

## Highlights

### **TRITON: A Multi-GPU Open Source 2D Hydrodynamic Flood Model**

M. Morales-Hernández, Md. B. Sharif, A. Kalyanapu, S. K. Ghafoor, T. T. Dullo, S. Gangrade, S.-C. Kao, M. R. Norman, K. J. Evans

- TRITON is released as a multi-GPU open source 2D hydrodynamic flood code
- It solves the 2D shallow water equations using a first order time-explicit scheme
- It runs efficiently for realistic configurations using heterogeneous architectures
- The runoff capability is demonstrated to be convenient for flood modelling
- Communication and I/O times may represent a bottleneck for operational purposes

# TRITON: A Multi-GPU Open Source 2D Hydrodynamic Flood Model

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## ABSTRACT

A new open source multi-GPU 2D flood model called TRITON is presented in this work. The model solves the 2D shallow water equations with source terms using a time-explicit first order upwind scheme based on an Augmented Roe's solver that incorporates a careful estimation of bed strengths and a local implicit formulation of friction terms. The scheme is demonstrated to be first order accurate, robust and able to solve for flows under various conditions. TRITON is implemented such that the model effectively utilizes heterogeneous architectures, from single to multiple CPUs and GPUs. Different test cases are shown to illustrate the capabilities and performance of the model, showing promising runtimes for large spatial and temporal scales when leveraging the computer power of GPUs. Under this hardware configuration, communication and input/output subroutines may impact the scalability. The code is developed under an open source license and can be freely downloaded in <https://code.ornl.gov/hydro/triton>.

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## 1. Software Availability

- 2 Name of the software: TRITON (Two-dimensional Runoff Inundation Toolkit for Operational Needs)  
3 Contact address: Oak Ridge National Laboratory, 1 Bethel Valley Road, TN 37830, USA / Tennessee  
4 Technological University, 1 William L Jones Dr, Cookeville, TN 38505, USA  
5 Email: [moraleshern2@ornl.gov](mailto:moraleshern2@ornl.gov), [akalyanapu@tntech.edu](mailto:akalyanapu@tntech.edu)  
6 Language: CUDA, C++  
7 Hardware: Desktop/Laptop or clusters of CPUs/GPUs  
8 Software: NVIDIA CUDA Toolkit, NetCDF (optional)  
9 Availability: <https://code.ornl.gov/hydro/triton>  
10 Year first available: 2020

## 11 2. Introduction

12 With the increasing frequency and intensity of extreme hydrologic events in a changing environment  
13 [36], faster and more accurate inundation models are particularly important tools for flood risk management.  
14 When translating the amount of rainfall (either from weather forecasting models or from rain gauge

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15 observations) all the way to surface inundation, coupled hydrologic-hydraulic models should be used, where  
 16 the flood inundation model represents “the last mile” that simulates flood wave propagation across high-  
 17 resolution terrain based on simulated runoff and streamflow from hydrologic models [65].

18 Flood inundation models can provide not just streamflow discharge but the temporal evolution of flood  
 19 location, depth and movement. However, this information is not always directly translated into practical  
 20 instructions to better support operators and emergency responders for more rapid decision making [52]. In  
 21 this regard, collaborative flood modeling is a great example for overcoming this challenge where end-users,  
 22 stakeholders and scientific knowledge meet and interact [19, 37]. Specifically, the use of high-resolution maps  
 23 built from flood inundation models together with non-technical terminology have proven to benefit decision-  
 24 making for end-users [50]. Beyond this methodology, integrated platforms using hydraulic modelling linked  
 25 with live geospatial information, remote sensing, flood visualization and community intercommunication  
 26 [66, 59], and other strategies such as probabilistic flood maps based on flood models and the Value of  
 27 Information (VOI) [1] have been also demonstrated to reduce the uncertainty and assess the consequences  
 28 of actions taken by decision-makers.

29 Despite the integrated flood risk management tools, large-scale operational hydrodynamics models are  
 30 still rarely used mainly because of their large computational cost. Simulation models must be particularly  
 31 fast (on the order of minutes) to meet decision-making needs resulting in the reliance on simplified and  
 32 analytical models. One example is the integrated version of Height Above Nearest Drainage (HAND) within  
 33 the US National Water Model (NWM) [34, 35]. HAND is based on Manning’s equation, some geometric  
 34 extrapolations, and precomputed rasters that are used to generate national flood maps at 10 m resolution.  
 35 Its European equivalent within the EFAS (European Flood Awareness System) is LISFLOOD-FP [4], a  
 36 spatially distributed rainfall-runoff-routing model. Its operational version [42, 63] uses the runoff generated  
 37 at a 5km grid spatial resolution as an input for a simplified shallow water model in which the convective term  
 38 is neglected. Flooding maps are derived from a catalog of flood hazard maps made of precalculated runs of  
 39 the LISFLOOD-FP model. The main limitation of these models is the range of applicability for all types of  
 40 flows and situations, which are restricted by the simplification hypothesis assumed, and consequently, the  
 41 validity and accuracy of the results.

42 One of the most complete inundation frameworks is the 2D full shallow water system [24], which solves  
 43 mass and momentum equations and provides water depth distribution and an accurate surface velocity  
 44 field. The resolution of the 2D shallow water equations is nevertheless computationally demanding at fine  
 45 resolutions and there is no obvious path for them to scale up to continental or global scales for operational  
 46 purposes. Two main efforts are highlighted in the last decades to overcome this constraint: efficient numerical  
 47 techniques and the adaptation to High Performance Computing (HPC). First, numerical improvements are  
 48 of crucial importance to reduce the computational burden. In the context of Augmented Riemann solvers,  
 49 a careful numerical estimation of topography and friction terms has been demonstrated to improve the  
 50 performance and accuracy of the solution [39, 40, 41]. Local time step methods [47, 12] are considered as a  
 51 worthwhile solution to improve the computational efficiency at the extra cost of having to deal with different  
 52 stages for flux and source computations, depending on the time level. As for the spatial discretization  
 53 – leaving aside adaptive mesh refinement techniques–, Discontinuous Galerkin (DG) schemes, as the one  
 54 proposed in [29], seem to deliver high quality solutions with desired scalability properties. On the same  
 55 page, a well-balanced no-neighbor method has recently been proposed for the 1D Saint Venant equations  
 56 [25]. Although the extension to the 2D framework is not clear, this family of schemes could open the door  
 57 to new efficient algorithms.

58 On the other side, parallel implementations, and the use of HPC on new architectures of modern super-  
 59 computers have become a fundamental requirement to study increasingly complex problems at large spatial  
 60 scale and high temporal resolution on water resources hydrodynamics [38]. Neal et al.[43] explored different  
 61 parallel strategies of LISFLOOD-FP across various types of architectures, stressing the efficiency, difficulty  
 62 and estimated development time of each implementation. The great majority of models are nevertheless  
 63 implemented on a single hardware type. One of the best exponents is PRIMO [48], a raster-based subgrid  
 64 flood model able to run on clusters of central processing units (CPUs) using both shared and distributed  
 65 memory. However, the use of Graphical Processing Units (GPUs) has become a new trend in the recent  
 66 decade [46, 7, 28, 6]. In the GPU context, the spatial discretization and efficiency have been studied for  
 67 regular [57] and irregular grids [44, 24, 17], seeking efficiency with i) different solvers [2], ii) different mem-

68 ory access patterns and mesh ordering algorithms for unstructured grids [31], iii) block uniform Quadtree  
 69 and adaptive mesh refinement on nested rectangular meshes [56], and iv) a local time stepping scheme to  
 70 improve performance [12]. Additional capabilities have been also reported and accelerated with the use of  
 71 GPUs: rainfall/runoff applications [32, 3], sediment transport and erosion processes [27, 8, 10], landslides  
 72 [30], hydraulic structures modelling [18, 11] and transport of contaminants and water quality models [58, 22].

73 Multi-GPU models could be the solution to improve the tradeoff among accuracy, speed and large scale  
 74 domains. The initial work by Sætra and Brodtkorb [46] studied both weak and strong scaling and the  
 75 effect of synchronizations of 2D shallow water equations using a 4-GPU machine. Xia et al. [65] used a  
 76 framework called HiPIMS to model a storm in a  $2500 \text{ km}^2$  catchment using 8 GPUs and 100 million grid  
 77 cells around 2.5 times faster than real time. In [55, 54] the equations are discretized in a BUQ (quadtree)  
 78 grid following the proposed scheme of [56]. Although this type of spatial discretization could be convenient  
 79 to improve performance with respect to regular Cartesian grids and to address high resolution problems, the  
 80 domain decomposition increases complexity and could add an overhead in large scale simulations. In [51],  
 81 the authors compare two versions of solvers for the shallow water equations (finite-difference versus finite  
 82 volume). Weak and strong scaling up to 272 million grid cells are analyzed together with the CUDA-Aware  
 83 MPI feature, designed to optimize communications between the different sub-domains.

84 TRITON is presented here as the first (to date) multi-architecture (multiple CPUs and GPUs) open-  
 85 source 2D hydrodynamic flood model based on the resolution of full shallow water equations with source  
 86 terms. Different free or open source 2D models can be found in the literature: besides the LISFLOOD model  
 87 [4, 42] and the well-known HEC-RAS model (2D version released in 2016), other CPU-based (or multi-  
 88 CPU) models such as FullSWOF [13] and BreZo [49] solve the 2D shallow water equations in structured  
 89 and unstructured triangular grids, respectively. Delft3D [15] also permits 2D flow computations for different  
 90 applications ranging from hydrodynamics to sediment transport and water quality. Few GPU models are  
 91 freely available: GeoClaw [5] for certain applications [45], IBER for 2D flood modeling [23] and ANUGA,  
 92 enabling the GPU-offloading using PyCUDA [61]. TRITON has been nevertheless designed for a multi-  
 93 architecture paradigm and is able to run on several configurations including: single or multiple CPUs and  
 94 single or multiple GPUs, using a combination of Open Multi-Processing (OpenMP), Compute Unified Device  
 95 Architecture (CUDA), and Message Passing Interface (MPI). In addition to this architectural flexibility, all  
 96 computing subroutines are programmed only once, regardless of the hardware type, minimizing error sources  
 97 and bolstering the software portability. Finally, a simple input/output configuration is implemented that  
 98 would avoid significant geographic information system (GIS) pre- and post- processing. As an example, a  
 99 digital elevation model (DEM) is directly used as the computational mesh, circumventing the necessity of  
 100 site-specific mesh building as with most existing models. These features would eventually enable the use of  
 101 2D hydrodynamic models for operational purposes and other applications that were not feasible before.

