# The SUMMA-SUNDIALS Earth System Model

Raymond Spiteri[1], Reza Zolfaghari[2], Wouter Knoben[3], and Martyn Clark[3]

[1]Numerical Simulation Lab, University of Saskatchewan
[2]University of Saskatchewan
[3]University of Saskatchewan Coldwater Laboratory

November 21, 2022

**Abstract**

The next generation of Earth System models promisesunprecedented predictive power through the application of improvedphysical representations, data collection, and high-performancecomputing. A key component to the accuracy, efficiency, and robustnessof the Earth System simulations is the time integration ofdifferential equations describing the physical processes. Manyexisting Earth System models are simulated using low-order,constant-stepsize time-integration methods with no error control,opening them up to being inaccurate, inefficient, or require aninfeasible amount of manual tweaking when run over multipleheterogeneous domains or scales. We have implemented the variable-stepize, variable-order differentialequation solver SUNDIALS as the time integrator within the Structurefor Unifying Multiple Modelling Alternatives (SUMMA) modelframework. The model equations in SUMMA were modified and augmented toexpress conservation of mass and enthalpy. Water and energy balanceerrors were tracked and kept below a strict tolerance. The resultingSUMMA-SUNDIALS software was successfully run in a fully automatedfashion to simulate hydrological processes on the North Americancontinent, sub-divided into over 500,000 catchments. We compared the performance of SUMMA-SUNDIALS with a version (calledSUMMA-BE) that used the backward Euler method with a fixed stepsize asthe time-integration method. We find that SUMMA-BE required two ordersof magnitude more CPU time to produce solutions of comparable accuracyto SUMMA-SUNDIALS. Solutions obtained with SUMMA-BE in a similar orshorter amount of CPU time than SUMMA-SUNDIALS often contained largediscrepancies. We conclude that sufficient accuracy, efficiency, and robustness ofnext-generation Earth System model simulations can realistically onlybe obtained through the use of adaptive solvers. Furthermore, wesuggest simulations produced with low-order, constant-stepsizesolvers deserve more scrutiny in terms of their accuracy.

University of Saskatchewan Numerical Simulation Research Lab

# The SUMMA–SUNDIALS Hydrological Model

**Raymond J. Spiteri**[†] Reza Zolfaghari[†] Wouter J.M. Knoben[‡] Kevin R. Green[†] Kyle Klenk[†] Ashley E. Van Beusekom[‡] Martyn P. Clark[‡]

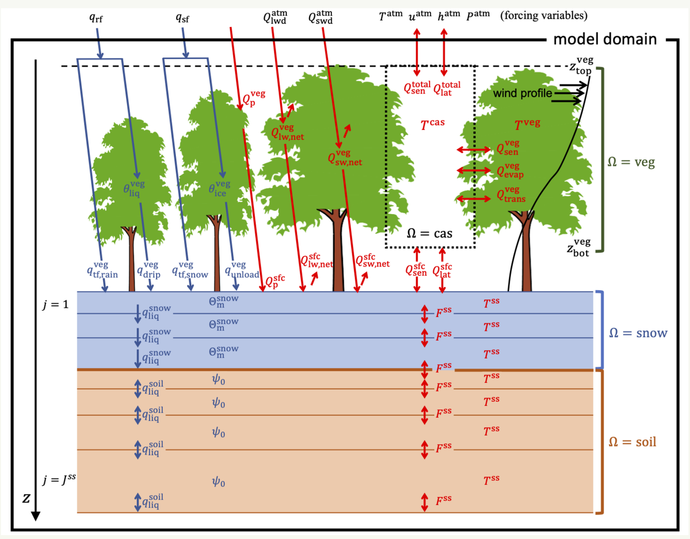
[†]Department of Computer Science, University of Saskatchewan
[‡]Coldwater Laboratory, University of Saskatchewan

## Motivation

- Upcoming Earth System models promise unmatched predictive power.
- A key component to the accuracy, efficiency, and robustness of Earth System simulations is the time integration of differential equations describing the physical processes.
- Many existing Earth System models use low-order, constant-stepsize time-integration methods with no error control.

## What is SUMMA?

The Structure for Unifying Multiple Modelling Alternatives (SUMMA) model is a software framework that enables the exploration and analysis of different hydrological models and their constituent components in a systematic way[1].




## What is SUNDIALS?

The SUite of Nonlinear and DIfferential/ALgebraic equation Solvers (SUNDIALS) is a set of six software librairies that provide robust numerical solutions and sensitivity analysis for nonlinear algebraic equations and ordinary and differential-algebraic equations[2].

