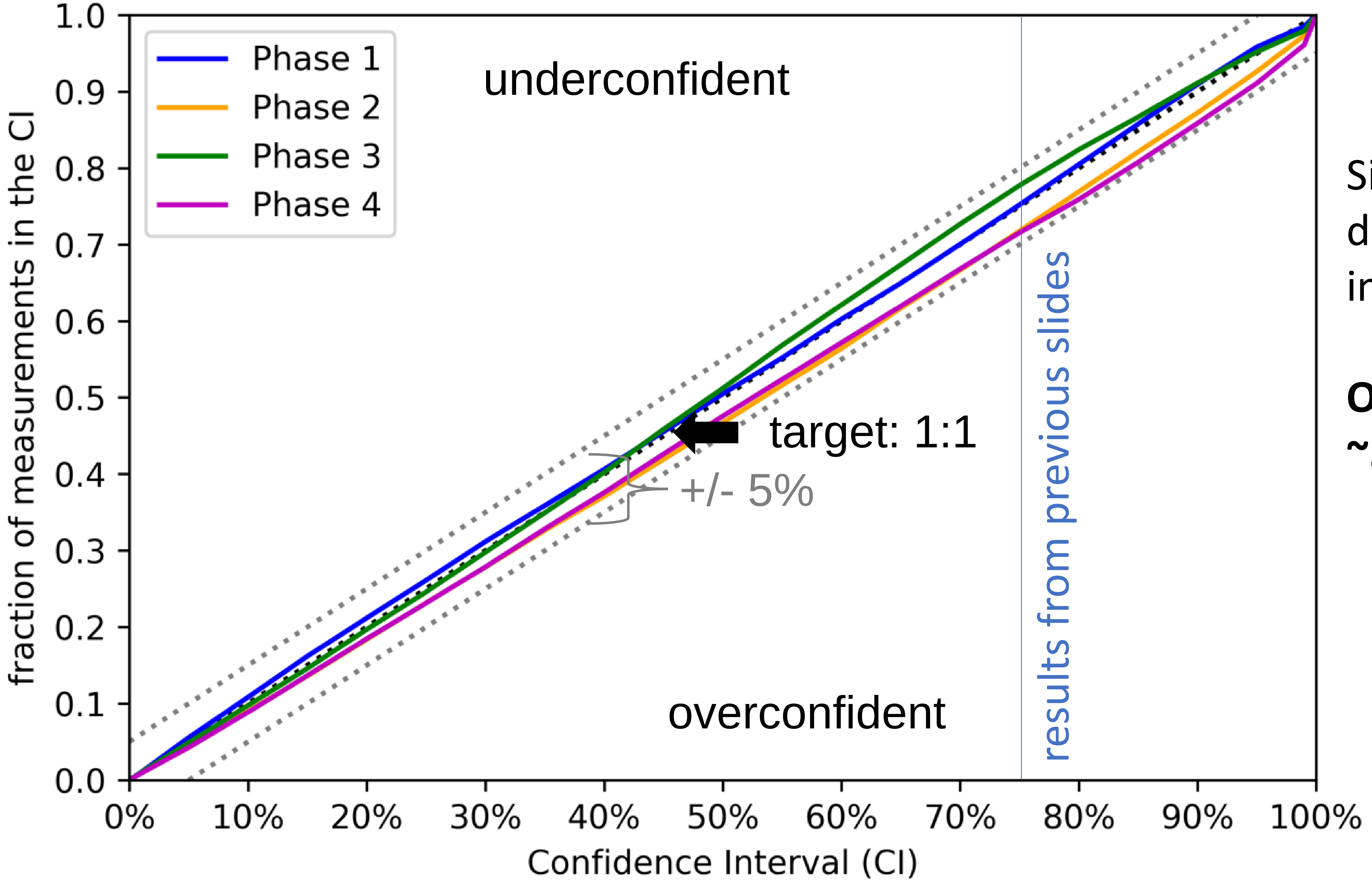


Ground Sites



