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Reply on RC1

Yunxiang Chen et al.

Author comment on "Modeling of streamflow in a 30 km long reach spanning 5 years using OpenFOAM 5.x" by Yunxiang Chen et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-313-AC1, 2022

[Reviewer comments]: The work in this paper uses relevant field data to provide appropriate calibrations and constraints in the development of a 3-D CFD model of the streamflow in a reach at large length and time scales. I applaud this 'grand challenge' effort to establish a significant bench-mark for the accurate long time/length scale prediction of streamflow.

[Response]:
We thank Prof. Vaughan Voller's recognition of the importance of this work. Yes, this work aims to demonstrate that river hydrodynamics at tens-kilometer and multiple-year scales can be accurately predicted by combining observation data (bathymetry, water stage, and discharge), open-source CFD code (OpenFOAM), carefully designed roughness calibration strategies, and high-performance computing (HPC). Additionally, we provide reproducible procedures and guidelines regarding data acquisition, mesh generation, distributed roughness calibration, and parallel computation leveraging commonly accessible survey techniques (e.g., LiDAR, water level logger, ADCP) and computing resources. These procedures, guidelines, techniques, and computing resources altogether provide a generic and repeatable framework for modeling the streamflow at spatiotemporal scales that are essential for both local-scale water infrastructure design, construction, and operation and evaluating the impacts of climate- and human-induced discharge variations on local river hydrodynamics.

[Reviewer comments]: I have a number of comments for the authors to consider. In my view, unless the authors so wish, none of these require changes to the current manuscript.

[Response]:
We thank the reviewer's invaluable suggestion. The references have been incorporated into the Introduction section in the revised version of the paper. Please check the red text between lines 65-70.

[Reviewer comments]: 1. The authors provide a comprehensive survey of the literature of the full range of previous modeling efforts for streamflow. One set of work which may have been overlooked is a series of papers by Kang, Sotiropoulos and others
Kang, S., A. Lightbody, C. Hill, and F. Sotiropoulos (2011), High-resolution numerical simulation of turbulence in natural waterways, Adv. Water Resour., 34(1), 98– 113.
Kang, S., and F.Sotiropoulos (2011), Flow phenomena and mechanisms in a field-scale

experimental meandering channel with a pool-riffle sequence: Insights gained via numerical simulation, J. Geophys. Res., 116, F03011, doi:10.1029/2010JF001814.
Kang, S., and F.Sotiropoulos (2011), Assessing the predictive capabilities of isotropic, eddy viscosity Reynolds-averaged turbulence models in a natural-like meandering channel, Water Resources Research, 48, https://doi.org/10.1029/2011WR011375
(full disclosure I was on Kang's PhD committee)

These works compare 3-D free surface/ turbulence (both RANS and LES) model predictions of streamflow with highly resolved measurements in a natural channel. The scale of these calculations is smaller than the current work (10 's m as opposed to 10's km) but the conclusion of the Kang et al work does point out possible accuracy issues in using time averaged turbulence models.
Some questions in this regard, Is a RANS model sufficient for the task at hand? Would LES improve predictive performance? Is LES currently feasible at the scale of the current simulation?

[Responses]:
We thank the reviewer's insightful questions. Here are our thoughts on these questions. From Kang et al's AWR and WRR work, they showed that the streamwise/transverse velocities and turbulent kinetic energy profiles are reasonably predicted using LES and SST-based RANS. The main differences between LES and RANS-SST lie in predicting the 3D secondary flows. They concluded that this discrepancy depends on the level of turbulence anisotropy that is further affected by streambed geometry (roughness and channel deepening) and flow rate. In particular, in the riffle regions, the 3D flow is dominated by the large-scale rough elements that generate large anisotropic turbulence and vortices; in the pool regions, the RANS can predict the curvature-induced secondary flow, but cannot predict the other features that are caused by the anisotropic turbulence induced by channel deepening at a bank full (with depth 0.3 m) flow rate. However, such a difference is reduced at a low flow (with depth 0.1 m) as shown in the ADW paper. From these results, it can be concluded that velocities and turbulence statistics can be reasonably predicted using both RANS-SST and LES, though the complex secondary flows induced by small-scale streambed sediments and local topography variations (e.g., channel deepening) are not well predicted by RANS. For the task reported in this paper, we argue that the RANS model is sufficient for predicting water surface elevation (or depth) and velocities, whose accuracy is supported by Figs. 5,6,8,9,10. Though Kang et al showed the 3D flow structures may not be predicted by RANS (at bank full), the comparison of velocity distributions at the 12 ADCP survey locations (Fig.7) indicates that no significant differences are observed between the model and measurements. Therefore, RANS with SST is likely sufficient for the current work.
Regarding if LES improves the performance, I would argue that LES may not improve the model performance due to (a) the limited accuracy in streambed topography surveys and (b) the uncertainties in velocity measurements. The three papers by Kang et al. demonstrated that the prediction of complex secondary flows can be improved if the small-scale (cm-scale) streambed rough elements can be accurately measured in topography surveys and their effects on the turbulence can be resolved by LES. Obtaining the details of rough elements in the field-scale lab facility with 0.1 to 0.3 m depth (as shown in Kang's work) is feasible, however, it is not practical to measure rough elements at km-scale natural rivers with water depth range 0-20 m (the river section studied in this work). In the current work, the river bathymetry is measured using a LiDAR whose spatial resolution cannot capture the sediment-scale (mm to dm) rough elements. Due to the missing information of small-scale rough elements, their effects on the flow must be calibrated by matching the model predicted water stage with observed ones. Replacing the RANS with LES cannot avoid such a calibration procedure. The ultimate model accuracy, therefore, depends on the accuracy of water stage observations and the roughness wall model (need to use rough wall model to account for the missing roughness effect), but not the scales resolved by LES. Additionally, the evaluation of a model's performance also