102 In addition to introducing this TRITON as a fast and flexible open source suite to simulate both pluvial  
 103 and fluvial flood events –together with some freely available pre- and post-processing tools –, this work aims  
 104 to answer the following research questions:

- 105 1. Is it possible to simulate large temporal and spatial scales in the order of minutes using a hydrodynamic  
 106 model based on the solution to the full 2D shallow water equations? Which are the most appropriate  
 107 architectural and parallelization strategies required to achieve this?
- 108 2. Does spatially distributed rainfall/runoff have an impact on the results of predictive hydrodynamic  
 109 models?
- 110 3. Could communication and I/O times represent a bottleneck for large scales?

111 The paper is organized as follows: after describing TRITON, including the equations, numerical scheme  
 112 and the HPC implementation, the software features are presented. Three test cases are included to demon-  
 113 strate the capabilities of the model, showing the accuracy and performance of TRITON on different config-  
 114 urations and architectures, including the simulation of the multi-day event of Hurricane Harvey over Harris  
 115 County in Texas, on 384 GPUs using Summit supercomputer at Oak Ridge National Laboratory. The  
 116 trade-offs among parallel computation, communication and input/output are also analyzed, revealing the  
 117 importance of the latter two for large temporal and spatial scales.

118 **3. The TRITON Model**

119 TRITON, the Two-dimensional Runoff Inundation Toolkit for Operational Needs, is a physically-based  
 120 hydrodynamic model that solves the 2D shallow water equations on a structured (Cartesian) grid. Based on  
 121 the initial GPU model developed by Kalyanapu et al. [28], a new conservative numerical scheme has been  
 122 implemented and integrated in an updated framework able run on multiple architectures.

123 **3.1. Governing equations**

124 The 2D shallow water equations express the depth-averaged conservation of mass and momentum in  $x$   
 125 and  $y$  directions of the space. They can be written in a compact differential conservative form as presented  
 126 in eq. (1):

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} = \mathbf{S}_r + \mathbf{S}_b + \mathbf{S}_f$$

$$\mathbf{U} = \begin{pmatrix} h \\ q_x \\ q_y \end{pmatrix} \quad \mathbf{F} = \begin{pmatrix} q_x \\ \frac{q_x^2}{h} + \frac{1}{2}gh^2 \\ \frac{q_x q_y}{h} \end{pmatrix} \quad \mathbf{G} = \begin{pmatrix} q_y \\ \frac{q_x q_y}{h} \\ \frac{q_y^2}{h} + \frac{1}{2}gh^2 \end{pmatrix} \quad (1)$$

$$\mathbf{S}_r = \begin{pmatrix} r \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{S}_b = \begin{pmatrix} 0 \\ -gh \frac{\partial z}{\partial x} \\ -gh \frac{\partial z}{\partial y} \end{pmatrix} \quad \mathbf{S}_f = \begin{pmatrix} 0 \\ -\frac{gn^2}{h^{7/3}} q_x \sqrt{q_x^2 + q_y^2} \\ -\frac{gn^2}{h^{7/3}} q_y \sqrt{q_x^2 + q_y^2} \end{pmatrix}$$

127 The vector  $\mathbf{U}$  represents the conserved variables (i.e. the unknowns of the system) and includes the water  
 128 depth,  $h$  [ $L$ ], and the  $x$  and  $y$  unit discharges, called  $q_x$  [ $L^2 T^{-1}$ ] and  $q_y$  [ $L^2 T^{-1}$ ] respectively. Eq. (1) also  
 129 contains the fluxes of these conserved variables ( $\mathbf{F}$  and  $\mathbf{G}$ ) –being  $g$  [ $LT^{-2}$ ] the gravity acceleration– and the  
 130 source terms. The latter encompass runoff terms,  $\mathbf{S}_r$ , expressed according to the runoff rate  $r$  [ $LT^{-1}$ ]; bed  
 131 slope terms,  $\mathbf{S}_b$ , accounting for the gradient of the elevation  $z$  [ $L$ ]; and friction terms,  $\mathbf{S}_f$ , modeled by means  
 132 of Gauckler-Manning’s law in terms of the Manning’s roughness coefficient  $n$  [ $TL^{-1/3}$ ]. Here runoff refers to  
 133 the effective rainfall (i.e., total rainfall minus losses due to infiltration, abstraction, and evapotranspiration)  
 134 plus baseflow that are typical outputs from hydrologic or land surface models.

135 **3.2. Numerical scheme**

136 A finite volume upwind explicit scheme is used to solve Eq. (1) in a squared (Cartesian) mesh of grid  
 137 spacing  $\Delta x$ . An Augmented Roe (ARoe) solver is implemented, based on [39, 17] for the fluxes and bed  
 138 slope source terms nevertheless a different estimation of bed slope source terms at each edge are proposed  
 139 in this work. This treatment also ensures the positivity of the solution without reducing the time step size.  
 140 For the sake of clarity, the derivation of this part of the scheme can be found in Appendix A. Friction terms  
 141 are discretized using a local implicit formulation [64] that does not alter the explicitness of the scheme.  
 142 Accordingly, a two-step algorithm is proposed for the update of a cell  $i$  from time  $t^n$  to time  $t^{n+1} = t^n + \Delta t$ :

$$\mathbf{U}_i^* = \mathbf{U}_i^n - \frac{\Delta t}{\Delta x} \sum_{k=1}^4 \sum_{m=1}^3 \frac{\tilde{\lambda}^-}{\tilde{\lambda}} \left[ (\tilde{\lambda} \tilde{\alpha} - \tilde{\beta}_b) \tilde{\mathbf{e}} \right]_{m,k}^n \quad \mathbf{U}_i^{n+1} = \mathcal{F}(\mathbf{U}_i^n, \mathbf{U}_i^*) + r_i^n \Delta t \quad (2)$$

143 where, at each interface  $k$ ,  $\tilde{\alpha}$  and  $\tilde{\beta}_b$  are the fluxes and bed slope source term linearizations, "minus"  
 144 superscript accounts for the upwind discretization and  $\tilde{\lambda}$  and  $\tilde{\mathbf{e}}$  are the eigenvalues and eigenvectors of the

<sup>145</sup> system of equations respectively (see Appendix A). The localized runoff rate is denoted by  $r_i$  while function  
<sup>146</sup>  $\mathcal{F}$  stands for the friction discretization, written as:

$$\mathcal{F}^1 = h^* \quad \mathcal{F}^2 = -(q_x^*) \left( \frac{1 - \sqrt{1 + 4S_f}}{2S_f} \right) \quad \mathcal{F}^3 = -(q_y^*) \left( \frac{1 - \sqrt{1 + 4S_f}}{2S_f} \right) \quad (3)$$

<sup>147</sup> where

$$S_f = \frac{\Delta t g n^2 \sqrt{(q_x^*)^2 + (q_y^*)^2}}{(h^n)^{7/3}} \quad (4)$$

<sup>148</sup> The explicit character of the scheme restricts the time step size according to the Courant-Friedrich-Lowy  
<sup>149</sup> (CFL) condition:

$$\Delta t = \text{CFL} \min_i \left\{ \frac{\Delta x}{\left| \frac{q_x}{h} \right|_i + \sqrt{gh}_i, \left| \frac{q_y}{h} \right|_i + \sqrt{gh}_i} \right\} \quad \text{CFL} \leq 0.5 \quad (5)$$

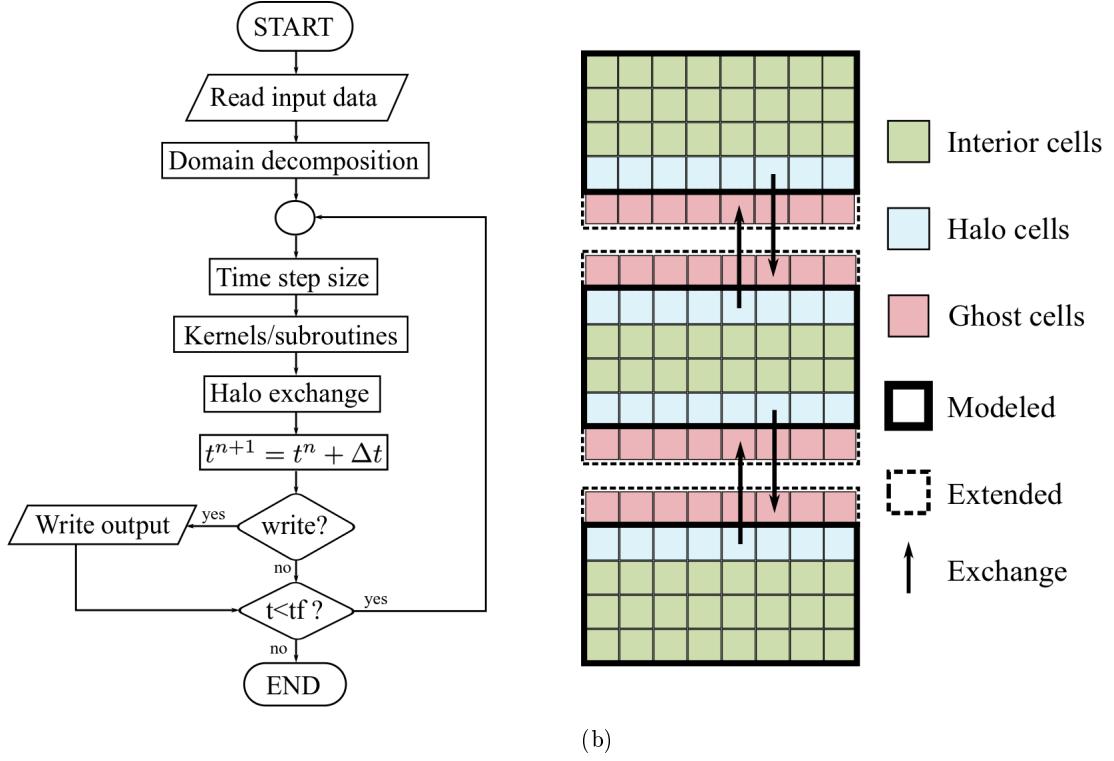
<sup>150</sup> where index  $i$  loops over the number of grid cells. Note that, although formally the maximum wave speed  
<sup>151</sup> should be estimated at the interfaces, the cell values are used instead in this work. Notwithstanding, this  
<sup>152</sup> approach does not compromise the stability of the scheme –in fact, a value equal to or less than the size of  
<sup>153</sup> the time step is selected using this formula– but it simplifies and ultimately accelerates the computations,  
<sup>154</sup> providing simultaneously a new way to estimate some corrections for the source terms (see Appendix A).