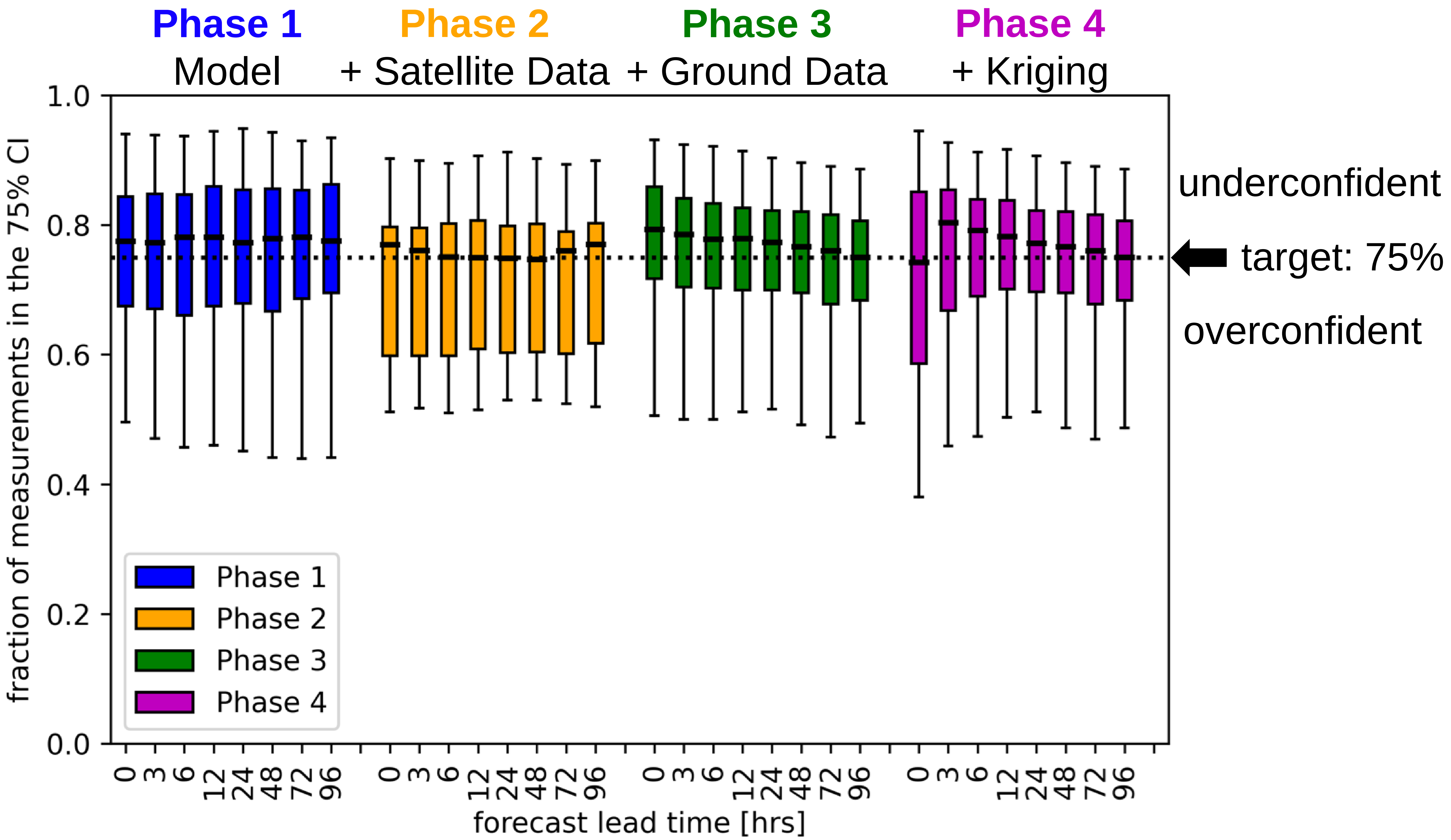


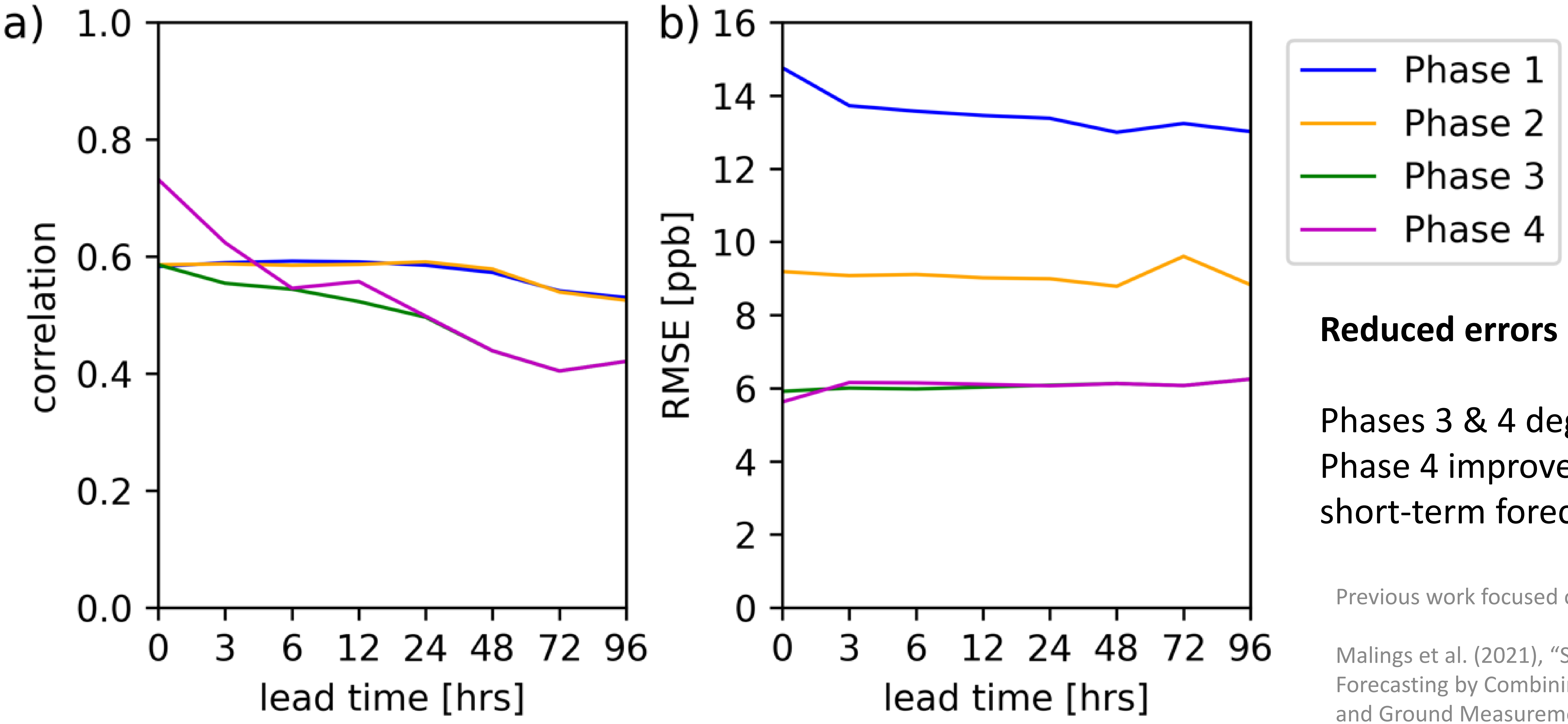
Similar performance for different confidence interval definitions