## Experiments

- 517,315 basins in North America (median 33 km$^2$; mean 40 km$^2$)
- Time span: 1986-01-01 00:00 to 1986-12-31 23:00; hourly forcing.
- SUMMA running backward Euler (BE) with constant step $\Delta t/64$ (BE64) is taken as the ground truth.

## Results

- BE with constant step size $\Delta t$ requires less computation time than SUNDIALS.
- SUNDIALS is generally more accurate than BE.

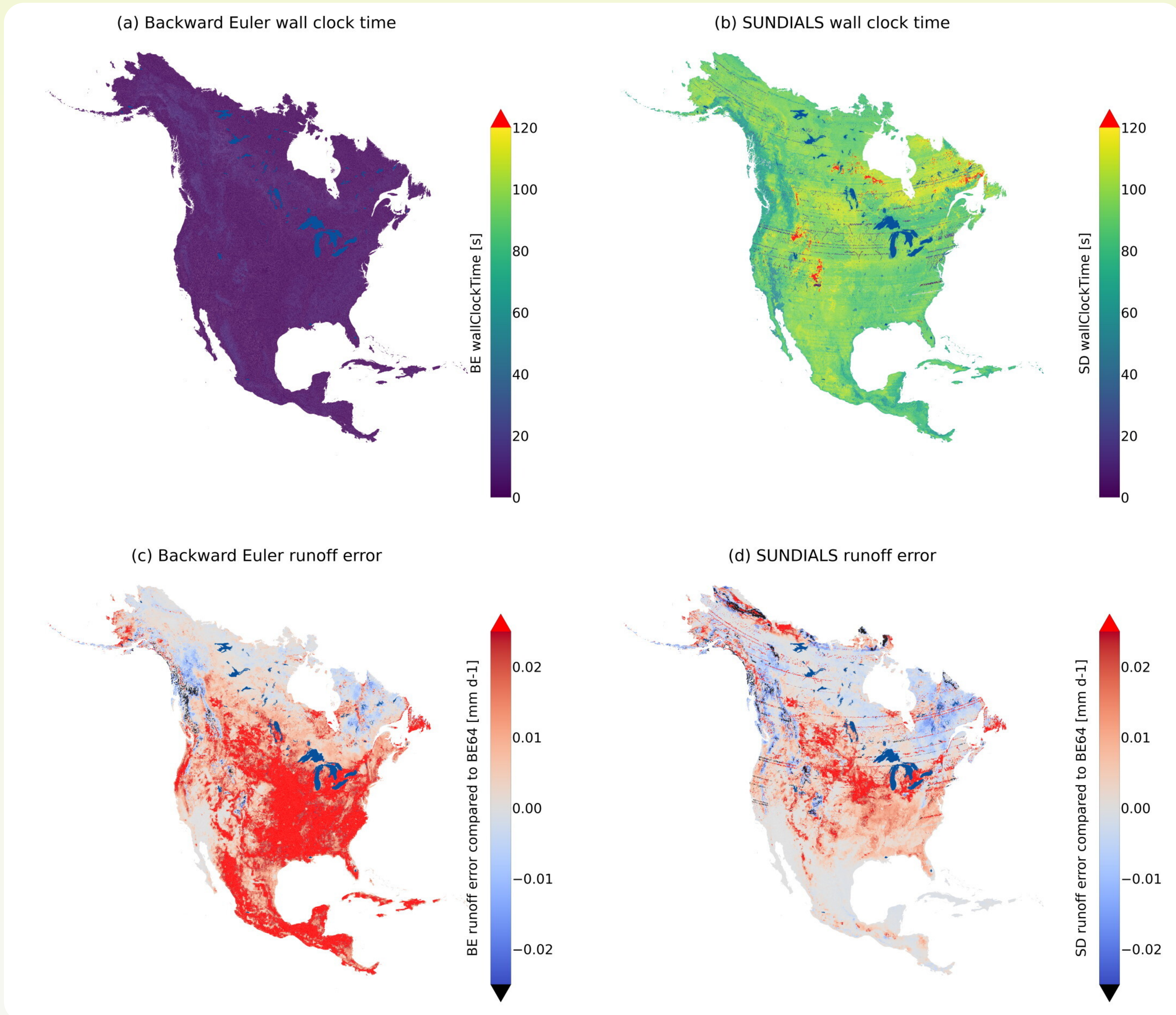
## Conclusions

- One-off time integration with low-order methods and constant step-sizes is fraught with risk of inaccuracy and inefficiency.
- State-of-the-art time-integration software with error control generally produces accurate solutions in an efficient manner and can be applied on large domains where manual tuning is infeasible.

