SWE – Anatomy of a Parallel Shallow Water Code

CSCS-FoMICS-USI Summer School on
Computer Simulations in Science and Engineering

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Teaching Parallel Programming Models . . .

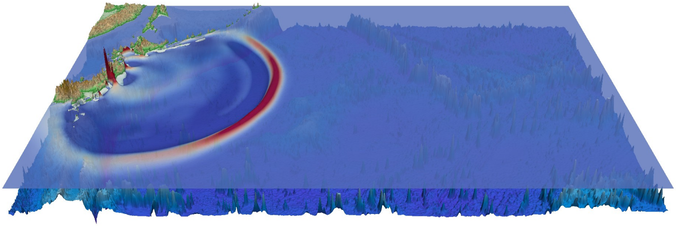
Starting Point: Lecture on Parallel Programming

- classical approaches for shared & distributed memory: OpenMP and MPI
- “something more fancy” $\rightarrow$ GPU computing (CUDA, e.g.)
- motivating example to teach different models and compare their properties

“Motivating Example”:

- not just Jacobi or Gauß-Seidel
- not the heat equation again . . .
- inspired by a CFD code: “Nast” by Griebel et al.
- turned out to become shallow water equations
- **and is heavily used for summer schools . . .**

Towards Tsunami Simulation with SWE

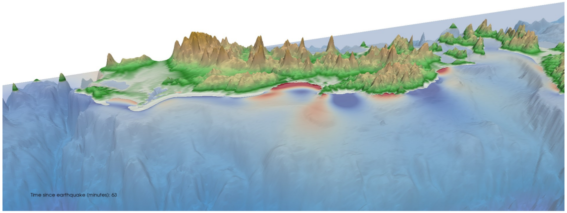


Time since earthquake (minutes): 78

Shallow Water Code – Summary

- Finite Volume discretization on regular Cartesian grids
  $\rightarrow$ simple numerics (but can be extended to state-of-the-art)
- patch-based approach with ghost cells for communication
  $\rightarrow$ wide-spread design pattern for parallelization

Towards Tsunami Simulation with SWE (2)

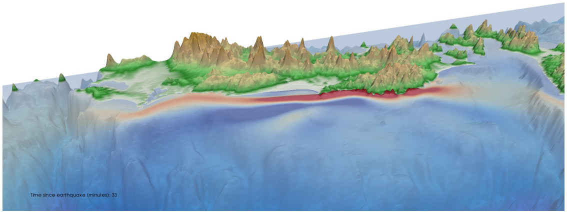


Shallow Water Code – Bells & Whistles

- included augmented Riemann solvers (D. George, R. LeVeque)
  $\rightarrow$ allows to simulate inundation
- developed towards hybrid parallel architectures
  $\rightarrow$ now runs on GPU clusters

Part I

Model and Discretization

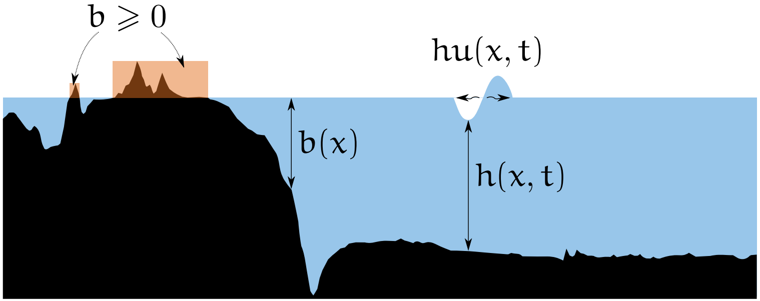


Model: The Shallow Water Equations

Simplified setting (no friction, no viscosity, no coriolis forces, etc.):

$$\frac{\partial}{\partial t}\begin{bmatrix} h \\ hu \\ hv \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \\ huv \end{bmatrix} + \frac{\partial}{\partial y}\begin{bmatrix} hv \\ huv \\ hv^2 + \frac{1}{2}gh^2 \end{bmatrix} = \begin{bmatrix} 0 \\ -\frac{\partial}{\partial x}(ghb) \\ -\frac{\partial}{\partial y}(ghb) \end{bmatrix}$$

Quantities and unknowns:



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Write as generalized hyperbolic PDE:

- 2D setting, three quantities: $q = (q_1, q_2, q_3)^T = (h, hu, hv)^T$

$$\frac{\partial}{\partial t}q + \frac{\partial}{\partial x}F(q) + \frac{\partial}{\partial y}G(q) = S(q, x, y, t)$$

- with flux functions:

$$F(q) = \begin{bmatrix} q_2 \\ q_2^2/q_1 + \frac{1}{2}gq_1^2 \\ q_2q_3/q_1 \end{bmatrix} \qquad G(q) = \begin{bmatrix} q_3 \\ q_2q_3/q_1 \\ q_3^2/q_1 + \frac{1}{2}gq_1^2 \end{bmatrix}$$