### <sup>155</sup> 3.3. HPC implementation

<sup>156</sup> Increased problem complexity motivates heterogeneous HPC for hydrodynamics codes in the new era  
<sup>157</sup> of parallel computing [38]. Computation time can be reduced effectively with the use of clusters of CPUs  
<sup>158</sup> and GPUs. On-demand cloud workstations are also becoming more popular and affordable, allowing the  
<sup>159</sup> simulation of larger spatial and temporal domains at finer scales. Varied programming paradigms have arisen  
<sup>160</sup> as a consequence of this heterogeneity: Open Multi-Processing (OpenMP) for multicore CPUs, Message  
<sup>161</sup> Passing Interface (MPI) for clusters, Compute Unified Device Architecture (CUDA) or Open Computing  
<sup>162</sup> Language (OpenCL) for GPUs. For that reason, TRITON has been designed as a multi-architecture single  
<sup>163</sup> code base, able to run on the following platforms through specific compilation instructions:

- <sup>164</sup> 1. Multi-core shared memory platform using OpenMP
- <sup>165</sup> 2. Multi-node cluster using MPI or MPI + OpenMP
- <sup>166</sup> 3. Single node GPU machine using CUDA
- <sup>167</sup> 4. Multi-node GPU cluster using MPI + CUDA

<sup>168</sup> The simplified flowchart for the current implementation is depicted in Figure 1(a). After reading and  
<sup>169</sup> parsing the input data (see Section 4.1), the domain is decomposed into different subdomains according to  
<sup>170</sup> the desired number of MPI sub-tasks. Then, the simulation starts and runs until the time reaches the final  
<sup>171</sup> simulation time, writing the output information (described in Section 4.2) each output interval. At each  
<sup>172</sup> time state, the time step size is first computed according to Eq. (5); then the computing kernels (GPU)  
<sup>173</sup> or subroutines (CPU) are executed, merely accounting for the numerical scheme in Eq. (2); finally the  
<sup>174</sup> information is exchanged between the corresponding subdomains. Details of the later three processes along  
<sup>175</sup> with the MPI decomposition are explained below.



**Figure 1:** TRITON flowchart (a) and row-wise domain decomposition (b)

### 3.3.1. Domain decomposition and halo exchange

Domain decomposition is an important factor for large-scale parallelization using MPI libraries (or similar) in design of portable and scalable communication between subdomains. Although there are different ways to partition the information, a 1D row-wise decomposition is applied here for simplicity [38]. As the stencil for the numerical scheme Eq. (2) involves neighbouring data (see Figure 9(a), Appendix A), the information has to be exchanged each time step and overlap computations are performed. Figure 1(b) shows a sketch of the row-wise approach, where north-south communication is required and the halo size is the number of columns of the whole domain. A two-step non-blocking algorithm is implemented using *MPI\_Isend* and *MPI\_Irecv*, with the aid of *MPI\_Wait* to wait for an MPI request. Let  $N$  be the number of ranks (e.g., the number of partitions of the domain). First, all subdomains  $n < N$  will send the halo data to the subdomain  $n + 1$  and receive from subdomain  $n - 1$ . Then, vice versa, each subdomain  $n > 1$  will receive information from subdomain  $n + 1$  and send to subdomain  $n - 1$ .

The subdomain exchange imposes a slightly greater level of complexity when dealing with a GPU implementation due to memory allocation. As computations are performed by a GPU, data are fully allocated in the device (GPU) memory. However, the regular MPI calls require pointers to host (CPU) memory, which requires an additional data copy between host and device, in addition to an extra host memory allocation. This might decrease the performance of the model. The CUDA-Aware MPI is used for halo exchange to overcome this challenge of possible performance degradation. CUDA-Aware MPI allows GPU to GPU direct communication via network, bypassing the CPU, if underlying hardware supports this technology. Specifically, Summit supercomputer has GPU direct communication support and the use of CUDA-Aware MPI has resulted in improved TRITON's performance. The impact of using CUDA-Aware MPI versus the conventional approach has been already studied in [51] (see results FVS and FVG) for a primitive version of TRITON. For the sake of flexibility, TRITON supports both approaches, allowing users to choose a preferred implementation according to their system requirements.

200 **3.3.2. Time step size computation**

201 In order to guarantee a stable and reliable solution at every time stage,  $\Delta t$  is limited according to  
 202 Eq. (5), which requires the computation of a global minimum time step size that will be imposed to  
 203 evolve the solution in time. To do that, each subdomain computes first its own local minimum time step  
 204 size for all its cells. Again, two different implementations can be distinguished here depending on the  
 205 architecture. The OpenMP approach is rather simple since it only consists of the computation of a *reduction*  
 206 operation. The equivalent reduction operation in GPU is more complicated. Although some CUDA standard  
 207 libraries (CuBlas, ThrusT) or third party (Cub) libraries can be used, a reduction *ad-hoc* function has been  
 208 implemented in CUDA. In contrast to the existing libraries, in which a global array of size the total number  
 209 of cells is required and then perform the reduction operation, we make use of shared memory and thread  
 210 synchronization at each kernel –where we calculate the time step size–, to launch multiple instances using  
 211 a reduced global array of size "thread block" times smaller than the original size. Then, the reduction  
 212 operation is done over the global reduced array, diminishing the global memory use, improving memory  
 213 coalescing and providing a better performance than the existing libraries for large scale problems. Once the  
 214 local minimum time step size is computed, the global minimum is found using *MPI\_AllReduce* across all  
 215 the processes (sub-tasks).

216 TRITON also offers the possibility of a constant time step size. This implementation does not require  
 217 any reduction operation –making it easier– nevertheless the accuracy and robustness of the results are not  
 218 ensured since the maximum allowed time step size, governed by Eq. (5) might be violated.

219 **3.3.3. Kernel/subroutine execution**

220 TRITON is written using C++ and CUDA. Each computing module has been implemented as a CPU  
 221 subroutine as well as a CUDA kernel. During compilation, based on the computing platform, appropriate  
 222 computing modules are compiled. A set of arrays with the same structure is allocated either in the CPU  
 223 or in the GPU so that the difference between CPU and GPU execution only consists of the memory where  
 224 the data is defined and the kernel/subroutine calls. Each kernel is then only programmed once, avoiding  
 225 duplicated information. This fact improves the readability of the code at the same time as reproducibility  
 226 and trustfulness between different architectures, minimizing or almost eliminating eventual human mistakes  
 227 usually made when porting the code from one to another architecture. Figure 2 depicts the source code for  
 228 the "wet/dry" kernel/subroutine, showing both the function call and declaration. As shown, the number of  
 229 arguments required by the CPU and GPU versions are exactly the same, although arrays reside either in the  
 230 device or the host memory according to the chosen architecture. Some `#ifdef`, `#else` and `#endif` directives  
 231 allow to switch between CPU and GPU in compilation time.

232 **4. Software Features**

233 TRITON is a UNIX-based model targeting laptops, desktops, and optimized for supercomputers, lever-  
 234 aging the current power of workstations. The code, pre-/post-processing tools and some samples can be  
 235 found in  
 236 <https://code.ornl.gov/hydro/triton>. The main features and tools are explained below.

237 **4.1. Input data**

238 The mandatory/optional TRITON input files include:

- 239 • **Configuration** (mandatory). A text file containing the path of all input files, output interval and  
 240 format, and all parameters and constants needed for simulation (e.g., number of streamflow sources,  
 241 external boundary conditions, initial and final time, CFL number, switches to enable/disable observa-  
 242 tion point and checkpointing, etc.). It can be configured either manually or with the aid of a Config  
 243 File Tool Generator.
- 244 • **Topography** (mandatory). TRITON is a DEM-based code. Consequently, the mesh used for com-  
 245 putation is a Cartesian (square) grid obtained directly from the DEM file (i.e., avoiding the ad-hoc  
 246 and site-specific task of computational mesh building). DEMs follow the ESRI raster file format –  
 247 both ASCII and binary formats are allowed, although binary format is recommended for large spatial

```

1 //variable definitions
2 ACTIVE_GPU: flag to enable GPU compilation
3 nrows: number of rows
4 THREAD_BLOCK: group of threads executed in parallel
5 device_vec: array containing all the GPU vectors
6 H,HU,HV,DEM: integers pointing to the beginning of
7 the water depth, x-unit discharge, y-unit-discharge
8 and elevation vectors respectively
9
10
11 //kernel/subroutine call
12 #ifdef ACTIVE_GPU
13   Kernels::wet_dry<< <(nrows*ncols+THREAD_BLOCK-1)/THREAD_BLOCK,THREAD_BLOCK,0,streams>> >(nrows*ncols,
14   nrows, ncols, global_dt, device_vec[H], device_vec[HU], device_vec[HV], device_vec[DEM]);
15 #else
16   Kernels::wet_dry(nrows*ncols, nrows, ncols, global_dt, host_vec[H], host_vec[HU], host_vec[HV],
17   host_vec[DEM]);
18 #endif
19
20 //kernel/subroutine declaration
21 template<typename T>
22 #ifdef ACTIVE_GPU
23   __global__
24 #endif
25 void wet_dry(int size, int nrows, int ncols, T dt, T *h_arr, T *hu_arr, T *hv_arr, T *dem)
26 {
27 #ifdef ACTIVE_GPU
28   int id = blockIdx.x * blockDim.x + threadIdx.x;
29   if (id >= size)
30     return;
31 #else
32   #pragma omp parallel for
33   for (int id = 0; id < size; id++)
34   {
35     .....
36     //Kernel/subroutine implementation. Note that this is common for both architectures
37 #ifdef ACTIVE_OMP
38   }
39 #endif
40 }
```

**Figure 2:** Source code for the call and declaration of "wet/dry" kernel/subroutine. GPU code is shown in green while CPU code is displayed in dark blue.

