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Enhancing long short-term memory (LSTM)-based streamflow prediction with a spatially distributed approach

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S1 Map of the streamflow gauging stations

Figure S1 below shows the modelled gauging station locations (by watershed outlet location). Notably, it emphasizes the positions of non-GRIP-GL stations in comparison to GRIP-GL stations.

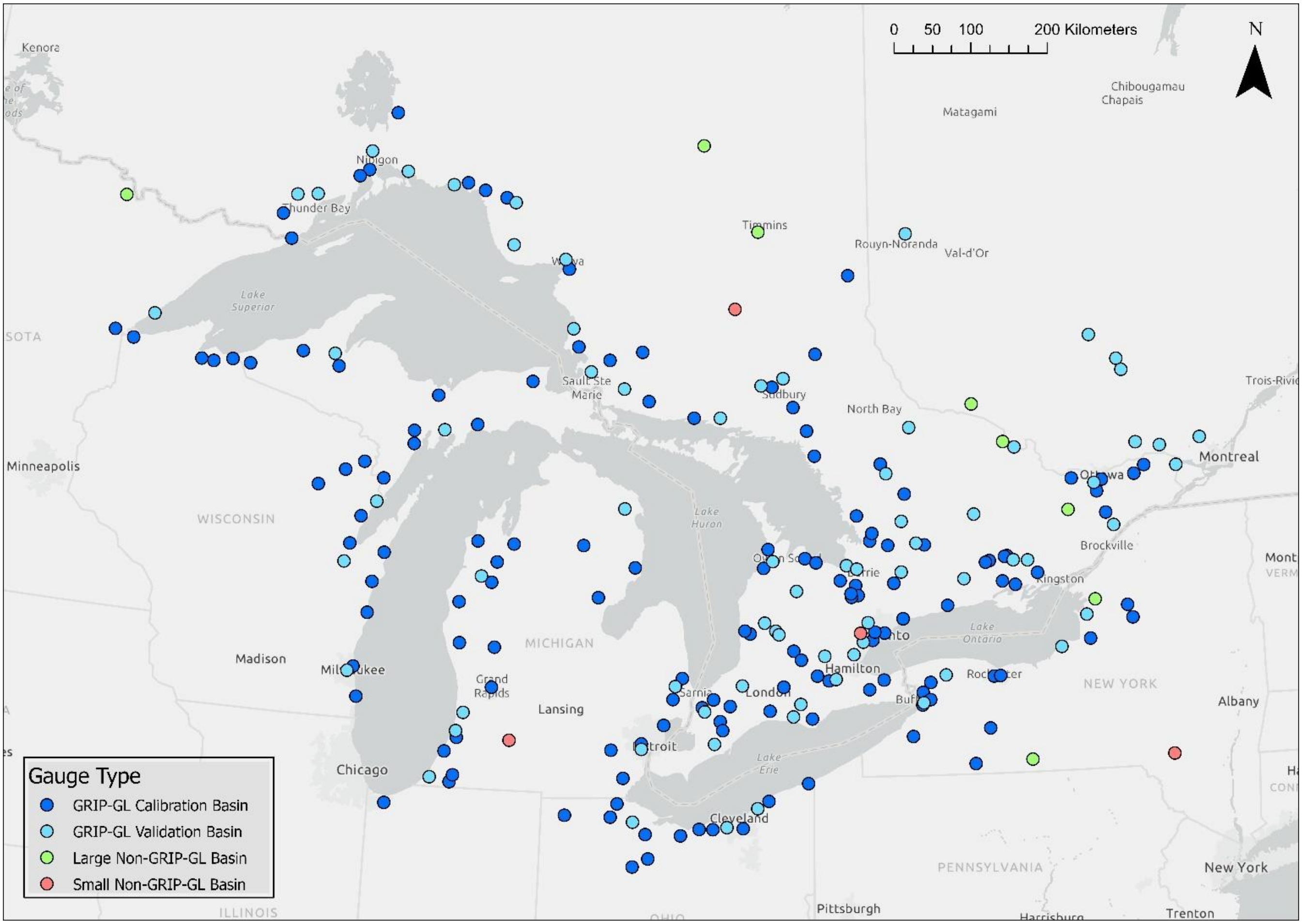

Figure S1. Locations of the streamflow gauging stations used in this study. In total, there are 224 streamflow gauging stations (shown as dots in the map). The 212 stations used in the GRIP-GL study are shown in dark blue dots (calibration) and light blue dots (validation). The stations of the 4 small Non-GRIP-GL basins (described in Sec 3.1 of the main article) are shown in light red dots, and the stations of the 8 large Non-GRIP-GL basins (described in Sec 3.2 of the main article) are shown in light green dots.