Model: The Shallow Water Equations

Simplified setting (no friction, no viscosity, no coriolis forces, etc.):

$$\frac{\partial}{\partial t}\begin{bmatrix} h \\ hu \\ hv \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \\ huv \end{bmatrix} + \frac{\partial}{\partial y}\begin{bmatrix} hv \\ huv \\ hv^2 + \frac{1}{2}gh^2 \end{bmatrix} = \begin{bmatrix} 0 \\ -\frac{\partial}{\partial x}(ghb) \\ -\frac{\partial}{\partial y}(ghb) \end{bmatrix}$$

Derived from conservations laws:

- h equation: conservation of mass
- equations for hu and hv: conservation of momentum
- $\frac{1}{2}gh^2$: averaged hydrostatic pressure due to water column h, similar: bathymetry terms $-\frac{\partial}{\partial x}(ghb)$ and $-\frac{\partial}{\partial y}(ghb)$
- may also be derived by vertical averaging from the 3D incompressible Navier-Stokes equations

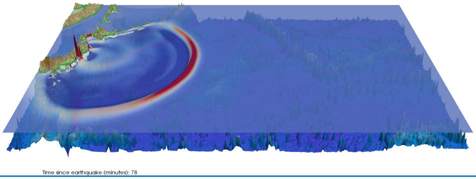
Model: The Shallow Water Equations

Simplified setting (no friction, no viscosity, no coriolis forces, etc.):

$$\frac{\partial}{\partial t}\begin{bmatrix} h \\ hu \\ hv \end{bmatrix} + \frac{\partial}{\partial x}\begin{bmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \\ huv \end{bmatrix} + \frac{\partial}{\partial y}\begin{bmatrix} hv \\ huv \\ hv^2 + \frac{1}{2}gh^2 \end{bmatrix} = \begin{bmatrix} 0 \\ -\frac{\partial}{\partial x}(ghb) \\ -\frac{\partial}{\partial y}(ghb) \end{bmatrix}$$

The ocean as “shallow water”??

- compare horizontal ($\sim$ 1000 km) to vertical ($\sim$ 4 km) length scale
- wave lengths large compared to water depth
- vertical flow may be neglected; movement of the “entire water column”



Finite Volume Discretisation

- discretise system of PDEs

$$\frac{\partial}{\partial t} q + \frac{\partial}{\partial x} F(q) + \frac{\partial}{\partial y} G(q) = S(t, x, y)$$

- results from integral equation:

$$\frac{\partial}{\partial t} \int_{t_n}^{t_{n+1}} \int_{\Omega} q \, d\omega \, dt + \int_{t_n}^{t_{n+1}} \int_{\partial\Omega} \vec{F}(q) \cdot \vec{n} \, ds \, dt = \ldots$$

- use averaged quantities $Q_{i,j}^{(n)}$ in finite volume elements Ω_{ij}:

$$Q_{ij}(t) := \frac{1}{|\Omega_{ij}|} \int_{\Omega_{ij}} q \, d\omega \quad \rightsquigarrow \quad \frac{\partial}{\partial t} \int_{t_n}^{t_{n+1}} \int_{\Omega} q \, d\omega \, dt = |\Omega_{ij}| \left(Q_{i,j}^{(n+1)} - Q_{i,j}^{(n)} \right)$$

- What about the flux integral?

Finite Volume Discretisation (2)

- flux integral on Cartesian grids:

$$\int_{t_n}^{t_{n+1}} \int_{\partial\Omega} \vec{F}(q)\cdot\vec{n}\,ds\,dt = \int_{t_n}^{t_{n+1}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} F(q(x_{i+\frac{1}{2}},y,t)) - F(q(x_{i-\frac{1}{2}},y,t))\,dy\,dt$$

$$+ \int_{t_n}^{t_{n+1}} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} G(q(x,y_{j+\frac{1}{2}},t)) - G(q(x,y_{i-\frac{1}{2}},t))\,dy\,dt$$

- leads to explicit time stepping scheme:

$$Q_{i,j}^{(n+1)} - Q_{i,j}^{(n)} = \frac{\Delta t}{\Delta y}\Big(F(q(x_{i+\frac{1}{2}},y,t_n)) - F(q(x_{i-\frac{1}{2}},y,t_n))\Big) + \frac{\Delta t}{\Delta x}\Big(G(q(x,y_{j+\frac{1}{2}},t_n)) - G(q(x,y_{i-\frac{1}{2}},t_n))\Big)$$

- how to compute $F_{i+\frac{1}{2},j}^{(n)} := F(q(x_{i+\frac{1}{2}},y,t_n))$?

Central and Upwind Fluxes

- define fluxes $F^{(n)}_{i+\frac{1}{2},j}$, $G^{(n)}_{i,j+\frac{1}{2}}, \ldots$ via 1D numerical flux function $\mathcal{F}$:

$$F^{(n)}_{i+\frac{1}{2}} = \mathcal{F}\left(Q^{(n)}_i, Q^{(n)}_{i+1}\right) \qquad G^{(n)}_{j-\frac{1}{2}} = \mathcal{F}\left(Q^{(n)}_{j-1}, Q^{(n)}_j\right)$$

