SUPPLEMENTAL MATERIALS

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Exploring Equity Challenges within Deeply Uncertain Water Supply Investment Pathways in the Federal District of Brazil

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Appendix S1. FDB Model: Mass Balance, Risks of Failure, and Performance Objectives

The FDB model design is based upon WaterPaths framework, initially applied to the Sedento Valley illustrative case (Trindade et al. 2020), and adapted for the FDB context by Giacomazzo (2020). Thus, the FDB model explicitly applies DU Pathways framework, incorporating rule systems that respond to observed system states. This is provided through a mass-balance model, solved for all water sources in each service area (summarized in Table S1) and mathematically represented by Eq. (S1):

$$\mathrm{x}_{\mathrm{s}}^{\mathrm{w+1}} = \mathrm{x}_{\mathrm{s}}^{\mathrm{w}} + \mathrm{NI}^{\mathrm{w}} + \mathrm{SE}^{\mathrm{w}} + \mathrm{URO}^{\mathrm{w}} - \mathrm{ER}^{\mathrm{w}} \cdot \mathrm{AR}(\mathrm{x}_{\mathrm{s}}^{\mathrm{w}}) - \mathrm{EO}^{\mathrm{w}} - \mathrm{S}^{\mathrm{w}} - \mathrm{RD}^{\mathrm{w}} \qquad \text{(S1)}$$

where $\mathrm{x}_{\mathrm{s}}^{\mathrm{w+1}}$ is the volume of water stored in the reservoir at the week after the current week w, NI is the natural inflow into the reservoir from all its tributaries, SE is a treated sewage effluent discharge directly or indirectly in the reservoir, URO is the upstream reservoir total outflow, ER is a non-dimensional evaporation rate, RA is the reservoir area as a function of stored volume, EO is the environmental outflow, RD is the total municipal demand drawn from that reservoir to the modelled service area, and S is the reservoir spillage, which is set to zero unless the reservoir is completely full. Eq. (S1) is solved on a weekly basis during all simulation time horizon (40 years).

Table S1 also summarizes the main features of the two services areas, Descoberto and Santa Maria, a division proposed by this work based upon FDB water supply infrastructure system. It is comprised of five main water production subsystems, divided according to water sources location and associated infrastructures (catchments, treatment plants and water networks). Descoberto and Santa Maria are the main subsystems, and together they provide water for over 80% of FDB population. As demonstrated in Fig. 1 of the main text, these two subsystems present wide socioeconomic disparities between the population they attend, leading to the definition of two service areas of study that spatially correspond to the water producing subsystems of Descoberto and Santa Maria.

Table S1. Main water sources' features in the Federal District supply system

Service area	Water Supply Infrastructure	Storage Capacity[a] (hm³)	% Storage allocated in water urban supply[a]	Water Treatment Plant (WTP)[a]	Water Production Capacity[a] (L/s)	Population served[b] (inhab)
Descoberto	Descoberto Resevoir	72,3	100	Descoberto Stream WTP	5,791.8	1,678,243
Santa Maria	Paranoa Lake	460,5	8	Lago Norte WTP	3,011.1	703,095
	Santa Maria Resevoir	61,3	100	Brasília WTP		
	Bananal Stream	-	-			
	Torto Stream	-	-			

[a]Data from ADASA (2018).
[b]Data from CODEPLAN (2018).

Another core component of the FDB WaterPaths model is the decision making through state-aware, risk monitoring metrics known as risk of failures (ROF). ROFs express the system's (or service area) ability to meet required water demand in each time basis. The FDB model presents two ROFs: first, the estimated probability that the service area total storage falls below a critical level in the next T_{rof} weeks, if hydrological conditions from the last 50 years occurs. Second, the estimated probability that service area demand exceeds 90% of its total treatment capacity. Short term ROFs are calculated with T_{rof} equals to 52 weeks, and triggers educational campaigns, rationing/contingency tariffs or water transfers if θ_{gr}, $\theta_{\Delta gr}$ or θ_{gt} thresholds are crossed, respectively. Long term ROFs are calculated when T_{rof} corresponds to 78 weeks, and trigger infrastructure construction in case θ_{ci} threshold is crossed. ROFs mathematical computation is based upon the work of Trindade et al. (2020), and expressed in Eqs. (S2)–(S4):

$$x_{rof,j}^{w} = \frac{1}{N_{rof}} \sum_{y'=0}^{N_{rof}} f_{y',j}^{w}(NI^{y'}, E^{y'}) \tag{S2}$$

where,

$$f_{y\prime,j}^{w} = \begin{cases} 0 \;\; \forall\, w' \epsilon \left\{(y', w), \ldots, \left(y', w + T_{rof}\right)\right\}: \dfrac{x_{s',j}^{y,w'}}{C_j} \geq s_c \\ 1 \; otherwise \end{cases} \tag{S3}$$

and,

$$x_{s',j}^{y,w'} = f\left(C_j, UD_j^{w}, NI_j^{y',w\prime}, E_j^{y',w\prime}, W_j^{y',w\prime} \,|\, \Psi_s\right) \tag{S4}$$

In Eqs. (S2)–(S4), w' and y' denote a week and a year simulated with historical data, $x_{rof,j}^{w}$ represents ROF for service area j (Descoberto or Santa Maria) in current week w, $f_{y\prime,j}^{w}$ is a binary variable that indicates failure or success during the simulation with data from past year y'. A failure is identified when the total water stored in realization y', $x_{s',j}^{y,w'}$, divided by storage capacity C_j, drops below a critical level. Variable $x_{s',j}^{y,w'}$ is the vector of storage states determined in one year-long ROF simulations, using recorded hydrologic data from past year y', defined considering storage capacity, C_j, unrestricted demand, UD_j^{w}, recorded natural inflows, evaporation rates and reservoir spillage, $NI_j^{y',w\prime}$, $E_j^{y',w\prime}$ and $W_j^{y',w\prime}$, respectively, calculated in year y' prior to current week w used in one of the N_{rof} simulations. Variable Ψ_S the the vector of DU factors. Fig. S1 presents a schematic view of the ROF calculation and mass balance loop in WaterPaths.