depends on the accuracy of the measurement data. This is especially true for validating the model with field velocity surveys because typical velocity survey techniques, e.g., boat towed ADCP, usually have large uncertainties. It is difficult to know whether the model performance improves or not without improving the velocity measurement accuracy. In Le, T. B. et al (Large-eddy simulation of the Mississippi River under base-flow condition: hydrodynamics of a natural diffluence-confluence region, JHR, 2019), they simulated the flow in a 3.2 km long reach to a quasi-steady state using LES with a mesh resolution 0.5 m, 2.37 m, and 0.094 m along x, y, z directions. Though the vertical mesh resolution is sufficient to resolve the effects of small-scale sediments (let's assume the sediment details are captured by the topography survey) on the flow, the velocity prediction accuracy is not improved compared to using a much coarser mesh with RANS in our paper (please compare Fig 12 in Le, T. B. et al with Fig. 8 in our paper). Please refer to lines 300-305 for the details of this discussion as well as Le, T.B. et al's paper.
To my best knowledge, the work by Le, T. B. is likely the largest spatial scale (3.2 km) where LES has been applied to. It is possible to extend such a scale to the scale (30 km) studied in the current work but will be likely not feasible to extend it to a multiple-year scale because of the limitation of the small time step required by LES. Modeling natural rivers using LES also needs to address the dynamically changing water surface that necessitates efficiently integrating LES with VOF. Additionally, LES likely improves the model's accuracy only if the details of streambed topography can be accurately measured. In recent years, structure-from-motion photogrammetry has demonstrated its capability in obtaining mm- to cm-scale resolution streambed at dry and shallow flow conditions up to 40 km reach. Integration LES with SfM-derived topography will likely be a key step to fully utilize the power of LES (in capturing the anisotropic turbulence induced by irregular strembed sediments). Discussions on this can be found in Section 4.1.4.

[Reviewer comments]: 2. The authors provide a nice explanation of how they balanced the modeling efforts between computational efficiency and predictive accuracy. Much of this focuses on how the code was constructed to segment the calculations and reduce the CPU requirement. Of course, in a large modeling study, of the scale reported here, the actual CPU time may only be a part of the overall effort used. Could the authors comment on the resources to set up the model (meshing, calibration etc) and the resources required to validate the model ; Were these of the same order as the CPU?

[Responses]:
We thank the reviewer raise these questions. In general, we divided the overall time costs into model setup time, simulation time, and post-processing time.
In the model setup step, we have some key tasks including (a1) converting DEM data (in ASC format) to a triangulated surface format (STL); (a2) setting up a script for the snappyHexMesh in OpenFOAM to generate a mesh based on the input STL; (a3) developing a Matlab code to extract the water depth and velocity data from a 1D hydrodynamics model (Mass1), (a4) writing these data as time-variable boundary conditions for velocity and volume fraction at the inlet and outlet for OpenFOAM; (a5) developing a Matlab code to read the OpenFOAM mesh, split the streambed boundary faces into N regions (see details between lines 405-425) based on the input water level logger location coordinates, and assign locally or globally optimal roughness values for each region through a rough wall model; (a6) copying the final globally optimal roughness value case for all months between 2013-2015 (36 months) and 2018-2019 (22 months), and setting up for the starting and ending time for each simulation in OpenFOAM; (a7) submitting all cases for parallel simulations.
Though most of the steps take little time, step a5 takes considerable time because we need to implement the local roughness optimization and adjustment strategy in this step (see Section 2.4). In the local roughness optimization step, we firstly run 8 simulations for the time period between Jan-20 to Feb-16, 2011 by assigning 8 different uniform roughness values (0, 0.025 m, 0.05 m, 0.1 m, 0.2 m, 0.3 m, 0.4 m, and 0.5 m) for the whole streambed. Then we determined the locally optimal values for each observation