- **central flux**:

$$F^{(n)}_{i+\frac{1}{2}} = \mathcal{F}\left(Q^{(n)}_i, Q^{(n)}_{i+1}\right) := \frac{1}{2}\left(F\left(Q^{(n)}_i\right) + F\left(Q^{(n)}_{i+1}\right)\right)$$

  leads to unstable methods for convective transport

- **upwind flux** (here, for h-equation, $F(h) = hu$):

$$F^{(n)}_{i+\frac{1}{2}} = \mathcal{F}\left(h^{(n)}_i, h^{(n)}_{i+1}\right) := \begin{cases} hu\big|_i & \text{if } u\big|_{i+\frac{1}{2}} > 0 \\ hu\big|_{i+1} & \text{if } u\big|_{i+\frac{1}{2}} < 0 \end{cases}$$

  stable, but includes artificial diffusion

(Local) Lax-Friedrichs Flux

- classical **Lax-Friedrichs method** uses as numerical flux:

$$F^{(n)}_{i+\frac{1}{2}} = \mathcal{F}\left(Q^{(n)}_i, Q^{(n)}_{i+1}\right) := \frac{1}{2}\left(F\left(Q^{(n)}_i\right) + F\left(Q^{(n)}_{i+1}\right)\right) - \frac{h}{2\tau}\left(Q^{(n)}_{i+1} - Q^{(n)}_i\right)$$

- can be interpreted as central flux plus diffusion flux:

$$\frac{h}{2\tau}\left(Q^{(n)}_{i+1} - Q^{(n)}_i\right) = \frac{h^2}{2\tau} \cdot \frac{Q^{(n)}_{i+1} - Q^{(n)}_i}{h}$$

  with diffusion coefficient $\frac{h^2}{2\tau}$, where $c := \frac{h}{\tau}$ is a velocity ("one grid cell per time step" $\rightarrow$ cmp. CFL condition)

- idea of **local Lax-Friedrichs** method: use the actual wave speed

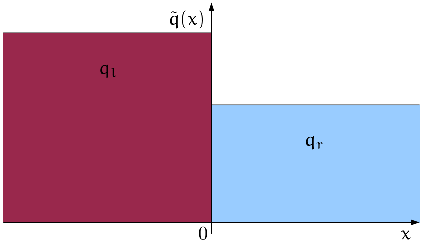
$$F^{(n)}_{i+\frac{1}{2}} := \frac{1}{2}\left(F\left(Q^{(n)}_i\right) + F\left(Q^{(n)}_{i+1}\right)\right) - \frac{a_{i+\frac{1}{2}}}{2}\left(Q^{(n)}_{i+1} - Q^{(n)}_i\right)$$

Riemann Problems

- solve **Riemann problem** to obtain solution $q(x_{i+\frac{1}{2}}, y, t_n)$, etc.:
- 1D treatment: solve shallow water equations with initial conditions

$$q(x_{i-\frac{1}{2}}, t_n) = \begin{cases} q_l = Q_{i-1}^{(n)} & \text{if } x < x_{i-\frac{1}{2}} \\ q_r = Q_i^{(n)} & \text{if } x > x_{i-\frac{1}{2}} \end{cases}$$

- solution: two (left or right) outgoing waves (shock or rarefaction)



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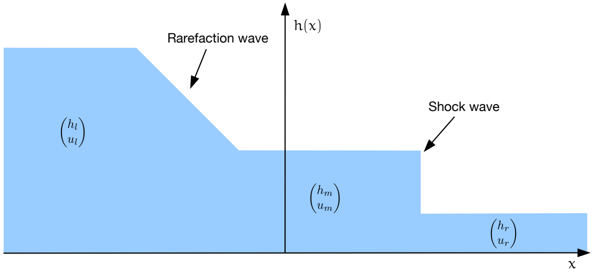
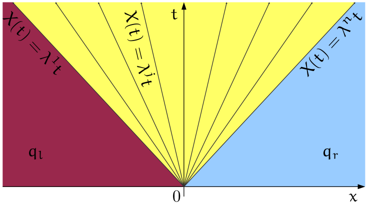


Riemann Problems (2)

- wave propagation approach: split the jump into fluxes

$$F(Q_i) - F(Q_{i-1}) - \Delta x \psi_{i-\frac{1}{2}} = \sum_p \alpha_p r_p \equiv \sum_p Z_p \qquad \alpha_p \in \mathbb{R}.$$

r_p the eigenvector of the linearised problem,
$\psi_{i-\frac{1}{2}}$ a fix for the source term (bathymetry)



- implementation will compute **net updates**:

$$\mathcal{A}^+\Delta Q_{i-1/2,j} = \sum_{p:\ \lambda_p>0} Z_p \qquad \mathcal{A}^-\Delta Q_{i-1/2,j} = \sum_{p:\ \lambda_p<0} Z_p$$

The F-Wave Solver

- use Roe eigenvalues $\lambda_{1/2}^{\text{Roe}}$ to approximate the wave speeds:

$$\lambda_{1/2}^{\text{Roe}}(q_l, q_r) = u^{\text{Roe}}(q_l, q_r) \pm \sqrt{g h^{\text{Roe}}(q_l, q_r)}$$