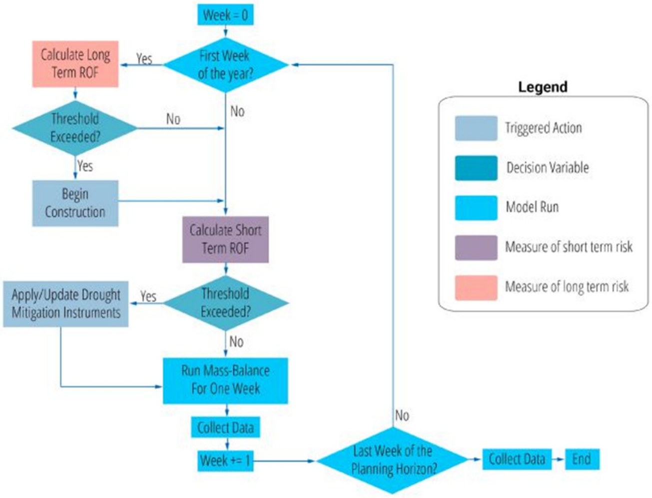

Fig. S1. WaterPaths ROF calculation, mass balance loop, and its relationship with decision-making associated with short- and long-term management actions. (Reprinted from *Environmental Modelling & Software*, Vol. 132, B. C. Trindade, D. F. Gold, P. M. Reed, H. B. Zeff, and G. W. Characklis, “Water pathways: An open source stochastic simulation system for integrated water supply portfolio management and infrastructure investment planning,” 104772, (c) 2020, with permission from Elsevier.)

As stated in Eq. (3) in the main text, a policy is defined as a set of risk tolerance limits for ROFs that, if crossed, trigger associated management measures. While short-term ROF thresholds are related to drought mitigation instruments (educational campaigns, rationing and contingency tariffs), long term ROF limits can trigger infrastructure construction, whose options for each service area are presented in Table S2. The ranges in which the decision variables that compose a candidate policy can vary are presented in Tables S3 and S4.

Table S2. Candidate supply infrastructure or supply expansion in Federal District water system

Service area	Water supply infrastructure	Description	Cost (10^6 R$)	Water Supply(L/s)
Descoberto	Corumba System - 1st phase	New Water Production System	276.50	1,400
	Corumba System - 2nd phase	Water Treatment Expansion	222.10	1,400
	Corumba System - 3rd phase	Water Treatment expansion/new pipelines	251.40	1,200
	Descoberto Resevoir Expansion	1.5 meter spillway level raise	7.50	400
Santa Maria	Paranoa System - 1st phase	New Water Treatment Plant in Paranoá Lake	60.30	700
	Paranoa System - 2nd phase	Water Treatment Expansion	60.30	700
	Paranoa System - 3rd phase	Water Treatment Expansion	60.30	700

Sources: Data from GDF (2017); CAESB (2019).

Table S3. Lower and upper thresholds for long- and short-term decision variables of the candidate policies

Decision variables	Lower bound	Upper bound
Water consumption restriction trigger for Descoberto - θ_{gr}	0.1%	100%
Water consumption restriction trigger for Santa Maria - θ_{gr}	0.1%	100%
Second stage water consumption restriction trigger for Descoberto - $\theta_{\Delta \mathrm{gr}}$	0.1%	100%
Second stage water consumption restriction trigger for Santa Maria - $\theta_{\Delta gr}$	0.1%	100%
Water transfer trigger for Descoberto - θ_{gt}	0.1%	100%
Water transfer trigger for Santa Maria - θ_{gt}	0.1%	100%
Annual reserve fund contribution for Descoberto as percentage of annual revenue - θ_{accf}	0%	10%
Annual reserve fund contribution for Santa Maria as percentage of annual revenue - θ_{accf}	0%	10%
Infrastructure construction long-term ROF trigger for Descoberto - θ_{ci}	0.1%	100%
Infrastructure construction long-term ROF trigger for Santa Maria - θ_{ci}	0.1%	100%

Table S4. Construction order ranges for each infrastructure option

Service area	Decision variables (ICO)	Lower bound	Upper bound
Descoberto	Corumba System - 1st phase	1st	4th
	Corumba System - 2nd phase	1st	4th
	Corumba System - 3rd phase	1st	4th
	Descoberto Resevoir Expansion	1st	4th
Santa Maria	Paranoa System - 1st phase	1st	3rd
	Paranoa System - 2nd phase	1st	3rd
	Paranoa System - 3rd phase	1st	3rd

DU many-objective optimization searches for best performing policies that minimizes function F [Eq. (1)], and thus maximizes water supply reliability (f_{REL}), minimizes water-use restriction frequency (f_{RF}), minimizes infrastructure net present value (f_{INPV}), minimizes the peak financial cost of drought mitigation and debt payments (f_{FC}), and minimizes the worst-case cost of drought mitigation actions (f_{WCC}). Each objective's formulation is presented as follows.

Reliability (REL) represents the fraction of states of the world in which reservoir levels drop below 20% of its maximum capacity in any given week (failure condition):

$$\max f_{REL} = min_j \left[min_y \left(\frac{1}{N_r} \sum_{i=1}^{N_r} g_{i,j}^{y} \right) \right] \tag{S5}$$

where,

$$g_{i,j}^{y} = \begin{cases} 0 & \forall\, w\colon \dfrac{x_{s,i,j}^{y,w}}{C_j} \geq s_c \\ 1\ otherwise \end{cases} \tag{S6}$$

where N_r is the number of realizations for one function evaluation and $g_{i,j}^{y}$ is a binary function that assumes zero value if, in a given year of a specific realization, there was a week when reservoir storage fell below s_c capacity, and 1 otherwise.

Restriction frequency (RF) is the fraction of years over the planning horizon (40 years for the FDB model) in which at least one week presents use of water restrictions:

$$\min f_{RF} = \ max_j \left[\frac{1}{N_{ys} \cdot \ N_r} \sum_{i=1}^{N_r} \sum_{y=1}^{N_{ys}} h_{i,j}^y \right] \tag{S7}$$

where

$$h_{i,j}^y = \begin{cases} 0 & \forall \, w\colon x_{s,i,j}^{y,w} \ \leq \ \theta_{rt,j} \\ 1 \, otherwise \end{cases} \tag{S8}$$

where $h_{i,j}^y$ represents the adoption of water use restrictions in a week of a given year of a particular realization, and 1 otherwise.

Infrastructure net present value (INPV) represents the average net present cost of all infrastructures built across all realizations:

$$\min f_{INPV} = \ \frac{1}{N_r} \sum_{i=1}^{N_r} \sum_{y=1}^{BM} \frac{PMT}{(1+d)^y} \tag{S9}$$

where BM is the bond term, d is the discount rate (4%), y is the year of the debt service payment (PMT) since the bond was issued, with PMT being calculated by:

$$PMT \ = \ \frac{P[BR(1+BR)^{BM}}{[(1+BR)^{BM} - 1]} \tag{S10}$$

where P is the principal, BR is the interest rate and BT is the bond term.