248 domains—that contains a header section with the number of columns, rows, origin coordinates and cell  
 249 size, as well as a matrix of elevation values. NODATA values are not allowed in the current version of  
 250 TRITON.

- 251 • **Streamflow hydrograph** (optional). Streamflow hydrograph is one of two possible hydrologic inputs  
 252 to TRITON. Streamflow here refers to the point discharge typically from upstream incoming river  
 253 channels (sources). When selecting streamflow hydrograph, two files are required: an  $(x, y)$  coordinate  
 254 list with the location of all inflow sources and a streamflow hydrograph table including the time (in  
 255 hours) and the timeseries of discharge (in cubic meters per second) at each source  $j$ ,  $Q_j(t)[L^3T^{-1}]$ .  
 256 The discharge is introduced in TRITON as a single mass release.
- 257 • **Runoff hydrograph** (optional). Runoff hydrograph is another possible hydrologic input to TRITON.  
 258 It is a common output from various hydrologic and land surface models (immediately before such  
 259 information is used for streamflow routing). By involving runoff in TRITON, the model can simulate  
 260 local (pluvial) floods and hence increases its functionality. When selecting runoff hydrograph, two  
 261 files are also required. The runoff regions (corresponding to the coarser hydrologic model grids) are  
 262 defined in the form of a matrix raster map with the same format with the DEM file (but without  
 263 the header). Each distinct area is labeled with a non-negative integer number that serves as a unique  
 264 region identifier (links to the runoff hydrograph table). As in the streamflow hydrograph table, the  
 265 runoff hydrograph table contains the time (in hours) and timeseries of runoff rate  $r$  (in mm per hour)

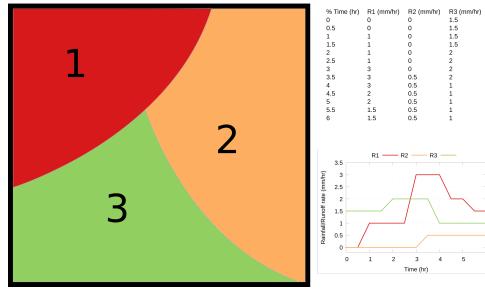


Figure 3: Example of runoff map and table

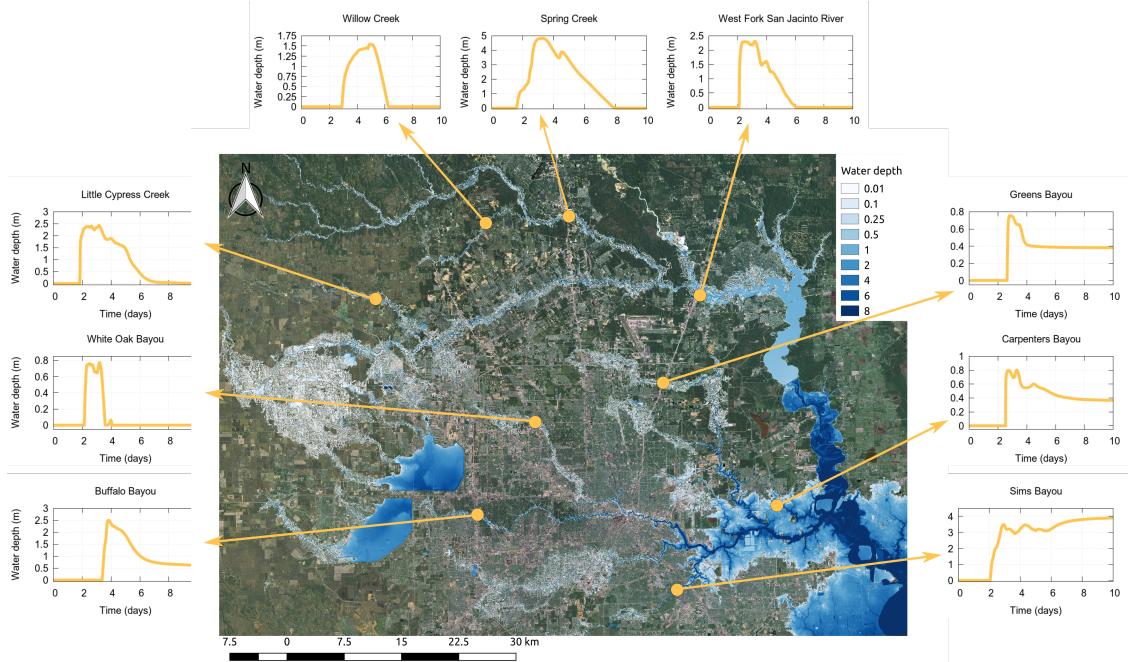
from all declared runoff regions. A sketch of the rainfall/runoff input files is depicted in Figure 3.

- **Roughness** (optional). The surface friction is represented by Manning's roughness coefficient  $n$ . It can be provided either as a constant number, specified in the configuration file and applied globally to the whole domain, or in the form of a matrix raster map (without header) matching the number of DEM grid cells. The latter choice allows the user to define spatially varied roughness coefficients to represent the site-specific land use and land cover conditions.
- **External boundary conditions** (optional). The boundaries of the domain (north, east, south and west) can be provided with five type of external boundary conditions. By default, all boundaries are closed (i.e., water flux is prevented from exiting the domain). Four alternative flow conditions can be then be imposed:

- Type 0: zero gradient. The original setup in [28].
- Type 1: level versus time. An additional file containing a table with the time and the timeseries of water level is mandatory.
- Type 2: normal slope. The desired slope is required.
- Type 3: Froude number. The Froude number defined as  $Fr = \frac{|\mathbf{q}|}{h \sqrt{gh}}$  is needed to be imposed across the external boundary, being  $\mathbf{q} = (q_x, q_y)$ .

More than one external boundary condition can be defined at each boundary edge. The user only has to provide the initial/ending  $(x, y)$  coordinates of the boundary and its corresponding boundary condition parameters according to the boundary type. The external boundary conditions are imposed at the ghost cells surrounding the whole domain. This implementation ensures the scalability of the solution for domain decomposition since no additional information has to be exchanged between the partitioned subdomains.

- **Initial conditions** (optional). A dry domain is the default initial condition. However, the user can also specify an initial condition for each conserved variable ( $h$ ,  $q_x$  or  $q_y$ ) in the configuration file, in the form of a matrix type file (without header). Furthermore, checkpointing/hotstart is also allowed. Backup files are written during the computation to retrieve the simulation from the last state in case it is necessary.
- **Point output** (optional). In addition to the default matrix output at user-specified time intervals, TRITON also supports output of timeseries at user-specified locations (to avoid data processing for known points of interest, such as locations with gauge observations). An  $(x, y)$  coordinate list file containing the location of the desired points is therefore required.



**Figure 4:** Example of output information obtained with TRITON

#### 4.2. Output data

The output from TRITON is intended to be easy to post-process by standard graphing and GIS tools. Two types of output data (spatial and temporal) are generated in a separate folder at each user-specified interval.

- **Matrix data** (spatial). A snapshot of water depth and unit discharge is written in the form of a matrix type file (without header) either in ASCII or in binary format (the latter is recommended for large scale domains [38]). Additionally, if the execution is run using domain decomposition (either multi-CPU or multi-GPU), a switch in the configuration file allows the user to choose the mode in which the data is written: 1) sequential that gathers all subdomain information in a single file during the computation, or 2) parallel that directly outputs subdomain data as separate files. For the latter, a separate script can then be used to combine all subdomain information into a single file during post-processing.
- **Water depth and unit discharge profiles** (temporal). The timeseries of water depth and unit discharge at the specified point locations (defined in the input files) can be outputted in a single file for each variable.

Figure 4 displays a style of output information that can be obtained. It corresponds to the Hurricane Harvey test case studied in Section 5.3 and condenses in a single panel the stage hydrograph for each predefined observation point as well as a 2D view of the whole spatial domain, showing the topography and the maximum flooded area. Note that to be consistent with Eq. (1), TRITON outputs unit discharge (rather than velocity). The user should conduct proper conversion to estimate velocity based on unit discharge and water depth.

#### 4.3. Other tools

A suite of tools is provided with TRITON in order to simplify some pre- and post-processing tasks. First, some bash scripts are included for the conversion between binary/ASCII formats and sequential/parallel mode. They can be used for both input and output data. Additionally, two programs containing a GUI

targeting Windows and Linux are included in the repository. The first one is a NetCDF converter, that takes both binary and ASCII files outputted from TRITON as input data, and converts them into NetCDF format. The second GUI software called Config File Tool Generator allows the user to generate the configuration file (mandatory input file for TRITON).