- with $h^{\text{Roe}}(q_l, q_r) = \frac{1}{2}(h_l + h_r)$ and $u^{\text{Roe}}(q_l, q_r) = \frac{u_l\sqrt{h_l} + u_r\sqrt{h_r}}{\sqrt{h_l} + \sqrt{h_r}}$
- eigenvectors $r_{1/2}^{\text{Roe}}$ for wave decomposition defined as

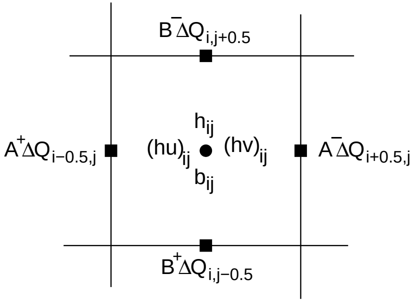
$$r_1^{\text{Roe}} = \begin{pmatrix} 1 \\ \lambda_1^{\text{Roe}} \end{pmatrix} \qquad r_2^{\text{Roe}} = \begin{pmatrix} 1 \\ \lambda_2^{\text{Roe}} \end{pmatrix}$$

- leads to net updates (source terms still missing):

$$A^- \Delta Q := \sum_{p:\{\lambda_p^{\text{Roe}}<0\}} \alpha_p r_p \qquad A^+ \Delta Q := \sum_{p:\{\lambda_p^{\text{Roe}}>0\}} \alpha_p r_p$$

- with $\alpha_{1/2}$ computed from $\begin{pmatrix} 1 & 1 \\ \lambda_1^{\text{Roe}} & \lambda_2^{\text{Roe}} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = F(Q_i) - F(Q_{i-1})$

Finite Volume on Cartesian Grids



Unknowns and Numerical Fluxes:

- (averaged) unknowns h, hu, hv, and b located in cell centers
- two sets of “net updates” or “numerical fluxes” per edge; here: $\mathcal{A}^+\Delta Q_{i-1/2,j}$, $\mathcal{B}^-\Delta Q_{i,j+1/2}$ (“wave propagation form”)

Flux Form vs. Wave Propagation Form

- numerical scheme in flux form:

$$Q_{i,j}^{(n+1)} = Q_{i,j}^{(n)} - \frac{\Delta t}{\Delta x}\left(F_{i+\frac{1}{2},j}^{(n)} - F_{i-\frac{1}{2},j}^{(n)}\right) - \frac{\Delta t}{\Delta y}\left(G_{i,j+\frac{1}{2}}^{(n)} - G_{i,j-\frac{1}{2}}^{(n)}\right)$$

  where $F_{i+\frac{1}{2},j}^{(n)}, G_{i,j+\frac{1}{2}}^{(n)}, \ldots$ approximate the flux functions $F(q)$ and $G(q)$ at the grid cell boundaries

- **Wave propagation form:**

$$\begin{aligned} Q_{i,j}^{n+1} = Q_{i,j}^{n} \quad & - \tfrac{\Delta t}{\Delta x}\left(\mathcal{A}^{+}\Delta Q_{i-1/2,j} + \mathcal{A}^{-}\Delta Q_{i+1/2,j}^{n}\right) \\ & - \tfrac{\Delta t}{\Delta y}\left(\mathcal{B}^{+}\Delta Q_{i,j-1/2} + \mathcal{B}^{-}\Delta Q_{i,j+1/2}^{n}\right). \end{aligned}$$

  where $\mathcal{A}^{+}\Delta Q_{i-1/2,j}$, $\mathcal{B}^{-}\Delta Q_{i,j+1/2}^{n}$, etc. are **net updates**

- difference in implementation: compute one “flux term” or two “net updates” for each edge

Time Stepping: Splitting or Not?

- With **Dimensional Splitting**:

$$\begin{aligned} Q^*_{i,j} &= Q^n_{i,j} \quad - \tfrac{\Delta t}{\Delta x}\left(\mathcal{A}^+\Delta Q^n_{i-1/2,j} + \mathcal{A}^-\Delta Q^n_{i+1/2,j}\right) \\ Q^{n+1}_{i,j} &= Q^*_{i,j} \quad - \tfrac{\Delta t}{\Delta y}\left(\mathcal{B}^+\Delta Q^*_{i,j-1/2} + \mathcal{B}^-\Delta Q^*_{i,j+1/2}\right). \end{aligned}$$

  two sequential “sweeps” of Riemann solves on horizontal vs. vertical edges

- vs. “un-split” method: (**currently used in SWE**)

$$\begin{aligned} Q^{n+1}_{i,j} = Q^n_{i,j} \quad &- \tfrac{\Delta t}{\Delta x}\left(\mathcal{A}^+\Delta Q^n_{i-1/2,j} + \mathcal{A}^-\Delta Q^n_{i+1/2,j}\right) \\ &- \tfrac{\Delta t}{\Delta y}\left(\mathcal{B}^+\Delta Q^n_{i,j-1/2} + \mathcal{B}^-\Delta Q^n_{i,j+1/2}\right). \end{aligned}$$

  allows to combine loops on horizontal and vertical edges

Time Stepping

CFL Condition:

- we only consider neighbour cells for a time step
  $\Rightarrow$ information must not travel faster than one cell per timestep!
- thus: timesteps need to consider characteristic wave speeds
- rule of thumb: wave speed depends on water depth, $\lambda = \sqrt{gh}$
- in SWE: Riemann solvers will compute local wave speeds
  $\Rightarrow$ maximum-reduction necessary to find global time step