The fourth objective, Peak Financial Cost (CF), represents the expected yearly cost of the portfolio applied to manage risks over the planning horizon, including revenue losses from restrictions, transfer costs, contingency funds contributions and debt repayment:

$$\min f_{CF} = \ max_j \left[\tfrac{1}{N_{ys} \cdot N_r} \textstyle\sum_{i=1}^{N_r} \sum_{y=1}^{N_{ys}} SYC_{i,j}^y \right] \tag{S11}$$

Next,

$$SYC_{i,j}^{y} = \frac{\sum_{C \in C_j} PMT_{\ i,j,c} + IP_{i,j}^{y} + \ \theta_{acfc,j} \cdot \ ATR_{i,j}^{y} + (RL_{i,j}^{y} + TC_{i,j}^{y} - IC_{i,j}^{y} - CF_{i,j}^{y}, 0)}{ATR_{i,j}^{y}} \tag{S12}$$

where $SYC_{i,j}^{y}$ correspond to yearly costs for service area j, $PMT_{\ i,j,c}$ is the debt payment for infrastructure option c, $ATR_{i,j}^{y}$ is the total annual volumetric revenue, $IP_{i,j}^{y}$ is the insurance contract cost in year y, $RL_{i,j}^{y}$ is revenue losses due to water restriction, $TC_{i,j}^{y}$ is the yearly water transfer costs, $IC_{i,j}^{y}$ represents insurance coverage value, and $CF_{i,j}^{y}$ is the value available in contingency fund.

The last objective, Worst First Percentile Cost (WCC) represents the 1% highest year drought management costs across the planning horizon of all SWOs:

$$\min f_{WCC} = \ max_j\{quantile_{i \in N_r}(SYC_{i,j}, 0.99)\} \tag{S13}$$

where

$$SYC_{i,j}^{y} = \ max \frac{RL_{i,j}^{y} + TC_{i,j}^{y} - \ \theta_{acfc,j} \cdot \ ATR_{i,j}^{y} - \ YIPO_{i,j}^{y}, 0}{ATR_{i,j}^{y}} \tag{S14}$$

where IP is the insurance contract cost in year y, YIPO is the total insurance payout over year y.

As already described in Many-Objective Optimization Section, the DU Optimization was executed using Borg MOEA (Hadka and Reed 2013), a multi-objective evolutionary algorithm that applies epsilon (ϵ)-dominance archiving (Laumanns et al. 2002), stagnation detection, and randomized restarts to avoid local optima and overcome dominance resistance (Hadka and Reed 2013; Hanne 2001). The significance for ϵ-dominance for each objective evaluation is presented in Table S5.

Table S5. The ε-dominance for objectives' evaluation

Objective	**ε-dominance**
Reliability	0.001
Restriction Frequency	0.005
Infrastructure Net Present Cost	10.000.000
Peak Financial Cost	0.002
Worst First Percentile Cost	0.005

Appendix S2. Building DU SOW Components

As already described in Methods Section, DU Optimization and Re-evaluation involves simulating each candidate policy over a large ensemble of DU SOWs, comprised of one vector of DU factors and one hydroclimatic realization (Natural Inflow, Natural Evaporation and Water Demand synthetic series). The DU vector is arranged as a row of the Ψ_s matrix, and presents one value for each DU of the FDB context. Each DU element is sampled using Latin Hypercube Sampling (LHS; McKay et al. 1979) within the ranges presented in Table S6. The boundaries in which DUs can vary were defined based upon technical meetings with the management and regulation agencies of the FDB water supply system, CAESB and ADASA, respectively.

The hydroclimatic realizations consist of a combination of 1,000 40-year long synthetic timeseries of natural inflows, natural evaporation, and water demands for each service areas. The inflows and evaporation timeseries were built using the Modified Gaussian Fraction Noise (mFGN) method (Kirsch et al. 2013), which bootstraps data from the historical record by accounting for temporal and spatial correlations to generate timeseries that represent realistic possible future alternatives. It's important to point out that the lack of large hydrologic historical data is a common obstacle in many Brazilian studies, and was overcome with the use of data filling and extension methodology presented in Souza (2022).

Fig. S2 shows the flow duration curves of historic and synthetic data for the water sources of the two service areas (Descoberto and Corumba reservoirs for Descoberto service area, Paranoa and Santa Maria reservoirs and Bananal/Torto streams for Santa Maria service area). The figures present the probability of exceedance based upon yearly data of the synthetic and historic flows. Since it has more extreme low and high values, the synthetic series appear to expand upon historic observations, without a bias and following the same hydrologic within-year behavior.

Table S6. Deep uncertainties and respective boundaries defined in a collaborative process with management and regulation agencies of the FDB water supply system

Deep uncertainties		**Reference Value**	**Lower Bound**		**Upper Bound**	
			MF[a]	**AV[b]**	**MF**	**AV**
Financial Indexes	Bond interest rate (% py)	12.00	0.84	10.08	1.16	13.92
	Bond term (years)	15.00	0.90	13.50	1.30	19.50
	Discount rate (%)	4.00	0.80	3.20	1.80	7.20
Water and Sanitation Tariffs (R$/m³)	Residential	4.43	1.02	4.52	1.16	5.14
	Commercial	13.08		13.34		15.17
	Industry	12.02		12.26		13.94
	Public services	13.08		13.34		15.17
	Sewage	4.80		4.89		5.57
Drought mitigation instruments effectiveness of water consumption restriction (%)	1st stage	2.00	0.80	1.60	1.20	2.40
	2nd stage	4.00		3.20		4.80
	3rd stage	10.00		8.00		12.00
Time to get Permitting (years)	Corumba - 1st stage	0.00	-	-	-	-
	Corumba - 2nd stage	0.00	-	-	-	-
	Corumba - 3rd stage	5.00	0.60	3.00	1.40	7.00
	Descoberto resevoir expansion	0.00	-	-	-	-
	Paranoa - 1st stage	0.00	-	-	-	-
	Paranoa - 2nd stage	0.00	-	-	-	-
	Paranoa - 3rd stage	0.00	-	-	-	-
Construction costs (in millions of R$)	Corumba - 1st stage	276.50	1.00	276.50	1.30	359.45
	Corumba - 2nd stage	222.10		222.10		288.73
	Corumba - 3rd stage	251.40		251.40		326.82
	Descoberto resevoir expansion	7.50		7.50		9.75
	Paranoa - 1st stage	60.30		60.30		78.39
	Paranoa - 2nd stage	60.30		60.30		78.39
	Paranoa - 3rd stage	60.30		60.30		78.39

Note: [a]MF: Multiplicative Factor - the value effectively applied as boundaries for sampling DU values used in WaterPaths. [b]AV: Absolute Value – value obtained when MF multiplies the Reference Value, and represents the actual value of a DU factor or boundary.