S2 Raven configurations for the routing-only mode

The routing-only model is defined within the Raven hydrologic modelling framework (Craig et al., 2020). It takes the LSTM-predicted subbasin-level streamflow as inputs, and then simulates the water routing through the delineated lake-river network. The mean daily subbasin-level streamflow is taken as precipitation at the hourly time-step (24 hours of constant precipitation intensity rate) and the precipitation in each subbasin is instantly flushed to the subbasin outlet. This approach ensures there is no in-catchment routing delay in the simulation, as would normally occur in a typical routing application that move surface runoff across a subbasin into the channel with a unit hydrograph. The model combines this subbasin-level streamflow at the subbasin outlet with in-channel routed streamflow that entered the subbasin from upstream subbasins. Figure S2 below shows the structure of the .rvi file (the primary input file of Raven) that defines the routing-only model.

```
# ----------------------------------------------
# Raven Input file
# ----------------------------------------------
:StartDate               2001-01-01 00:00:00
:EndDate                 2017-12-31 00:00:00
:Method                  ORDERED_SERIES
:TimeStep                01:00:00
:RunName                 02HC017

:CatchmentRoute          ROUTE_DUMP
:Routing                 ROUTE_DIFFUSIVE_WAVE
:PrecipIceptFract        PRECIP_ICEPT_NONE
:PotentialMeltMethod     POTMELT_NONE
:SoilModel               SOIL_ONE_LAYER

:HydrologicProcesses
  :Precipitation     PRECIP_RAVEN            ATMOS_PRECIP     PONDED_WATER
  :Flush             RAVEN_DEFAULT           PONDED_WATER     SURFACE_WATER
:EndHydrologicProcesses

:EvaluationMetrics                     NASH_SUTCLIFFE    PCT_BIAS    KLING_GUPTA

:EvaluationPeriod TRAINING 2001-01-01 2010-12-31
:EvaluationPeriod TESTING 2011-01-01 2017-12-31
```

Figure S2. The .rvi file structure for implementing the routing-only setup in this study.

The ‘:CatchmentRoute’ command specifies the in-catchment routing method, which is used to represent how water is transported from the subbasin tributaries to the subbasin outlets. Since subbasins are the smallest response unit in this study, we choose the ‘ROUTE_DUMP’ algorithm as the in-catchment routing method, in which all of the water is instantly dumped to the subbasin outlet.

The ‘:Routing’ command specifies the in-channel routing method, which is used to represent how water is transported from upstream to downstream within the primary subbasin channels. We choose the ‘ROUTE_DIFFUSIVE_WAVE’ algorithm as the in-channel routing method, which applies an analytical solution to the diffusive wave equation through the reach using a constant reference celerity (Raven Development Team, 2023).

The ':PrecipIceptFract' command specifies the method for estimating the fraction of precipitation intercepted by canopy. Since the LSTM-predicted subbasin-level streamflow inputs are taken as precipitation in Raven, we used the 'PRECIP_ICEPT_NONE' algorithm to indicate that there are no canopy interception processes.

The ':PotentialMeltMethod' command specifies the method for estimating the potential snow melt. We adopted the 'POTMELT_NONE' algorithm because snow melt processes are not considered in the routing-only mode.

The ':SoilModel' command specifies the soil structure model used for routing. We used the 'SOIL_ONE_LAYER' mode which defines single soil layer structure. It is worth mentioning that soil water is not simulated in the routing-only mode but Raven requires an input for the ':SoilModel' option, even if it is not used.

The ':HydrologicProcesses' block defines the hydrologic processes to be simulated. The routing-only mode only included two hydrologic processes, ':Precipitation' and ':Flush'. As mentioned previously, the subbasin-level streamflow inputs are taken to mimic precipitation, and then flushed on the land surface to the stream reach.

```
#----------------------------------------------
# This is a Raven lake rvh file generated
# by BasinMaker v2.0
#----------------------------------------------
#############################################
# New Lake starts
#############################################
:Reservoir   Lake_108369
  :SubBasinID  3047150
  :HRUID   26
  :Type RESROUTE_STANDARD
  :WeirCoefficient  0.6
  :CrestWidth    10.7983
  :MaxDepth 12.7
  :LakeArea    7515656.781559977
  :SeepageParameters   0   0
:EndReservoir
```

Figure S3. The .rvh file structure for representing lakes/reservoirs in the routing model.