Adaptive time step control forces sequential main loop:

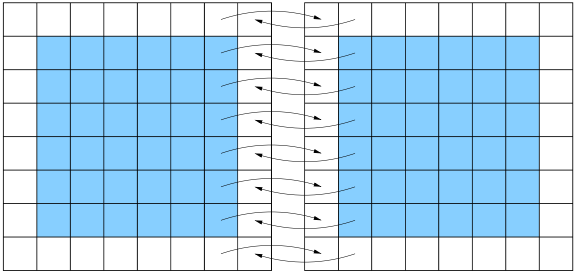
1. solve Riemann problems, compute wave speeds
2. compute maximum wave speed and infer global Δt
3. update unknowns

References & Literature

- LeVeque: *Finite Volume Methods for Hyperbolic Problems*, Cambridge University Press, 2002
- Toro: *Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction*, Springer, 2009
- Bale, LeVeque, Mitran, Rossmanith: *A wave propagation method for conservation laws and balance laws with spatially varying flux functions*, SIAM Journal on Scientific Computing 24 (3), 2003
- George: *Augmented Riemann solvers for the shallow water equations over variable topography with steady states and inundation*, Journal of Computational Physics 227 (6), 2008
- Breuer, Bader: *Teaching Parallel Programming Models on a Shallow-Water Code*, Proc. of the ISPDC 2012

Part II

Parallel Programming Patterns



Reference: Mattson, Sanders, Massingill, Patterns for Parallel Programming. Addison-Wesley, 2005.

Finding Concurrency

Common rule:

Before you start parallelising your code, make sure the serial version is perfectly optimised!

Pro:

- parallelising a badly optimised serial algorithm leads to a badly optimised parallel algorithm
- **use an asymptotically optimal algorithm!**
  for large problems (that are worth being parallelised) asymptotics is crucial

Contra:

- **exploit all available concurrency in your problem**
  (your optimised serial code might have unneccessary sequential parts)
- the fastest serial algorithm is not necessarily the fastest parallel algorithm

Finding Concurrency – Task Decomposition

Decompose your problem into tasks that can execute concurrently!

Consider "un-split" time stepping:

$$\forall i,j\colon\ Q_{i,j}^{n+1} = Q_{i,j}^{n} \quad - \frac{\Delta t}{\Delta x}\left(\mathcal{A}^{+}\Delta Q_{i-1/2,j}^{n} + \mathcal{A}^{-}\Delta Q_{i+1/2,j}^{n}\right) - \frac{\Delta t}{\Delta y}\left(\mathcal{B}^{+}\Delta Q_{i,j-1/2}^{n} + \mathcal{B}^{-}\Delta Q_{i,j+1/2}^{n}\right)$$

Concurrent tasks:

1. compute net updates (i.e., solve Riemann problems) $\mathcal{A}^{+}\Delta Q_{i-1/2,j}^{n}$, $\mathcal{B}^{+}\Delta Q_{i,j-1/2}^{n}$ for all (vertical and horizontal) edges
2. update quantities $Q_{i,j}^{n+1}$ in all cells

or: for all cells, compute net updates (on local edges) and update quantities $Q_{i,j}^{n+1}$ (requires two arrays for $Q_{i,j}^{n}$ and $Q_{i,j}^{n+1}$, resp.)

Finding Concurrency – Task Decomposition

Decompose your problem into tasks that can execute concurrently!

Consider Dimensional Splitting:

$$\begin{aligned} Q^*_{i,j} &= Q^n_{i,j} \quad - \tfrac{\Delta t}{\Delta x}\left(\mathcal{A}^+\Delta Q^n_{i-1/2,j} + \mathcal{A}^-\Delta Q^n_{i+1/2,j}\right) \\ Q^{n+1}_{i,j} &= Q^*_{i,j} \quad - \tfrac{\Delta t}{\Delta y}\left(\mathcal{B}^+\Delta Q^*_{i,j-1/2} + \mathcal{B}^-\Delta Q^*_{i,j+1/2}\right). \end{aligned}$$

Concurrent tasks:

1. compute net updates on all vertical edges ($\mathcal{A}^+\Delta Q^n_{i-1/2,j}$, etc.)

1a. update intermediate quantities $Q^*_{i,j}$ in all cells

2. compute net updates on all horizontal edges ($\mathcal{B}^+\Delta Q^n_{i,j-1/2}$, etc.)

2a. update quantities $Q^{n+1}_{i,j}$ in all cells

Finding Concurrency – Data Decomposition

Decompose your data into units that can operated on relatively independently!