## 5. Test Cases

A set of test cases are proposed here to demonstrate certain desired characteristics such as consistency, stability, convergence and robustness, and model capabilities. As TRITON is intended to be a reference software for the computation of large scale flood problems, reliability on the output results is mandatory. The first test case is therefore included as a verification and to show how the model behaves on a classic literature test case that involves all kind of flows (subcritical, supercritical, and sonic transitions), and to test the accuracy and grid convergence of the model. Once the model is able to provide a robust and trustworthy solution, the second test is designed to test the capability of a model to accept runoff hydrograph as a hydrologic input and illustrate its importance. This feature also allows users to simulate the effects of local (pluvial) floods that occur due to highly intense local precipitation in a non-floodplain region. The final test case is oriented to evaluate the performance of the model on different architectures (multiple CPUs and GPUs), analyzing the possible bottlenecks in large temporal and spatial scales. All test cases introduced below can be found in the repository. Additional test cases will be included as they are developed to provide users with further examples.

### 5.1. Test case 1: paraboloid bed topography

This test case consists of a square domain  $[0, 4] \times [0, 4]$  with a frictionless paraboloid topography. The initial water depth condition is a planar surface with velocity in the y-direction. The domain boundaries are closed and after one period ( $t=1T$ ), the numerical solution should recover the initial condition due to the rotating velocity field. This configuration is considered to be a challenge test where some numerical methods fail when trying to reproduce it, mainly due to an incorrect treatment of wet/dry interfaces or a non-balanced source terms/fluxes implementation. More details about the analytical periodic solution are described in [14]. The package provided there is used to generate four different resolution grids:  $\Delta x = 0.04, 0.02, 0.01, 0.005m$ . The tolerance  $h_{tol}$  (see Appendix A) is set to  $10^{-4}$  in this particular case without friction and CFL=0.45.

Three periods ( $t=3T$ ) are simulated and the numerical results obtained by each grid resolution are compared to the exact solution, understood as the projection of the analytical solution on each computational grid. Figure 5 depicts those comparisons at  $t=1T$ ,  $t=2T$  and  $t=3T$ .

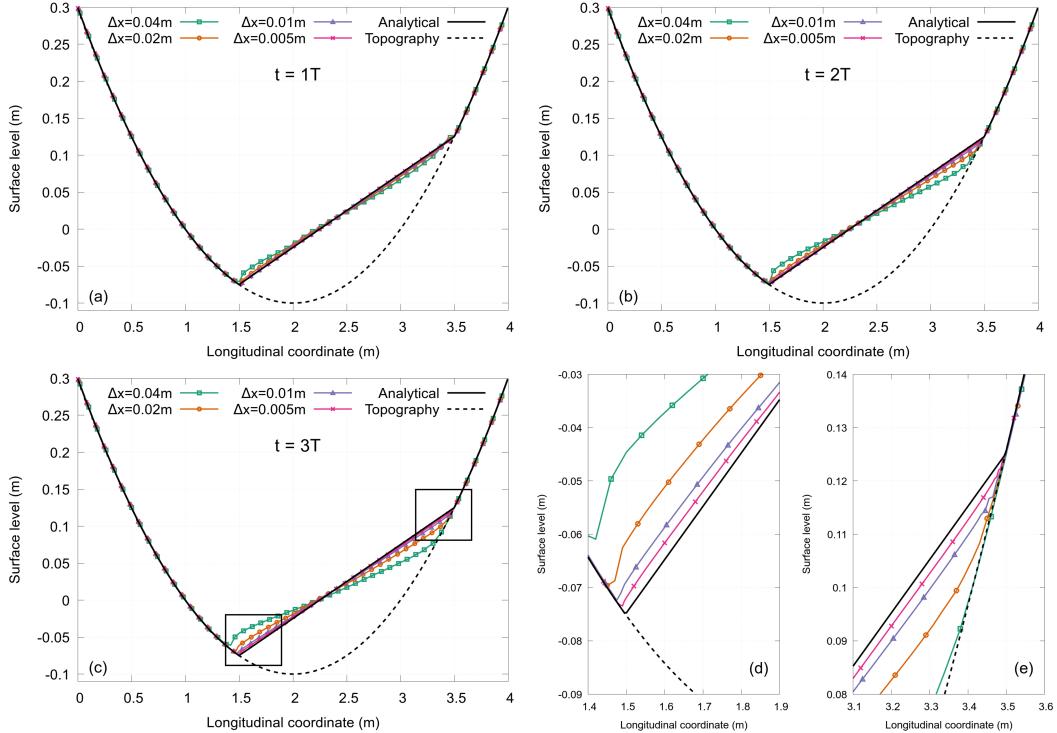
Accuracy decreases as time advances, especially with lower resolution. This is a consequence of the first order only numerical diffusion, which is resolution dependent. That said, the use of higher order schemes is not recommended since both pressure and dissipative terms usually dominate over the convective terms with the roughness of realistic applications. Also, the presence of wet/dry discontinuities would downgrade the accuracy to first order so that the cost of the implementation is not justified. Nonetheless, a correct estimation of the source strengths is mandatory to avoid dramatic reductions in the time step size and to ensure a correct well-balanced implementation [39, 41, 17].

To provide a quantitative measure of the error made for each resolution and to check the convergence rate,  $L_1$ ,  $L_2$  and  $L_\infty$  error norms are computed with respect to the analytical solution at  $t=3T$ . Table 1 contains those error norms computed as:

$$L_1(y_{\Delta x}) = \frac{1}{N} \sum_{i=1}^N |(y_n - y_e)_i| \quad L_2(y_{\Delta x}) = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_n - y_e)_i^2} \quad L_\infty(y_{\Delta x}) = \max_i |(y_n - y_e)_i| \quad (6)$$

where N is the number of grid cells and  $y_n$  and  $y_e$  are the numerical and exact solutions respectively.

These errors confirm the consistency of the scheme for a first order method. Even though this test case involves water depth values on the order of centimeters, millimeters, or below, together with strong velocities, the scheme is demonstrated to be robust and accurate enough, providing a solution free of oscillations, which is particularly of interest when dealing with wet/dry boundaries – a key factor in 2D flood models–.



**Figure 5:** Exact and numerical solutions for different grid resolutions at (a)  $t=1T$ , (b)  $t=2T$  and (c)  $t=3T$ . Panels (d) and (e) show a zoom of the left and right wet/dry interfaces respectively, at  $t=3T$ .

$\Delta x$	$L_1$ norm	$L_2$ norm	$L_\infty$ norm
0.04	3.943e-03	9.612e-03	4.630e-02
0.02	2.065e-03	5.137e-03	2.405e-02
0.01	9.724e-04	2.457e-03	1.090e-02
0.005	4.433e-04	1.117e-03	5.311e-03

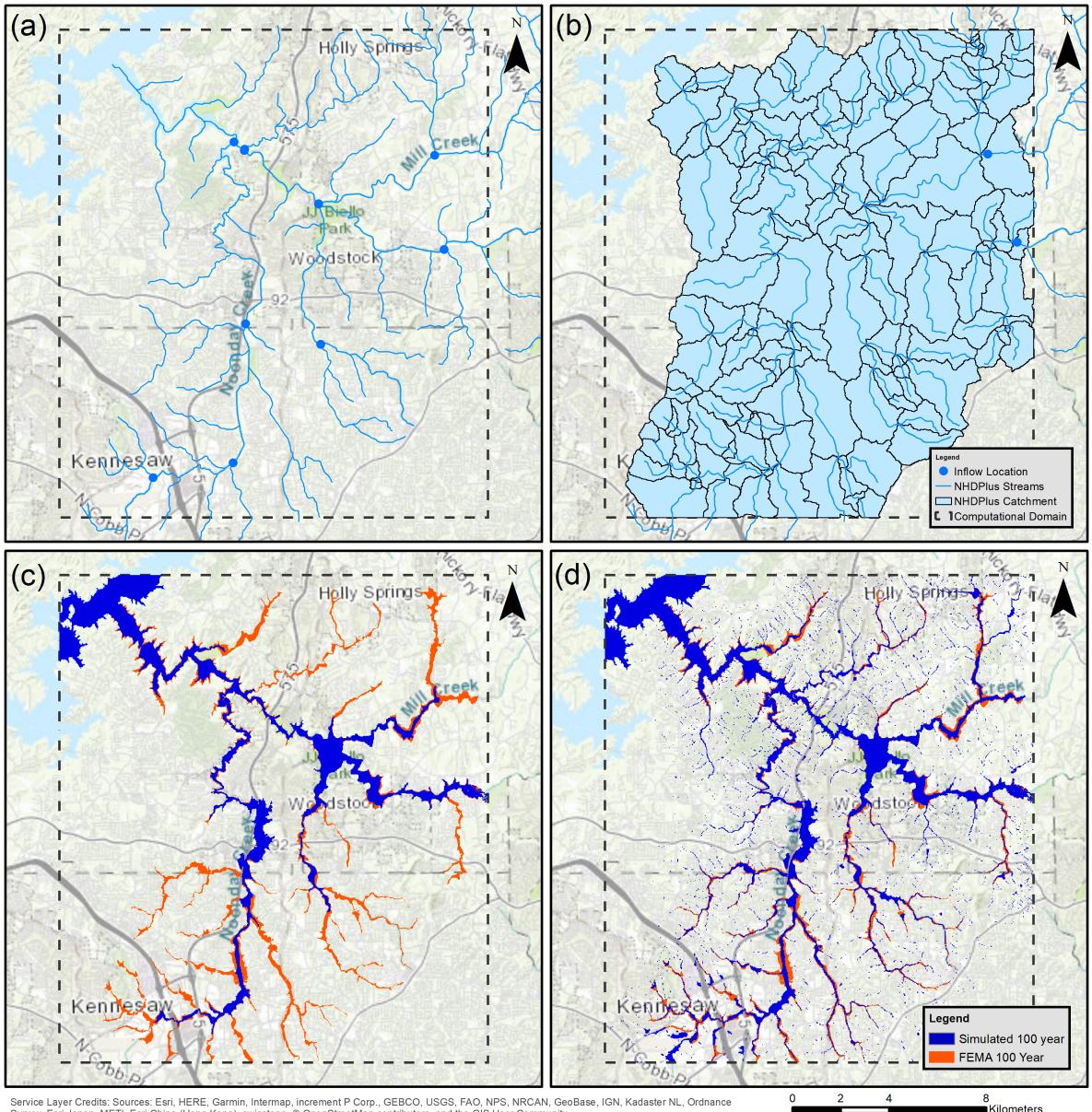
**Table 1**

$L_2$  ,  $L_1$  and  $L_\infty$  error norms for each resolution for the paraboloid test problem

### 5.2. Test case 2: runoff capability

TRITON admits runoff hydrographs to provide spatiotemporally distributed runoff as an input. Typically, a hydraulic model is driven by providing streamflow hydrographs at user-specified locations to simulate riverine (fluvial) floods. These locations can be where the observations of streamflow were made or can match a river routing model. However, the lack of sufficient streamflow source locations, due to hydrologic model limitations or other factors, may lead to the underestimation of flood extents, especially at smaller tributaries. To overcome this issue, users can utilize the “runoff function” within TRITON.