It's important to emphasize that the aspect of evaporation curves is due to the lack of available daily records in the reservoirs' region. Thus, given that the FDB has only two well defined seasons – one rainy, hot summer and one dry, cold winter (CODEPLAN 2020) – the assumption of equal daily evaporation rates across the months is reasonable for the purposes of this work.

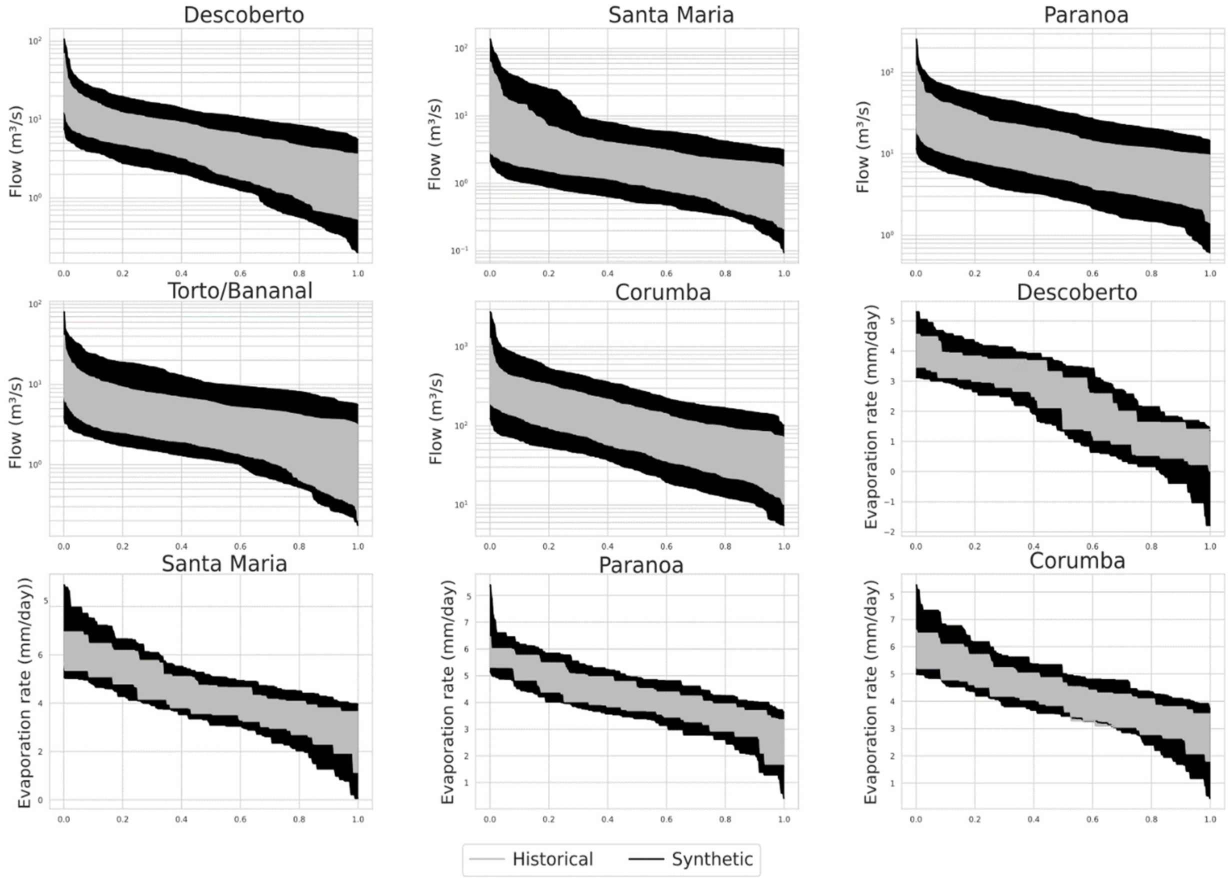

Fig. S2. Flow duration curves for natural inflow and natural evaporation synthetic series.

Figs. S3–S11 present statistic comparisons of observed and synthetic data, generated from one-hundred ensemble of synthetic series with 100-years length, and a bootstrapped historical data with the same size and length. We can denote that, for all water sources, streamflow and evaporation synthetic series present reasonably close behavior if compared to historical data.

Given the non-parametric nature of the method applied for synthetic series generation, Wilcoxon rank-sum test and Levene's test were used to test if synthetic monthly medians and variances were statistically different from observations. The associated p-values indicate that none of the synthetic momentum differ from the historical at significance level of 0.05.

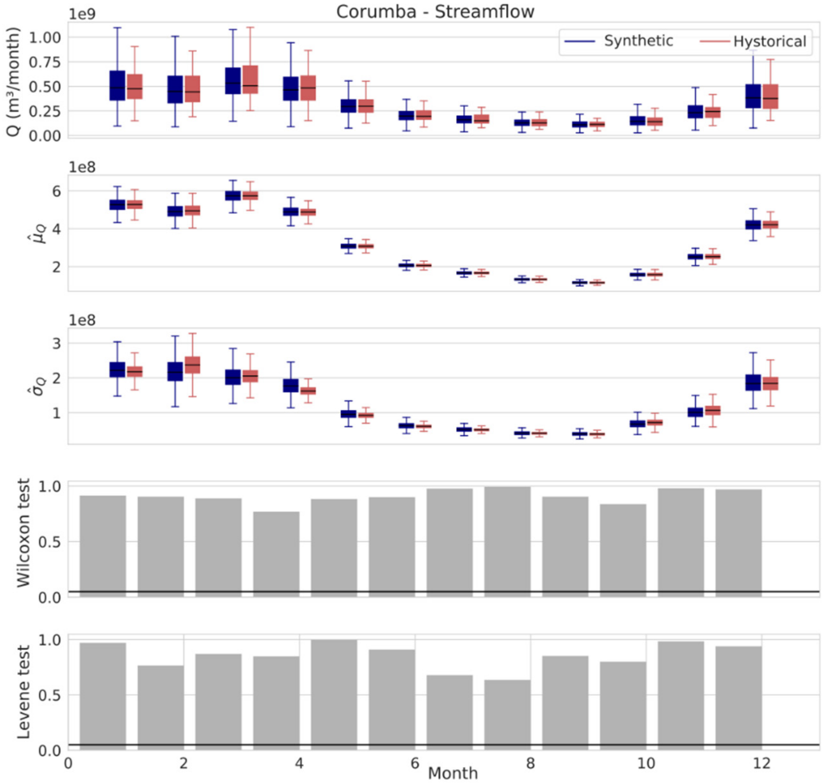

Fig. S3. Statistical evaluation for the Corumba synthetic streamflow timeseries.