Consider Dimensional Splitting:

$$
\begin{aligned}
Q^{*}_{i,j} &= Q^{n}_{i,j} \quad - \tfrac{\Delta t}{\Delta x}\left(\mathcal{A}^{+}\Delta Q^{n}_{i-1/2,j} + \mathcal{A}^{-}\Delta Q^{n}_{i+1/2,j}\right)\\
Q^{n+1}_{i,j} &= Q^{*}_{i,j} \quad - \tfrac{\Delta t}{\Delta y}\left(\mathcal{B}^{+}\Delta Q^{*}_{i,j-1/2} + \mathcal{B}^{-}\Delta Q^{*}_{i,j+1/2}\right).
\end{aligned}
$$

Data Decomposition:

1. computation of $Q^{*}_{i,j}$: distribute data row-wise, as computation is independent for different j
2. update of $Q^{n+1}_{i,j}$: distribute data column-wise, as computation is independent for different i

Finding Concurrency – Data Decomposition

Decompose your data into units that can operated on relatively independently!

Consider "un-split" time stepping:

$$\forall i,j\colon\ Q_{i,j}^{n+1} = Q_{i,j}^{n} \quad - \frac{\Delta t}{\Delta x}\left(\mathcal{A}^{+}\Delta Q_{i-1/2,j}^{n} + \mathcal{A}^{-}\Delta Q_{i+1/2,j}^{n}\right) - \frac{\Delta t}{\Delta y}\left(\mathcal{B}^{+}\Delta Q_{i,j-1/2}^{n} + \mathcal{B}^{-}\Delta Q_{i,j+1/2}^{n}\right)$$

Concurrent tasks:

- compute net updates requires left/right and top/down neighbours $\Rightarrow$ no "perfect" data decomposition possible
- partitioning of data will require extra care at **boundaries** of the partitions
- **and:** (seemingly trivial) do not decompose quantities in $Q_{i,j}$

Task and Data Decomposition – “Forces”

Flexibility:

- be flexible enough to adapt to different implementation requirements
- for example: do not concentrate on a single parallel platform or programming model

Efficiency:

- solution needs to scale efficiently with the size of the computer
- task and data decomposition need to provide enough tasks to keep all processing elements busy

Simplicity:

- complex enough to solve the task, but simple enough to keep program maintainable

Identifying Dependencies Between Tasks

Group Tasks:

Group your tasks to simplify the managing of dependencies

Order Tasks:

Given a collection of tasks into logically related groups, order these task groups to satisfy constraints

Data Sharing:

Given a data and task decomposition, how is data shared among the tasks?

Element Updates as Task Groups

Consider “un-split” time stepping:

$$\begin{aligned}\forall i,j:\ Q_{i,j}^{n+1} = Q_{i,j}^{n} \quad &- \frac{\Delta t}{\Delta x}\left(\mathcal{A}^{+}\Delta Q_{i-1/2,j}^{n} + \mathcal{A}^{-}\Delta Q_{i+1/2,j}^{n}\right)\\ &- \frac{\Delta t}{\Delta y}\left(\mathcal{B}^{+}\Delta Q_{i,j-1/2}^{n} + \mathcal{B}^{-}\Delta Q_{i,j+1/2}^{n}\right)\end{aligned}$$

Grouped Tasks:

- solve Riemann problems on the four cell edges
- update quantities $Q_{i,j}$ from the net updates

Data Dependencies:

- tasks access quantities $Q_{i\pm1,j\pm1}^{n}$ of neighbour cells
  $\Rightarrow$ two copies required for $Q_{i,j}^{n}$ and $Q_{i,j}^{n+1}$
- Riemann problem computed twice for each edge?

Riemann Solves and Updates as Task Groups

Consider Dimensional Splitting:

$$\begin{aligned} Q^*_{i,j} &= Q^n_{i,j} \quad - \tfrac{\Delta t}{\Delta x}\left(\mathcal{A}^+\Delta Q^n_{i-1/2,j} + \mathcal{A}^-\Delta Q^n_{i+1/2,j}\right) \\ Q^{n+1}_{i,j} &= Q^*_{i,j} \quad - \tfrac{\Delta t}{\Delta y}\left(\mathcal{B}^+\Delta Q^*_{i,j-1/2} + \mathcal{B}^-\Delta Q^*_{i,j+1/2}\right). \end{aligned}$$

Separate Task Groups (for each of the two steps):

- solve Riemann problems on all horizontal (vertical) cell edges
- update quantities $Q_{i,j}$ of an entire column (row)

Data Dependencies:

- tasks access neighbours in either row or column direction
- requires extra storage to compute the net updates (results of the Riemann problems)

Computation of the CFL Condition

Consider “un-split” time stepping:

$$\begin{aligned}\forall i,j\colon\ Q_{i,j}^{n+1} = Q_{i,j}^{n} \quad &- \frac{\Delta t}{\Delta x}\left(\mathcal{A}^{+}\Delta Q_{i-1/2,j}^{n} + \mathcal{A}^{-}\Delta Q_{i+1/2,j}^{n}\right)\\ &- \frac{\Delta t}{\Delta y}\left(\mathcal{B}^{+}\Delta Q_{i,j-1/2}^{n} + \mathcal{B}^{-}\Delta Q_{i,j+1/2}^{n}\right)\end{aligned}$$

where Δt results from wave propagation speeds

Sequential Order of Tasks:

1. solve Riemann problems on the four cell edges (compute wave propagation speeds as partial results)
2. determine maximum wave speed for CFL condition $\rightsquigarrow \Delta t$
3. update quantities $Q_{i,j}$ from the net updates

The Geometric Decomposition Pattern

How can your algorithm be organized around a data structure that has been decomposed into concurrently updatable "chunks"?