## Future Work

- Global simulations.
- Adaptive error control in space.
- Fault tolerance and automatic restart.
- Dynamic load balancing.

## One-off time integration with low-order methods and constant step-sizes is fraught with risk of inaccuracy and inefficiency.




## Details: SUMMA

SUMMA solves coupled conservation equations for thermodynamics and hydrology for the sub-domains of the canopy air space (cas), vegetation (veg), snow, and soil. For a given model sub-domain $\Omega$, the state equations for thermodynamics and hydrology can be written as

$$\frac{\partial H^\Omega}{\partial t} = -\frac{\partial F^\Omega}{\partial z} + \mathcal{F}^\Omega_{\text{sink}}, \qquad \Omega = \text{cas, veg, snow, soil}, \tag{1a}$$

$$\frac{\partial \Theta^\Omega_{\text{m}}}{\partial t} = -\frac{\partial q^\Omega_{\text{ice}}}{\partial z} - \frac{\partial q^\Omega_{\text{liq}}}{\partial z} + \mathcal{M}^\Omega_{\text{sink}}, \qquad \Omega = \text{veg, snow, soil}. \tag{1b}$$

## Details: SUNDIALS

Equations (1) are discretized vertically in space à la method of lines.
Time integration of the resulting system is performed using the IDA package from SUNDIALS that solves initial-value problems for implicit ordinary and differential-algebraic equations of the form $\mathbf{f}(t, \mathbf{y}, \dot{\mathbf{y}}) = \mathbf{0}$ via variable-stepsize, variable-order backward differentiation formulas.

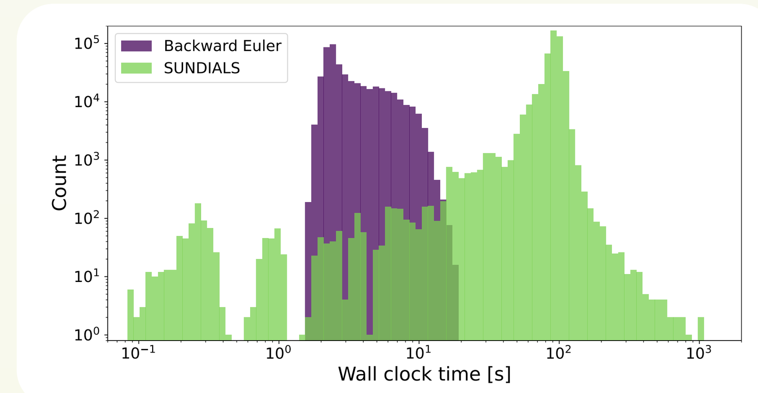
## Details: Experiments

Model configuration was generated through the Community Workflows to Advance Reproducibility in Hydrologic Modeling (CWARHM) project: `https://github.com/CH-Earth/CWARHM`.

## Details: Results

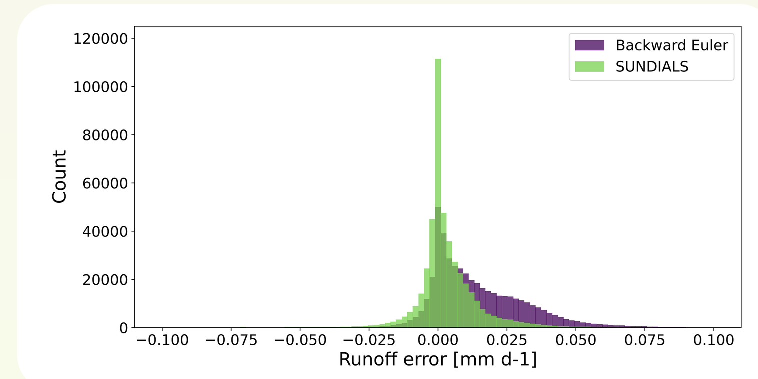
**Distribution of runtimes**

- Note logarithmic scales.
- Many SUNDIALS runs are much slower than BE.




**Distribution of errors**

- Many BE runs have larger errors than SUNDIALS.
- BE runs are biased to overestimate runoff.




## References

1. Clark, M. P., et al. (2015), A unified approach for process-based hydrologic modeling: 1. Modeling concept, Water Resour. Res., **51**, 2498– 2514, Research, doi:10.1002/2015WR017198.
2. Hindmarsh, A. C., et al. (2005), SUNDIALS: Suite of nonlinear and differential/algebraic equation solvers. ACM Trans. Math. Softw. **31**, 3, 363–396. doi:10.1145/1089014.1089020