As an example to illustrate this capability, we select an area located upstream of Allatoona Reservoir in the northwest Georgia, US. The region was previously modelled by [21] [20] to study probable maximum flood using the Distributed Hydrologic Soil Vegetation Model (DHSVM) and Flood2D-GPU [28]. The 100-year peak streamflow was estimated at the outlet of the computational domain following the guidelines of Bulletin 17B [60], and then used to prepare 100-year return level streamflow hydrographs. For a detailed description, readers are referred to Section 3.1 of [20]. In TRITON, the 100-year flood is simulated with two different model configurations: Scenario A (no runoff) - using 13 streamflow source locations along the river network (Figure 6(a)), and Scenario B (with runoff) - using 2 upstream streamflow source locations and runoff simulated at various catchments (Figure 6(b)). The computational domain spans 358 sq. km and consists of 400,000 grid cells at a 30m DEM resolution. In both scenarios, a 5-day simulation is conducted



**Figure 6:** Comparison of runoff functionality. Panel (a) shows streamflow source locations for Scenario A (no runoff), and panel (b) shows streamflow source locations and runoff regions for Scenario B (with runoff). Panels (c) and (d) are the TRITON simulated 100-year flood plain against FEMA 100-year flood plain for Scenarios A and B, respectively.

(with peak streamflow occurring at day-3). The water depth is written in raster maps every 30 minutes. The maximum flood inundation extents for both scenarios, compared against a benchmark dataset from FEMA (100-year flood zones), are presented in Figure 6(c) and Figure 6(d), respectively. A qualitative comparison reveals that just using streamflow inputs (Scenario A, Figure 6(c)) may lead to the underestimation of flood extents, especially in tributaries where no upstream streamflow inputs are specified. In Scenario B, since the model is driven by runoff hydrograph across the entire domain, it can better capture the flood extents especially in the tributary areas. To evaluate the two scenarios quantitatively, we use a metric called "hit rate" which is a measure of model tendency to accurately predict the benchmark flood extents [20] [62]. Using FEMA 100-year flood plain as a benchmark, we obtain a hit rate of 0.50 for Scenario A and an

Summit nodes	multi-CPU			multi-GPU		
	# hardware cores	#MPI tasks	Runtime (h)	# devices	#MPI tasks	Runtime (h)
1	168	1	107.99	6	6	2.40
2	336	2	56.73	12	12	1.44
4	672	4	28.78	24	24	0.90
8	1344	8	14.39	48	48	0.63
16	2688	16	7.57	96	96	0.49
32	5376	32	3.68	192	192	0.43
64	10752	64	2.73	384	384	0.42

**Table 2**

Hardware configuration and runtimes for the Harvey test problem

improved rate of 0.68 for scenario B. Not only demonstrating a better floodplain simulation, local pluvial floods can also be simulated in Figure 6(d). The results showcase the advantage of using runoff for better and easier flood regime simulation.

### 5.3. Test case 3: Hurricane Harvey

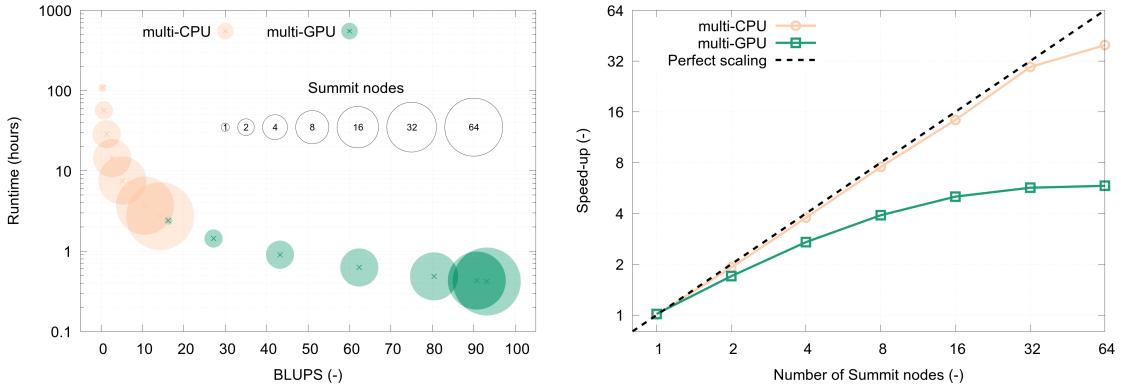
The last test case is intended to evaluate the performance and applicability of TRITON using different architectures (multiple CPUs and GPUs) in a realistic configuration. In this scenario, we simulate the massive flood that Hurricane Harvey caused in the summer of 2017 along the US Gulf Coast. The spatial domain encompasses around  $6800 \text{ km}^2$  of Harris County, Texas, US. The simulation covers ten days, with the heaviest rainfall occurring during day 7-to day-9. The runoff data are generated using the Variable Infiltration Capacity (VIC) hydrologic model [33] driven by hourly 4km radar-based Stage IV Quantitative Precipitation Estimate. This runoff is then routed using the Routing Application for Parallel computation of Discharge (RAPID) model [9] through the river network to generate streamflow input at 69 inflow source locations. Information from the US Geological Survey National Elevation Dataset is used to build a corrected DEM in which we included Addicks and Barker's reservoir capacities, incorporated the bathymetry of the main river segments and eliminated some noise present in the original data. The DEM resolution is 10m, with a total of around 68 million grid cells, and the Manning's roughness coefficient is set to a constant value of  $n = 0.035s/m^{1/3}$ . The output is configured in sequential binary format, with an output interval of 1800s. More information about this test case can be found in [16].

The purpose of this test case is to evaluate the efficiency and scalability of the model on different hardware configurations. Simulations are carried out on Summit supercomputer at Oak Ridge National Laboratory. Summit is comprised of 4,608 compute nodes, each of them containing six NVIDIA Volta V100 GPUs and 42 physical cores (168 hardware cores using Simultaneous Multithreading). In order to make a fair comparison between multiple architectures, a Summit compute node is chosen and seven numerical experiments are performed using up to 64 nodes. Two TRITON hardware configurations are used: multiple CPUs using MPI + OpenMP and multiple GPUs using MPI+CUDA, each of them with the aim of minimizing the number of MPI tasks per configuration. Consequently, the multi-CPU version uses one MPI task per node, while the multi-GPU version uses one MPI tasks per GPU. CUDA-Aware MPI is used for the multi-GPU simulations. Table 2 condenses both hardware configurations as well as displays the runtimes. Following [51] we also define the following metrics: Billion Lattice Updates per Second (BLUPS) and speed-up:

$$\text{BLUPS} = \frac{N_c \times N_{ts}}{T_n \times 10^9} \quad \text{speed-up} = \frac{T_1}{T_n} \quad (7)$$

where  $N_c$  is the number of grid cells,  $N_{ts}$  is the number of time steps done and  $T_n$  is the runtime achieved using  $n$  computing nodes. The speed-up in this case measures how fast the simulation is compared to the runtime using 1 node. Figure 7 (left) depicts the runtime in log scale ( $y$ -axis) and the number of BLUPS ( $x$ -axis) achieved by each hardware configuration (plotted in circles of different sizes).

The main result is that a very large problem for a serial code can be computed more reasonably with a multi-GPU system, with runtimes of less than 30 minutes. Even with the lowest hardware configuration



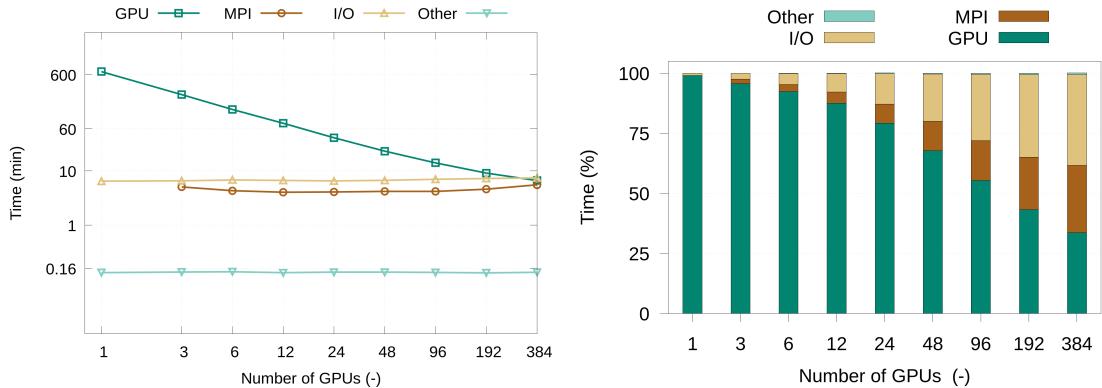
**Figure 7:** Runtime and BLUPS (left) and speed-up (right) achieved by each configuration for the Harvey test problem

(1 node, 6 GPUs), the multi-GPU version is able to achieve a lower runtime than the most demanding multi-CPU hardware configuration (64 nodes, 10752 OpenMP threads). Accordingly, the maximum BLUPS achieved by the multi-CPU system is still lower than the 1-node multi-GPU configuration. Additionally, given a fixed number of Summit nodes, the average BLUPS ratio between the multi-GPU and multi-CPU versions is 25x, with a maximum of 45x for 1 node, revealing the convenience of using this architecture. The circle series turns horizontal when the strong scaling limit is reached, and the asymptote is representative of the absolute fastest runtime expected for each configuration in this problem. With this, the multi-CPU system has not reach its maximum using 64 nodes while the multi-GPU version tails off significantly beyond 8 or 16 nodes.