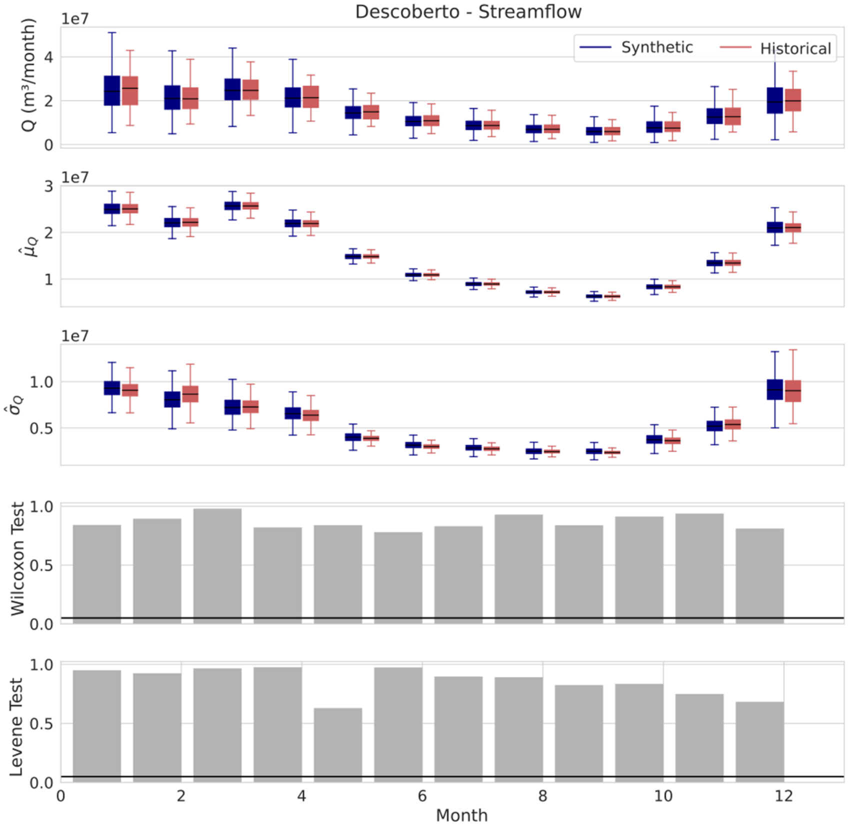

Fig. S4. Statistical evaluation for the Descoberto synthetic streamflow timeseries.

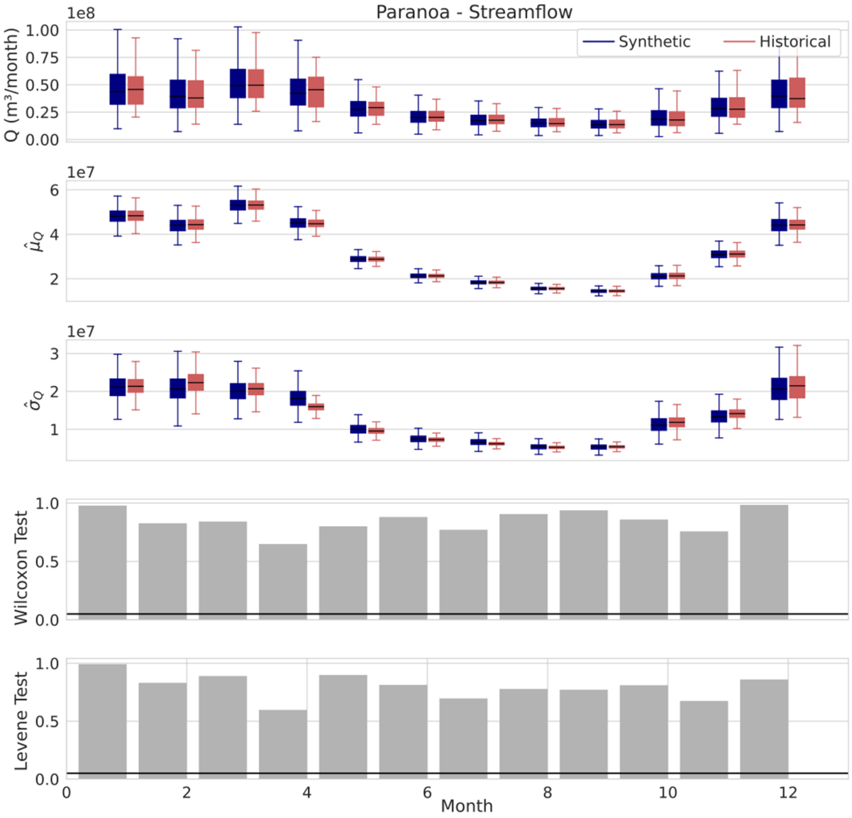

Fig. S5. Statistical evaluation for the Paranoa synthetic streamflow timeseries.

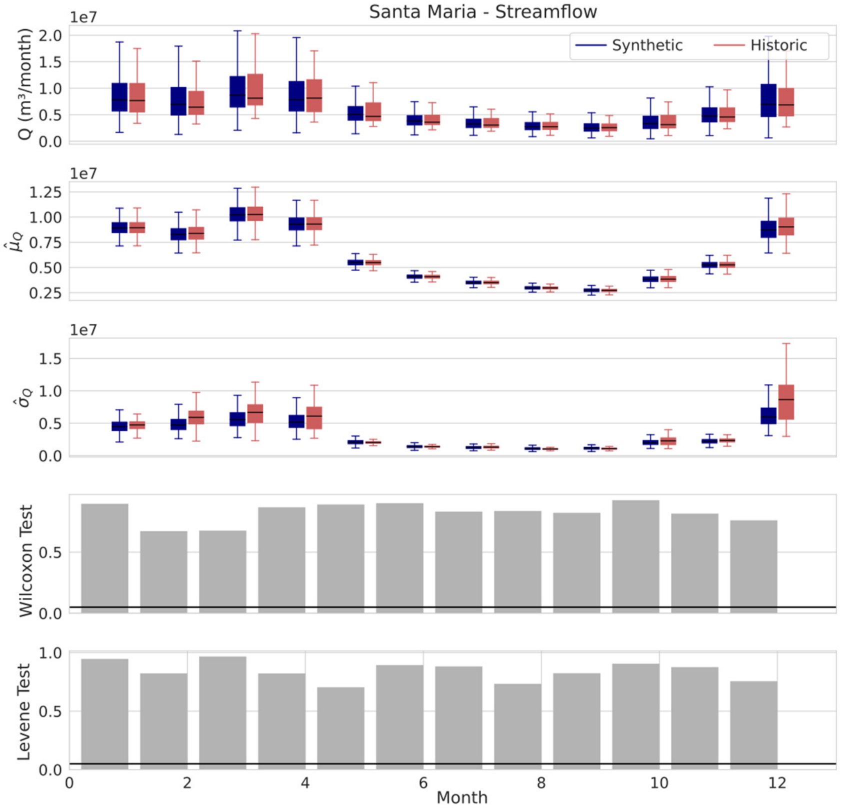

Fig. S6. Statistical evaluation for the Santa Maria synthetic streamflow timeseries.