location based on Fig. 3b., which finally results in the case OF0 as shown in Table 1. In the roughness adjustment step, 5 additional simulations are conducted based on the case OF0 to adjust the roughness values at upstream locations as shown in cases OF1-OF5 in Table 1. The roughness values derived via this step are used in step a6 for parallel simulations. In total, the 8 simulations conducted in the roughness optimization step consumed 254,000 CPU hours with each case consuming around 32,000 CPU hours. The 7 simulations implemented in the roughness adjustment step used 52,000 CPU hours with each case consuming 7,400 CPU hours. The cases in the adjustment step spend around 4.3 times less time compared to those used in the roughness optimization step because larger time step (3s vs 0.95 s) and improved linear solvers are used in the adjustment step. With the optimal distributed roughness values, we run the Matlab code developed in step a4 to generate 58 OpenFOAM cases for all months during 2013-2015 and 2018-2019 for parallel simulations. The total time required in this step is around 6 days (or 1.1 million CPU hours) as reported in Section 4.4. Combining the time used in the calibration step, the overall computing cost is around 1.4 million CPU hours with around 21% used for model setups and calibration. The ratio of model calibration time to the model running time is around 28%.

When all simulations are completed, it takes extra time to post-process the results from OpenFOAM. The time consumed in post-processing depends on the dimension of the data we need to use. For the water stage data reported in Figs. 5,6,9,10, they are interpolated from the OpenFOAM results at 6 locations, which takes a few hours to obtain the data. For the velocity data reported in Figs. 7-8, the OpenFOAM results are interpolated to 12 cross-sections (thousands of coordinates) at two specific hours. This post-processing takes less than 1 hour using a Matlab code developed for this purpose. For the pressure data reported in Fig. 11, they are interpolated from the OpenFOAM results to a 2D uniform grid with 1.2 million points using a Matlab code. It takes around 8-12 hours to extract all pressure data during 2013-2019.

In our work, we have developed a series of Matlab functions and scripts to automate the model setups, parallel job submissions, and post-processing. The actual time required for the simulations and post-processing depends on the spatiotemporal scales to be investigated. But for the model setups and calibration, it only takes 2-3 days to finalize the case setups for final simulations by running our scripts step by step. This conclusion has been demonstrated in another work where we apply the same framework to another 30 km-long reach in the Columbia River.

To apply the framework for other rivers, the following resources are necessary: (1) digital elevation model of the target river; (2) water stage surveys at a few locations along the target river; (3) velocity measurements at a few cross-sections along the river; (4) velocity and depth information at the inlet and outlet locations for the target river (a 1D hydrologic model was used to extract this information in this work); (5) computing resources. For practical applications, it is better to first check with national or local water agencies or open data repositories regarding the availability of these resources.

[Reviewer comments]: 3. The authors close by correctly pointing out the possible benefit of their approach in assessing impacts of climate change. They could be a little more specific here. In particular, are the space and time domains presented here sufficient for meaningful climate change scenario modeling? If not, what time scales and reach sizes would be meaningful?

[Response]:

We thank the reviewer's insightful comments. A natural river system is strongly affected by the discharge that is further controlled by the overall water balance, human usage, and climate forcing such as precipitation. Existing global hydrological models such as the Variable Infiltration Capacity (VIC) model have enabled predicting global stream discharge at a spatial scale of 5-10 km and a time scale of 3 hours to one day spanning 40 years with precipitation as the main climate forcing (Yang, Y. et al., Global Reach-Level 3-Hourly River Flood Reanalysis (1980–2019, BAMS, 2021). The impact of human activities on global water resources has also been evaluated by integrating the VIC model with anthropogenic modules, though at coarser (55 km) resolution (Droppers, B., et al., Simulating human impacts on global water resources using VIC-5, GMD, 2020). With the discharge output from these models, it is straightforward to evaluate the impacts of climate and human activities on river hydrodynamics by constraining the river CFD model with the discharge from global hydrologic models. In the present work, the space and time domains are 30 km and around 9 years (2011-2019) with a spatial resolution of 20 m and a temporal resolution of 3 seconds. This information means that the space and time scale studied in this work fall within the scales (global 5 km and 3-hour resolution discharge data available according to Yang, Y. et al) of the latest global hydrological modeling. Therefore, the current CFD framework can be meaningfully linked to global hydrologic models to understand their impacts on river hydrodynamics and associated biogeochemical processes. We have incorporated this message into the revised version of the paper (see red texts between 570-575).

[Reviewer comments]: 4. While outside of the scope of the current paper. In future work it might be worthwhile to compare the performances (CPU/predictions) of the proposed 3D RANS/fee surface calculations with the more widely used 1-D and 2-D streamflow codes noted in the literature review. Vaughan Voller, University of Minnesota.

[Response]:
We thank the reviewer's suggestion for future work. To keep the paper short, this paper only compared the water stage prediction from the proposed 3D model with another 1D (Mass1) and 2D (Mass2) model. But it will be of great practical value to compare our model with other widely used 1D/2D models in terms of their long-term performance and computational costs.