Furthermore, the routing-only model is configured to simulate lakes/reservoirs (water levels and outflows) with a surface area greater than 5 km^2. Figure S3 shows the Raven command block that define a lake/reservoir in the routing network, the command block is automatically generated by the BasinMaker library (Han et al., 2023). All lakes are assumed to be vertically prismatic and are simulated with a lake outlet structure that is a broad-crested weir. Raven applies Equation S1 below to simulate the lake/reservoir outflow:

$$Q(s) = \frac{2}{3}\sqrt{2g} * C * L * s^{3/2} \quad \text{(S1)}$$

Where g is the gravitational constant, C represents the weir coefficient, L is the crest width, and s is the lake stage relative to the weir crest elevation. All lakes are initialized with a water level of zero. The weir coefficient is a fixed value of 0.6. The crest width is assigned with a region-dependent value according to the delineation methodology employed in the BasinMaker library. Each lake is represented by its corresponding 'lake subbasin' in the routing network and there are no channels within the lake subbasin. All lake inlets are defined as upstream subbasin outlets, and the single lake outlet corresponds to the lake subbasin outlet.

S3 Lumped LSTM configurations

Recall that the lumped LSTM is a replicate of the LSTM built for the GRIP-GL study (Mai et al., 2022) and the settings/input description below is taken from the supplemental information from that study.

Table S1. Hyperparameter settings used for the lumped LSTM.

Hyperparameter	value/range
Hidden size	256
Batch size	64
Epochs	30
Learning rate[1]	(**0**: 0.0005, **20**: 0.0001, **30**: 0.00005)
Sequence length	365 days
Dropout	0.4
Loss function	Nash-Sutcliffe efficiency (NSE)[2]

[1](**0**: x_1, **5**: x_2, **10**: x_3) denotes learning rate x_1 for epoch 0 to 4, learning rate x_2 for epoch 5 to 9, and learning rate x_3 after epoch 10.
[2]Basin-averaged NSE loss – the average of the NSE values across the calibration/training basins (Kratzert et al., 2019).

The loss function is shown in Equation S2 below:

$$\mathrm{NSE} = \frac{1}{B} + \sum_{b=1}^{B} \sum_{n=1}^{N} \frac{(\hat{y}_n - y_n)^2}{(s(b)+\epsilon)^2} \qquad \text{(S2)}$$

Where B is the number of basins, N is the number of samples (days) per basin B, $\hat{y}_n$ is the prediction of sample n ($1 \leq \mathrm{n} \leq N$), y_n is the observation, and $s(b)$ is the standard deviation of the discharge in basin b ($1 \leq b \leq B$), calculated from the training period (Kratzert et al., 2019).

The input variables required to drive the LSTM are grouped into dynamic attributes (Table S2) computed at the daily time step, and static attributes (Table S3) which are taken as constant through the LSTM training period.

Table S2. CaSR-v2/RDRS-v2 forcing variables used for the lumped LSTM. For initial lumped LSTM training, these variables are derived for each of the gauged basins. For the SR-model, these variables are derived for each of subbasins in the routing network.

Variable name	Unit
Quantity of precipitation	m
Downward solar flux	W/m^2
Minimum air temperature	°C
Maximum air temperature	°C
Specific humidity	kg/kg
U wind component	kts
V wind component	kts
Surface pressure	mb
Potential evapotranspiration (PET)	mm/day

Table S3. Static attributes defining lumped LSTM input variables. For initial lumped LSTM training, these variables are derived for each of the gauged basins. For the SR-model, these variables are derived for each of subbasins in the routing network.

Attribute Name	Unit
Mean daily precipitation	mm/day
Mean daily PET	mm/day
Aridity (ratio of mean PET to mean precipitation)	-
Mean daily temperature	°C
Fraction of precipitation falling on days with mean daily temperatures below 0°C	-
Frequency of days with high precipitation (≥ 5 times the mean daily precipitation)	days/year
Average duration of high-precipitation events	days
Frequency of dry days (daily precipitation less than 1 mm/day)	days/year
Average duration of dry periods	days
Catchment mean elevation	meter
Standard deviation of catchment elevation	meter
Catchment mean slope	meter/kilometre
Standard deviation of catchment slope	meter/kilometre

Catchment area	km^2
Fraction of land covered by ‘Temperate-or-sub-polar-needleleaf-forest’	-
Fraction of land covered by ‘Temperate-or-sub-polar-grassland’	-
Fraction of land covered by ‘Temperate-or-sub-polar-shrubland’	-
Fraction of land covered by ‘Temperate-or-sub-polar-grassland’	-
Fraction of land covered by ‘Mixed-Forest’	-
Fraction of land covered by ‘Wetland’	-
Fraction of land covered by ‘Cropland’	-
Fraction of land covered by ‘Barren-Lands’	-
Fraction of land covered by ‘Urban-and-Built-up’	-
Fraction of land covered by ‘Water’	-
Soil bulk density	g/cm^3
Soil clay content	% of weight
Soil gravel content	% of volume
Soil organic carbon	% of weight
Soil sand content	% of weight
Soil silt content	% of weight

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