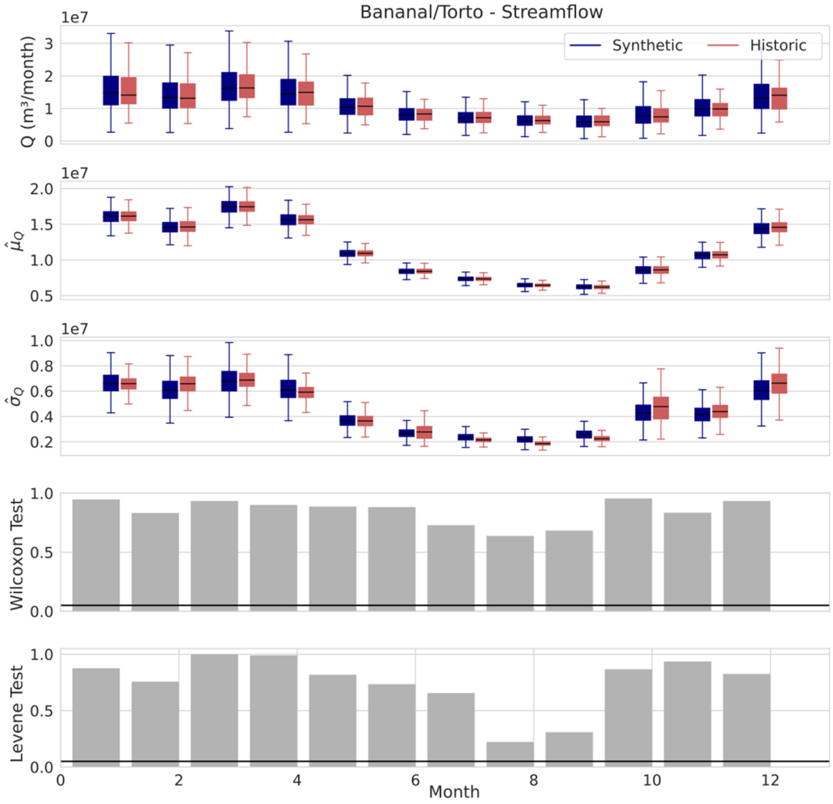

Fig. S7. Statistical evaluation for the Bananal-Torto the synthetic streamflow timeseries.

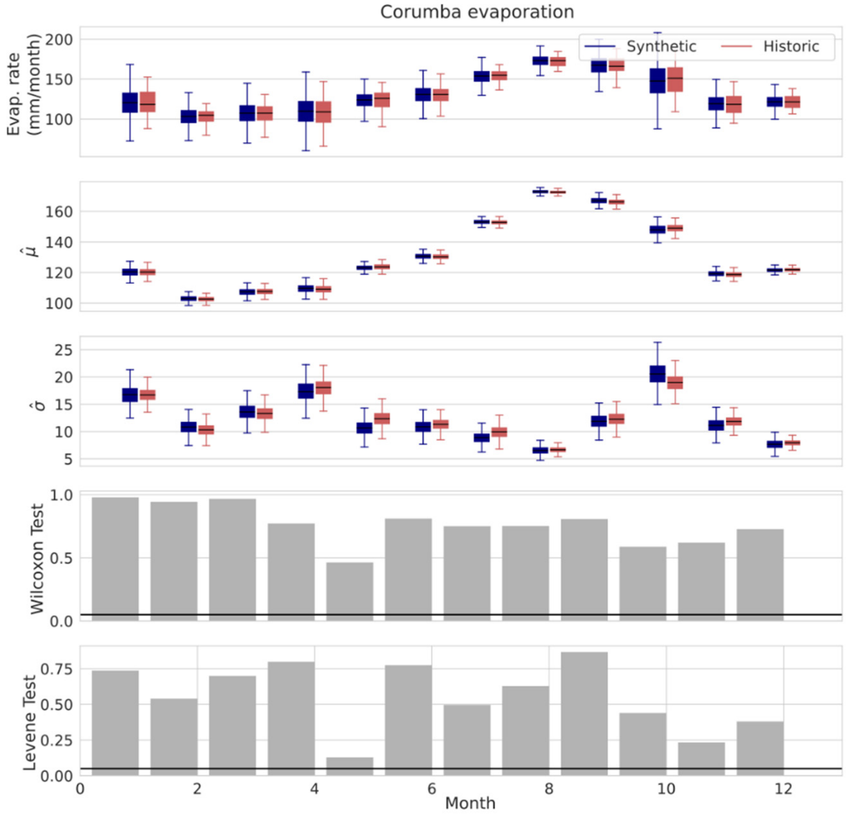

Fig. S8. Statistical evaluation for the Corumba synthetic evaporation timeseries.

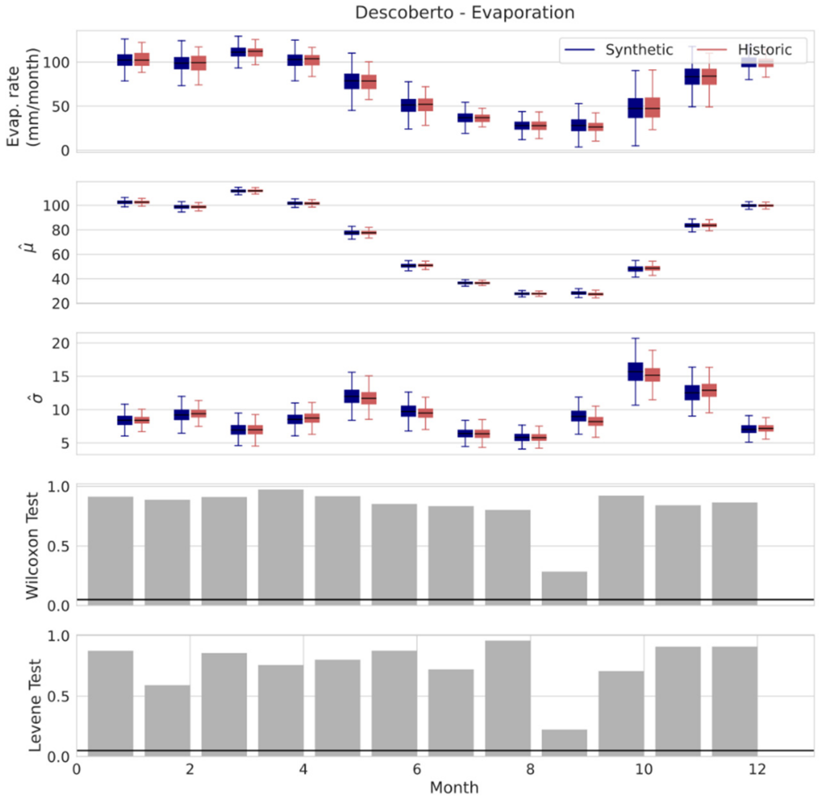

Fig. S9. Statistical evaluation for the Descoberto synthetic evaporation timeseries.