Overall coverage within ~5% of target

Similar performance for different forecast lead times

Widest spread in phase 4 coverage at 0 lead time





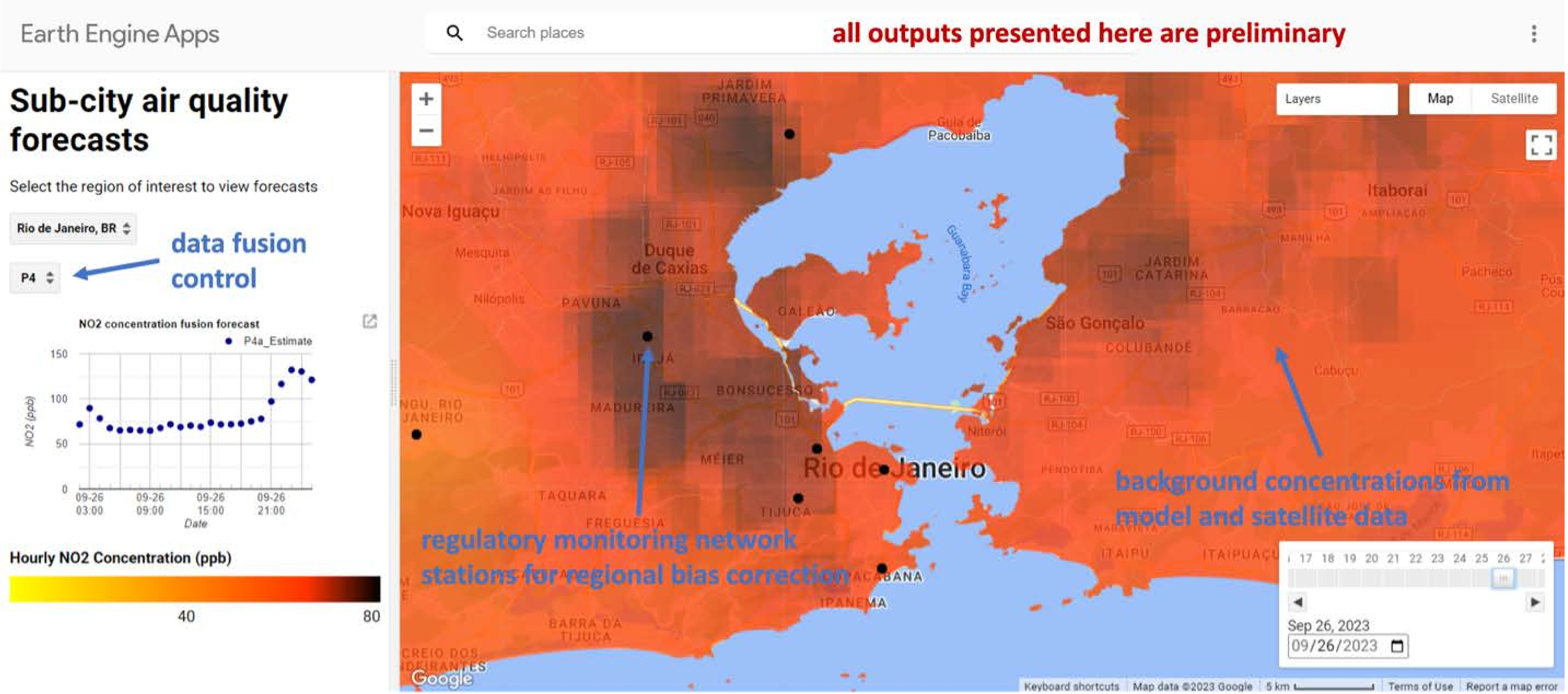
Reduced errors as phase increases

Phases 3 & 4 degrade correlation, Phase 4 improves correlations for short-term forecasts

Previous work focused on performance assessment:

Malings et al. (2021), "Sub-City Scale Hourly Air Quality Forecasting by Combining Models, Satellite Observations, and Ground Measurements" *Earth & Space Science.* DOI: 10.1029/2021EA001743

- Theoretical
  - Better approach to uncertainty quantification near sources
    - Include ancillary data, experiment with non-linear (machine learning) methods
  - Better approach to uncertainty quantification at Phase 4
    - Non-isotropic correlation functions?
  - Incorporating low-cost air quality sensors
    - Possibility to regionally re-calibrate sensors based on Phase 3 outputs
- Practical
  - Implement data fusion system in Google Earth Engine
    - Efficiency improvements needed!
  - Design the user interface
    - How to display uncertainty in an intuitive way?



Source: NASA GMAO Science Snapshot [“Google Earth Engine Data Fusion Tool to support Air Quality Managers”]

Global Modeling and Assimilation Office
GESTAR II Cooperative Agreement

Partner

Thank you!

Questions?

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