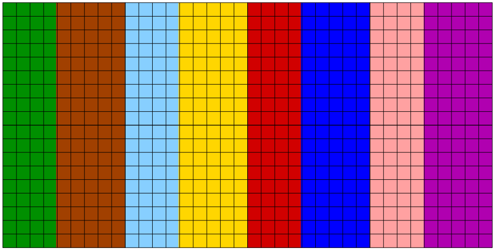
Partitioning (how to select your "chunks"):

- w.r.t. size, shape, etc. ("granularity" of parallelism)
- multiple levels of partitioning necessary?

Organization of parallel updates:

- need to access water height, momentum components and bathymetry from neighbour cells (possible in other partition)
- need to access net updates from neighbour partition? (alternative: compute on all involved partitions?)

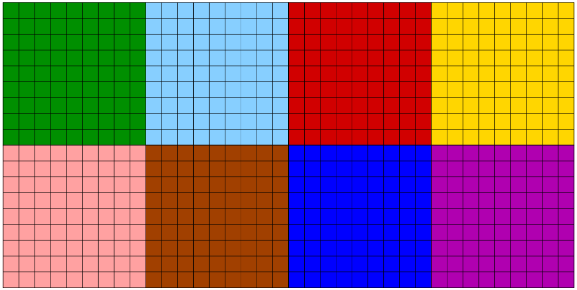
1D Domain Decomposition – Slice-Oriented



Discussion:

- degenerates for large number of partitions: thin slices, lots of data exchenge required at (long!) boundaries
- for dimensional splitting: slices match dependencies (vertical or horizontal) but alternating slices required for the two update steps

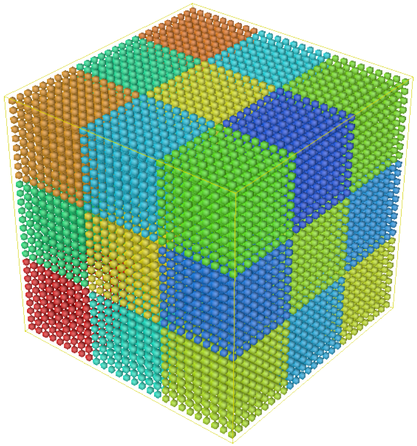
2D Domain Decomposition – Block-Oriented



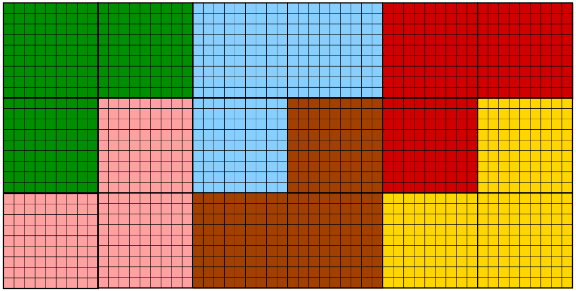
Discussion:

+ length of domain boundaries (communication volume)
– fit arbitrary number of partitions to layout of boxes

3D Domain Decomposition – Cuboid-Oriented



“Patches” Concept for Domain Decomposition

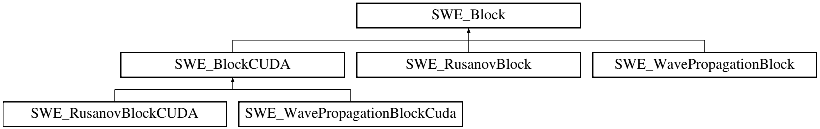


Discussion:

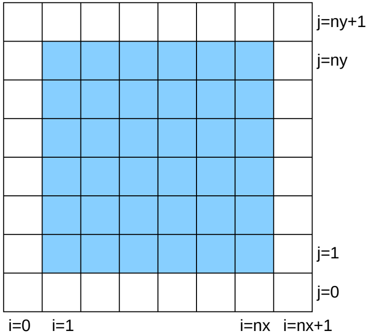
+ more fine-grain load distribution
+ “empty patches” improve representation of complicated domains
– overhead for additional, interior boundaries
– requires scheme to assign patches to processes

Part III

SWE Software Design



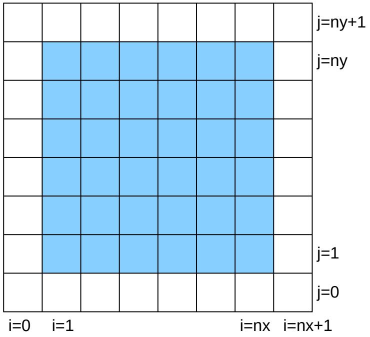
Basic Structure: Cartesian Grid Block



Spatial Discretization:

- regular Cartesian meshes; later: allow multiple patches
- ghost layers to implement boundary conditions;
  connect multiple patches (complicated domains, parallelization)

Basic Structure: Cartesian Grid Block



Data Structure:

- arrays h, hu, hv, and b to hold water height, momentum components and bathymetry data
- “column major” layout: j the “faster running” index in h[i][j]