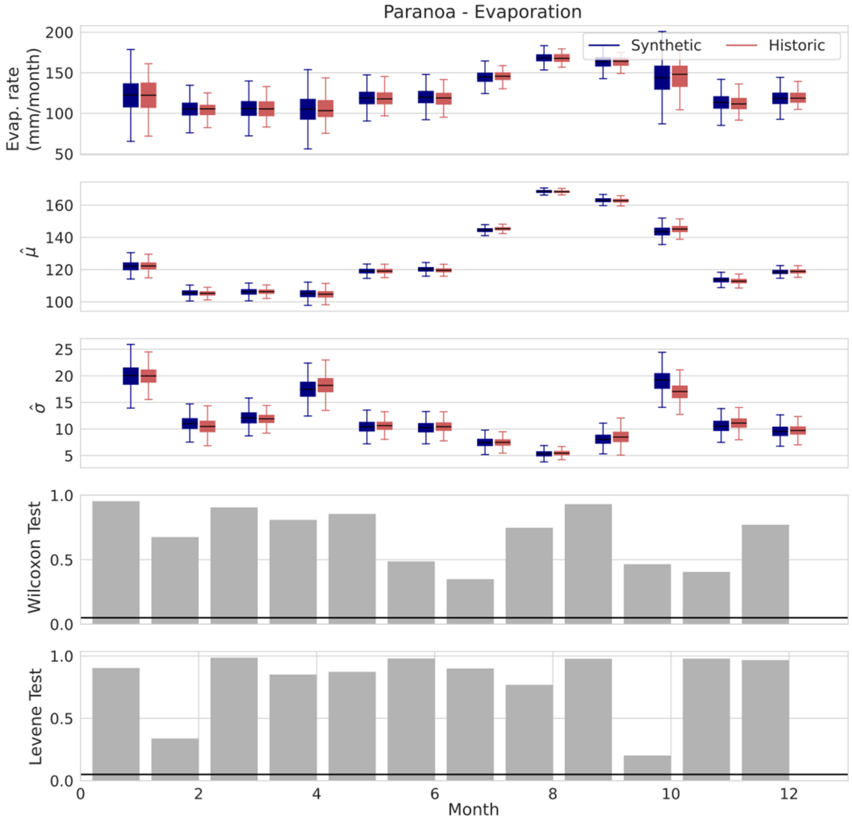

Fig. S10. Statistical evaluation for the Paranoa synthetic evaporation timeseries.

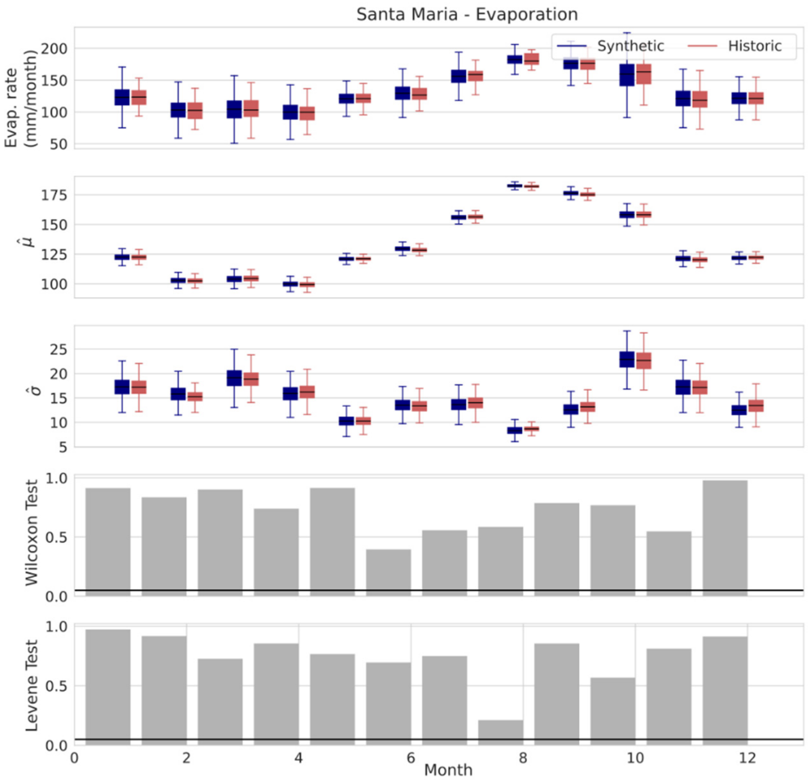

Fig. S11. Statistical evaluation for the Santa Maria synthetic evaporation timeseries.

The 1,000 demand time series were built applying different multiplicative factors to a reference demand projection. This reference series, in turn, was obtained by taking the Federal District population projection for the next 40 years in IBGE, and associating it with demand estimatives extracted from Federal District Sanitation Plan of 2017 (GDF 2017). Figures S12 and S13 show the highest and lowest demand synthetic series for Descoberto and Santa Maria service area, suggesting reasonable variability given population projections for each set of the FDB Administrative Regions.

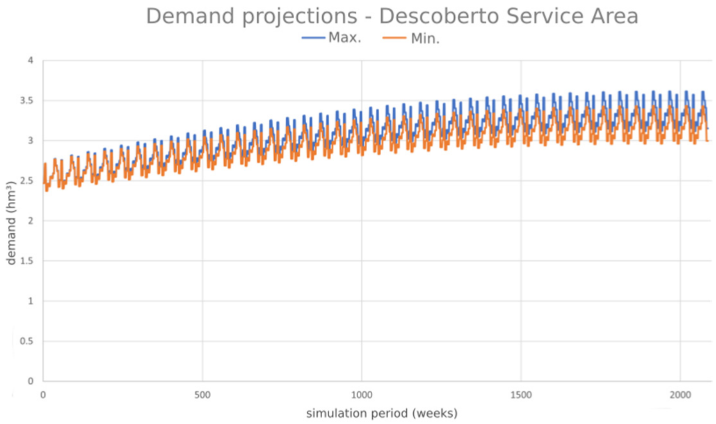

Fig. S12. Upper- and lower-bounds of the demand projections for the Descoberto service area.