Figure 7 (right) shows in log-log scale the speed-up relative to the simulation using 1 node ( $y$ -axis) as a function of node count ( $x$ -axis), compared with the perfect scaling. As shown, the multi-CPU version is able to achieve a satisfactory scaling factor up to 32 nodes (32 MPI tasks) although a performance hit is observed for 64 nodes. This might be due to the row-wise (1D) MPI partitioning. On the other hand, the multi-GPU speed-up does not scale acceptably. Although 6 MPI tasks are used per Summit node (1 per GPU), a lower speed-up is observed even for 32 MPI tasks (extrapolation between 4 and 8 nodes), where adequate speed-ups were achieved for the multi-CPU version. Many factors are responsible for this: first, this test case does not have runoff as an inflow and only around 20% (as an average) of the domain is wet. A loss of efficiency is therefore caused by thread divergence due to an “if statement” implemented in the code to avoid the computations on dry cells. This is an issue reported for CUDA and it is not the case with OpenMP since each CPU core runs like a single-threaded subroutine, executing its own independent set of instructions. Additionally, a static MPI subdomain partitioning aggravates this fact since some subdomains could not have a significant computational burden, resulting in an imbalance among MPI processes [38]. To investigate other sources of scaling limitations in the multi-GPU system, the computation time (GPU), the MPI communication time, the I/O time and the rest are plotted in Figure 8. Two additional simulations are carried out using 1 and 3 GPUs. The left panel shows (in log-log scale) the absolute number (in minutes) while the right plot displays the percentage of the time consumed by each process against the GPU count.

Note that memory copies between the host and the device are counted within the GPU time and the “Other” time stands for subroutine calls and basic operations run on the CPU. As observed on the left plot, the GPU time is reduced at almost the same rate for each configuration, meaning that it actually scales according to the number of GPUs. A slightly lower rate is detected for the last two values (192 and 384 GPUs) due to the low number of grid cells per GPU –each GPU does not have enough work to leverage its computing power. I/O and other (CPU) time remain almost constant for all configurations as expected. Communication time using a blocking algorithm and CUDA-Aware MPI does not increase noticeably as the number of GPUs grows, indicating that communicating every time step carries significantly more weight than the number of GPUs.

The right panel demonstrates that MPI and I/O times govern this problem for large GPU count. In particular, from 40% to 66% of the time in this test case is consumed by these processes at 96 GPUs and



**Figure 8:** GPU, MPI, I/O and "other" time (left) and percentage (right) achieved by each configuration for the Harvey test problem

beyond. This fact suggests that the operational scale bottleneck is not with computation but on communication and I/O tasks. Parallel I/O should improve these results, and a more efficient communication strategy should be designed. These results motivate even larger test cases to leverage the massive parallelization in a substantial number of GPUs, paving the way to even larger temporal and spatial scales.

## 6. Conclusions and Perspectives

A new open-source 2D flood model, TRITON, is available to run on heterogeneous architectures using single and multiple CPUs and GPUs to enable hydraulic computations at large temporal and spatial scales. It consists of a simple input file structure (meshless, standard GIS formats and a configuration text file) and provides spatiotemporal information of water depths and velocities as output information.

Three test cases have been provided to demonstrate the TRITON capabilities. The accuracy, consistency and robustness of the scheme has been proved by means of the paraboloid test case. The importance of runoff capability in TRITON has been highlighted using a flood test case in northwest Georgia, US. Results with and without runoff have been compared against the 100-year flood extension provided by FEMA, revealing the benefit of considering the runoff capability for this sort of studies. Finally, the Hurricane Harvey test case has been used to show the performance on the scheme on different architectures: multi-CPU using OpenMP + MPI and multi-GPU with CUDA + MPI. The numerical experiments highlight the convenience of using the multi-GPU version against the multi-CPU, achieving a low runtime (less than 30 mins) for real-world configurations –a large spatial domain at 10m resolution and a 10-day hydrograph – and unlocking operational purposes at even larger spatial and temporal scales.

Although the runtimes are promising, the scalability of the multi-GPU version is nevertheless unsatisfactory for large number of GPUs. Many aspects are responsible for this: thread divergence for dry cells, poor load balancing between MPI ranks with a static decomposition, and principally the execution time consumed by I/O and MPI communication for a large scale problem, with respect to the computation time. Although these times (in the order of minutes each) are almost constant and does not depend on the number of GPUs, they represent a great percentage of the total runtime when trying to achieve operational purposes. Future perspectives are therefore aimed at designing optimized I/O parallel algorithms and exploring new communication techniques such as a 2D MPI decomposition or overlapping strategies. Particularly, the latter would considerably improve the performance as communication between subdomains would not be required to be every time step.

TRITON is under continuous development. Future planned improvement includes, besides new efficient I/O and communication algorithms, support for other GPU libraries such as OpenACC. All of these efforts will be regularly documented in the repository. We provide this baseline to enable the use of a fully 2D hydraulic model for new science questions such as uncertainty quantification or climate change problems beyond the studied temporal and spatial scales heretofore. The extension to very high resolution contin-

500 nental/global scale flood modeling will require multi-GPU computations so new algorithms are obviously  
 501 planned to extend these capabilities to operational scales.

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 510 public access to these results of federally sponsored research in accordance with the DOE Public Access Plan  
 511 (<http://energy.gov/downloads/doe-public-access-plan>).

## 512 A. Numerical Scheme

513 The derivation of the numerical scheme from (1) to (2) is detailed here. First, integrating the hyperbolic  
 514 system of equations (1) in  $\Omega_i \times [t^n, t^*]$ , where  $\Omega_i$  is referred to the  $i$ -th computational cell of the domain  
 515 and  $t^* = t^n + \Delta t$ , and applying the Gauss theorem:

$$\int_{t^n}^{t^*} \int_{\Omega_i} \frac{\partial \mathbf{U}}{\partial t} dSdt + \int_{t^n}^{t^*} \int_{\Omega_i} (\nabla \cdot \mathbf{E}) dSdt = \int_{t^n}^{t^*} \int_{\Omega_i} \mathbf{S}_b dSdt \quad (8)$$

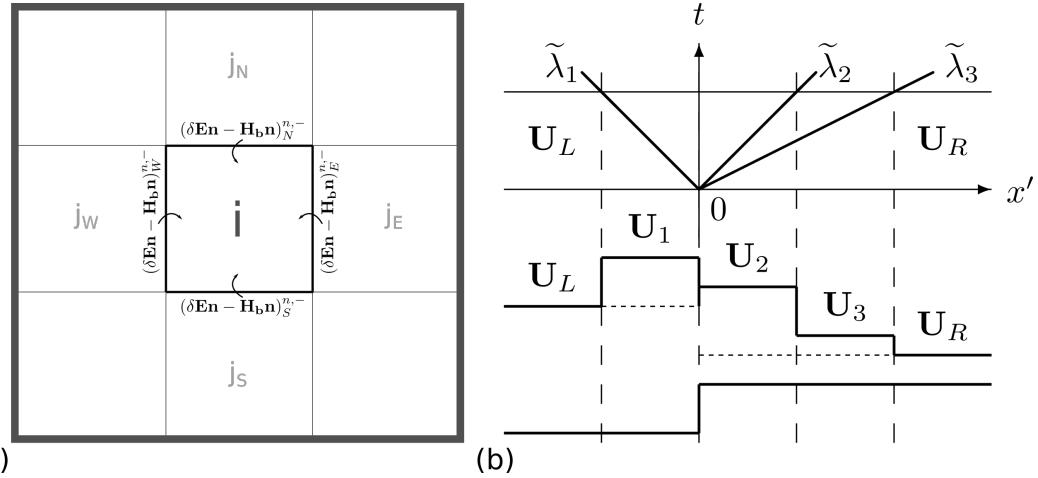
where  $\mathbf{E} = (\mathbf{F}, \mathbf{G})$ . Applying the Gauss theorem and replacing the contour integral by the sum across its four edges (Cartesian square grid of size  $\Delta x$ ):

$$\int_{t^n}^{t^*} \int_{\Omega_i} \frac{\partial \mathbf{U}}{\partial t} dSdt + \int_{t^n}^{t^*} \sum_{k=1}^4 \mathbf{E} \mathbf{n} \Delta x dt = \int_{t^n}^{t^*} \int_{\Omega_i} \mathbf{S}_b dSdt \quad (9)$$

516 with  $\mathbf{n} = (n_x, n_y)$  the outward normal direction. Assuming a piecewise discretization and a Roe's solver  
 517 with an upwind discretization of fluxes and source terms, the updating of the conserved variables can be  
 518 written in flux-difference splitting form as [26]:

$$\mathbf{U}_i^* = \mathbf{U}_i^n - \frac{\Delta t}{\Delta x} \sum_{k=1}^4 (\delta \mathbf{E} \mathbf{n} - \mathbf{H}_b \mathbf{n})_k^{n,-} \quad (\delta \mathbf{E} \mathbf{n})_k^- = (\tilde{\mathbf{P}} \tilde{\Lambda}^- \tilde{\mathbf{A}})_k \quad (\mathbf{H}_b \mathbf{n})_k^- = (\tilde{\mathbf{P}} \frac{\tilde{\Lambda}^-}{\tilde{\Lambda}} \tilde{\mathbf{B}}_b)_k \quad (10)$$