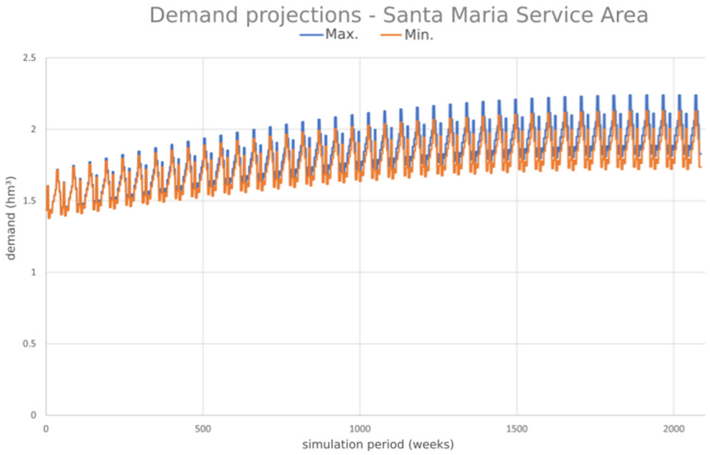

Fig. S13. Upper- and lower-bounds of the demand projections overview for the Santa Maria service area.

Appendix S3. MOEA Runtime Diagnostics

We run multiple instances of the Borg MOEA to ensure the algorithm has overcome any biases generated by the random sampling of the initial population (Salazar et al. 2017). In this experiment, we ran 5 random seeds using the Master-Worker configuration of the Borg MOEA. The true Pareto set for this problem is not known, so we used the relative hypervolume metric to assess the convergence of each seed (Zitzler et al. 2003). The relative hypervolume compares the performance of the Pareto sets discovered at set checkpoints within each seed to the final “reference set”, which contains non-dominated solutions across all seeds. We conclude that the algorithm has converged to a satisfactory approximation of the true Pareto set when the hypervolume of each reference set plateaus. Runtime diagnostics for all seeds are shown in Fig. S14. There was some variance across seeds, but the hypervolume of each optimization run plateaued after approximately 10,000 function evaluations.

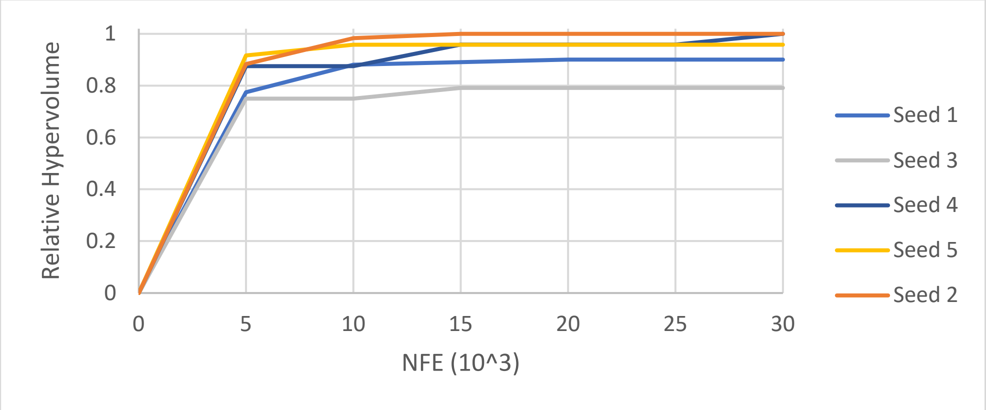

Fig. S14. Runtime diagnostics for optimization.

Appendix S4. Gradient Boosted Trees Feature Importance

We measure feature importance by evaluating how each DU factor reduces leaf impurity during Gradient Boosted Trees classification. Leaf impurity provides a measure of how "mixed" a leaf of a classification tree is. A leaf containing all scenarios with the same classification will have a leaf impurity of 0, and leaf impurity will increase with the increasing faction of scenarios classified differently. We calculate the percentage of the total decrease in leaf impurity across all trees due to splits from each DU factor in the performance of a policy to calculate feature importance. Feature importance for the High infrastructure and Moderate infrastructure policies are shown in Table S7.

Table S7. Feature importance ranking for the High infrastructure and Moderate Infrastructure compromises

Factor	Feature importance for High Infrastructure compromise	Feature importance for Moderate Infrastructure compromise
Demand Growth	0.432	0.527
Permitting Time	0.001	0.000
Construction Time	0.002	0.000
Bond Term	0.002	0.002
Bond Interest Rate	0.001	0.002
Discount Factor	0.001	0.002
Restriction Effectiveness	0.561	0.467

Appendix S5. Scenario Discovery for Santa Maria

The compromise policies perform extremely well for Santa Maria across all SOWs. Santa Maria does not fail the robustness criteria (90% reliability, 20% restriction frequency) under any sampled SOW. An factor map showing Santa Maria's performance for the moderate infrastructure compromise is shown in Fig. S15.

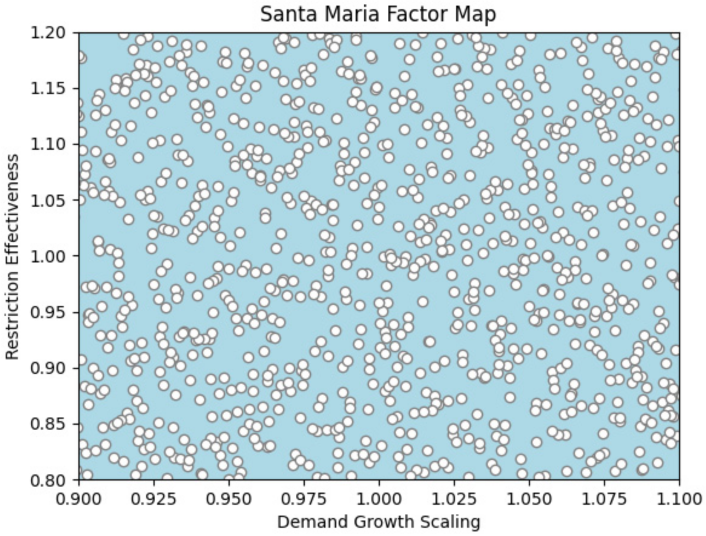

Fig. S15. Factor map for Santa Maria. Each point represents a sampled SOW, with white points representing SOWs where the policy meets performance criteria, and red points representing SOWs where the policy fails to meet performance criteria. The policy meets performance criteria under all sampled SOWs.

References

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