519 The meaning of this expression is simple: the conserved variables  $\mathbf{U} = (h, q_x, q_y)$  at each grid cell  $i$  will  
 520 be updated according to the in-going contributions that come from its four edges  $k$  (east, north, west and  
 521 south) shared by the four neighbouring cells  $j$ . A sketch of the scheme is shown in Figure 9(a).  
 522 Equation (10) includes the matrices and vectors coming from Roe's linearization:  $\tilde{\mathbf{P}}$  is the matrix containing  
 523 the three right eigenvectors  $\tilde{\mathbf{e}}_k$  of the Jacobian Matrix,  $\tilde{\Lambda}$  represents the diagonal matrix of the three  
 524 eigenvalues  $\lambda_k$  – the minus superscript denotes the upwind discretization – and  $\tilde{\mathbf{A}}_k$  and  $\tilde{\mathbf{B}}_{bk}$  account for the  
 525 three wave and source strengths respectively. With this, it is easy to derive equation (2) from (10). The



**Figure 9:** Stencil for the proposed numerical scheme (a) and approximate solution for  $\tilde{\lambda}_1 < 0$ ,  $\tilde{\lambda}_2, \tilde{\lambda}_3 > 0$  (b)

expressions for those matrices and vectors are detailed here:

$$\tilde{\mathbf{P}}_k = (\tilde{\mathbf{e}}_1, \tilde{\mathbf{e}}_2, \tilde{\mathbf{e}}_3)_k = \begin{pmatrix} 1 & 0 & 1 \\ \tilde{u} - \tilde{c} n_x & -\tilde{c} n_y & \tilde{u} + \tilde{c} n_x \\ \tilde{v} - \tilde{c} n_y & \tilde{c} n_x & \tilde{v} + \tilde{c} n_y \end{pmatrix}_k$$

$$\tilde{\mathbf{\Lambda}}_k = \begin{pmatrix} \tilde{\lambda}_1 & 0 & 0 \\ 0 & \tilde{\lambda}_2 & 0 \\ 0 & 0 & \tilde{\lambda}_3 \end{pmatrix}_k = \begin{pmatrix} \tilde{\mathbf{u}}\mathbf{n} - \tilde{c} & 0 & 0 \\ 0 & \tilde{\mathbf{u}}\mathbf{n} & 0 \\ 0 & 0 & \tilde{\mathbf{u}}\mathbf{n} + \tilde{c} \end{pmatrix}_k \quad \tilde{\mathbf{\Lambda}}_k^- = \frac{\tilde{\mathbf{\Lambda}}_k - |\tilde{\mathbf{\Lambda}}_k|}{2}$$

$$\tilde{\mathbf{A}}_k = (\tilde{\mathbf{P}}^{-1} \delta \mathbf{U})_k = \begin{pmatrix} \tilde{\alpha}_1 \\ \tilde{\alpha}_2 \\ \tilde{\alpha}_3 \end{pmatrix}_k = \begin{pmatrix} \frac{\delta h}{2} - \frac{\delta \mathbf{q}\mathbf{n} - \tilde{\mathbf{u}}\mathbf{n}\delta h}{2\tilde{c}} \\ \frac{1}{\tilde{c}} [(\delta q_y - \tilde{v}\delta h)n_x - (\delta q_x - \tilde{u}\delta h)n_y] \\ \frac{\delta h}{2} + \frac{\delta \mathbf{q}\mathbf{n} - \tilde{\mathbf{u}}\mathbf{n}\delta h}{2\tilde{c}} \end{pmatrix}_k \quad (11)$$

$$\tilde{\mathbf{u}}_k = (\tilde{u}, \tilde{v})_k = \left( \frac{u_i \sqrt{h_i} + u_j \sqrt{h_j}}{\sqrt{h_i} + \sqrt{h_j}}, \frac{v_i \sqrt{h_i} + v_j \sqrt{h_j}}{\sqrt{h_i} + \sqrt{h_j}} \right)_k \quad \tilde{c} = \sqrt{g \frac{h_i + h_j}{2}}$$

$$\delta h_k = h_j - h_i \quad \delta \mathbf{q}_k = (\delta q_x, \delta q_y)_k = (q_{x_j} - q_{x_i}, q_{y_j} - q_{y_i})_k$$

where  $\mathbf{u} = (u, v) = (q_x/h, q_y/h)$  is the flow velocity.

The term  $\tilde{\mathbf{B}}_{bk}$  accounts for the bed slope source estimation. In this work, the integral formulation proposed in [39] is adopted, leading to the following definition of  $\tilde{\mathbf{B}}_{bk}$ :

$$\tilde{\mathbf{B}}_{bk} = \begin{pmatrix} \tilde{\beta}_{b1} \\ \tilde{\beta}_{b2} \\ \tilde{\beta}_{b3} \end{pmatrix}_k = \begin{pmatrix} \frac{g}{2\tilde{c}} \left( h_p - \frac{|\delta z'|}{2} \right) \delta z' \\ 0 \\ -\frac{g}{2\tilde{c}} \left( h_p - \frac{|\delta z'|}{2} \right) \delta z' \end{pmatrix} \quad h_p = \begin{cases} h_i & \delta z \geq 0 \\ h_j & \delta z < 0 \end{cases} \quad \delta z' = \begin{cases} h_i & \delta z \geq 0 \text{ and } h_i + z_i < z_j \\ -h_j & \delta z < 0 \text{ and } h_j + z_j < z_i \\ z_j - z_i & \text{otherwise} \end{cases}$$

530 Although this estimation is more accurate than the conventional ‘finite-difference-like’ approach, it can still  
 531 lead to non-physical solutions when dealing with complex flows. When these problems arise, the conventional  
 532 solution consists in reducing CFL and consequently the time step size, impacting directly on the performance  
 533 of the computation. Another approach is adopted here, based on the augmented approach, which allows us  
 534 to reconstruct the cell-averaged approximate solution with the objective of avoiding negative water depth  
 535 values at time  $t^*$ . This can be particularly useful for the treatment of wet/dry fronts, a key factor for reliable  
 536 2D hydraulic models. In this work, the wet/dry treatment detailed in [17, 39] is implemented. Following  
 537 this approach, the intermediate states of the Riemann problem are analyzed and, depending on their sign,  
 538 the information is sent to the left or the right side of the discontinuity. This has been proved to be mass  
 539 conservative and robust for any kind of flows [17, 39].

540 Besides the wet/dry fronts, stiff source terms can lead to negative water depth values, even in the presence  
 541 of wet/wet problems -i.e., thin layers of water with strong bed discontinuities and high friction terms. In  
 542 order to consider these situations in our numerical scheme, a similar technique of that followed in [39] is  
 543 adopted here. However, as the time step is computed before the source terms estimation, a new limitation  
 544 based on the final integration –rather than zero the intermediate states– is proposed in this work. As detailed  
 545 in [39], only wet/wet subcritical cases are analyzed. Let us denote  $L$  and  $R$  the left and right states of a  
 546 discontinuity and assume  $\tilde{\lambda}_2 > 0$  –the derivation does not change for  $\tilde{\lambda}_2 < 0$  due to the properties of the  
 547 intermediate states for the water depth in the augmented approach–. The numerical solution at time  $t^*$   
 548 should guarantee  $h_L^* \geq 0$  and  $h_R^* \geq 0$ . Then, according to Figure 9(b), the following inequations must be  
 549 fulfilled:

$$h_L \left( \frac{\Delta x}{2} - |\tilde{\lambda}_1| \Delta t \right) + |\tilde{\lambda}_1| \Delta t h_1 \geq 0 \quad \tilde{\lambda}_2 \Delta t h_2 + (\tilde{\lambda}_3 - \tilde{\lambda}_2) \Delta t h_3 + h_R \left( \frac{\Delta x}{2} - \tilde{\lambda}_3 \Delta t \right) \geq 0 \quad (13)$$

550 In agreement with the definitions of the intermediate states [53, 39]:

$$h_1 = h_L + \tilde{\alpha}_1 - \frac{\tilde{\beta}_{b_1}}{\tilde{\lambda}_1} \quad h_2 = h_3 = h_R - \tilde{\alpha}_3 - \frac{\tilde{\beta}_{b_1}}{\tilde{\lambda}_3} \quad (14)$$

551 and doing some simple algebraic manipulations, the following restrictions are derived for  $\tilde{\beta}_{b_1}$  –and conse-  
 552 quently for  $\tilde{\beta}_{b_3}$ –:

$$\tilde{\beta}_{min} \leq \tilde{\beta}_{b_1} \leq \tilde{\beta}_{max} \quad \tilde{\beta}_{min} = -h_L \frac{\Delta x}{2\Delta t} + \tilde{\alpha}_1 \tilde{\lambda}_1 \quad \tilde{\beta}_{max} = \frac{\Delta x}{2\Delta t} h_R - \tilde{\lambda}_3 \tilde{\alpha}_3 \quad \tilde{\beta}_{b_3} = -\tilde{\beta}_{b_1} \quad (15)$$

553 These conditions are implemented in TRITON, minimizing the appearance of negative water depths.  
 554 Additionally, this scheme needs an entropy correction for transonic rarefactions hence the Harten-Hyman  
 555 entropy fix is used here. As this approach is based on decomposing the existing jump into two new jumps,  
 556 a special emphasis should be put in the source term split [39].

557 Two additional assumptions are considered. First, a cell is considered dry if its water depth is below  
 558  $10^{-12}$ . Second, velocities are set to zero for water depths below a tolerance. This value depends on the  
 559 characteristics of the problem study (spatial scales and roughness mainly). As a physical explanation for this  
 560 parameter, dissipation terms (in practical applications with realistic roughness values) dominate at this scale  
 561 over convective and inertial terms. Therefore, it is not arbitrary to model this phenomenon as a tolerance  
 562 under which velocities are considered null. A value of  $10^{-3}$  is suggested for real-world scenarios as a general  
 563 recommendation, although it can be also modified in TRITON for every configuration. The scheme has  
 564 been proved to be well-balanced, robust and reliable for flows under various conditions, according to Section  
 565 5.

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