Main Loop – Euler Time-stepping

```
while( t < ... ) {
   // set boundary conditions
   splash.setGhostLayer();

   // compute fluxes on each edge
   splash.computeNumericalFluxes();

   // set largest allowed time step:
   dt = splash.getMaxTimestep();
   t += dt;

   // update unknowns in each cell
   splash.updateUnknowns(dt);
};
```

$\rightarrow$ **defines interface for abstract class SWE_Block**

Set Ghost Layers – Boundary Conditions

Split into two methods:

- setGhostLayer(): interface function in SWE_Block, needs to be called by main loop
- setBoundaryConditions(): called by setGhostLayer(); sets "real" boundary conditions (WALL, OUTFLOW, etc.)

```
switch(boundary[BND_LEFT]) {
  case WALL:
  {
    for(int j=1; j<=ny; j++) {
      h[0][j] = h[1][j];       b[0][j] = b[1][j];
      hu[0][j] = -hu[1][j];  hv[0][j] = hv[1][j];
    };
    break;
  }
  case OUTFLOW:
  { /* ... */
```

(cmp. file SWE_Block.cpp)

Compute Numerical Fluxes

main loop to compute net updates on **left/right edges**:

```
for(int i=1; i < nx+2; i++) {
  for(int j=1; j < ny+1; j++) {
    float maxEdgeSpeed;
    wavePropagationSolver.computeNetUpdates(
        h[i−1][j], h[i][j],
        hu[i−1][j], hu[i][j],
        b[i−1][j], b[i][j],
        hNetUpdatesLeft[i−1][j−1], hNetUpdatesRight[i−1][j−1],
        huNetUpdatesLeft[i−1][j−1], huNetUpdatesRight[i−1][j−1],
        maxEdgeSpeed
    );
    maxWaveSpeed = std::max(maxWaveSpeed, maxEdgeSpeed);
  }
}
```

(cmp. file SWE_WavePropagationBlock.cpp)

Compute Numerical Fluxes (2)

main loop to compute net updates on **top/bottom edges**:

```
for(int i=1; i < nx+1; i++) {
  for(int j=1; j < ny+2; j++) {
    float maxEdgeSpeed;
    wavePropagationSolver.computeNetUpdates(
        h[i][j-1], h[i][j],
        hv[i][j-1], hv[i][j],
        b[i][j-1], b[i][j],
        hNetUpdatesBelow[i-1][j-1], hNetUpdatesAbove[i-1][j-1],
        hvNetUpdatesBelow[i-1][j-1], hvNetUpdatesAbove[i-1][j-1],
        maxEdgeSpeed
    );
    maxWaveSpeed = std::max(maxWaveSpeed, maxEdgeSpeed);
  }
}
```

(cmp. file SWE_WavePropagationBlock.cpp)

Determine Maximum Time Step

- variable maxWaveSpeed holds maximum wave speed
- updated during computation of numerical fluxes in method computeNumericalFluxes():

```
maxTimestep = std::min( dx/maxWaveSpeed, dy/maxWaveSpeed );
```

- simple “getter” method defined in class SWE_Block:

```
float getMaxTimestep() { return maxTimestep; };
```

- hence: getMaxTimestep() for current time step should be called *after* computeNumericalFluxes()
- in general: in many situations, the maximum computation inhibits certain optimizations $\rightarrow$ fixed time step probably faster!

Update Unknowns – Euler Time Stepping

```
for(int i=1; i < nx+1; i++) {
   for(int j=1; j < ny+1; j++) {
      h[i][j] -= dt/dx * (hNetUpdatesRight[i-1][j-1]
                         + hNetUpdatesLeft[i][j-1] )
               + dt/dy * (hNetUpdatesAbove[i-1][j-1]
                         + hNetUpdatesBelow[i-1][j] );
      hu[i][j] -= dt/dx * (huNetUpdatesRight[i-1][j-1]
                          + huNetUpdatesLeft[i][j-1] );
      hv[i][j] -= dt/dy * (hvNetUpdatesAbove[i-1][j-1]
                          + hvNetUpdatesBelow[i-1][j] );
      /* ... */
   }
}
```

(cmp. file SWE_WavePropagationBlock.cpp)

Goals for (Parallel) Implementation

Spatial Discretization:

- allow different parallel programming models
- and also to switch between different numerical models

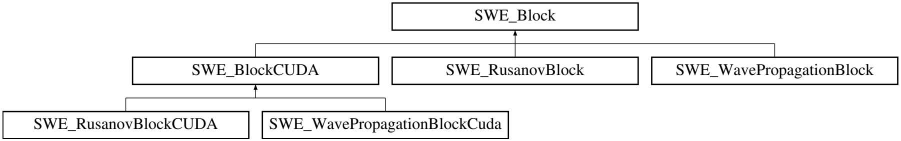
$\Rightarrow$ **class hierarchy of numerical vs. programming models**

Hybrid Parallelization:

- support two levels of parallelization (such as shared/distributed memory, CPU/GPU, etc.)
- coarse-grain parallelism across Cartesian grid patches
- fine-grain parallelism on patch-local operations

$\Rightarrow$ **separate fine-grain and coarse-grain parallelism** (plug&play principle)

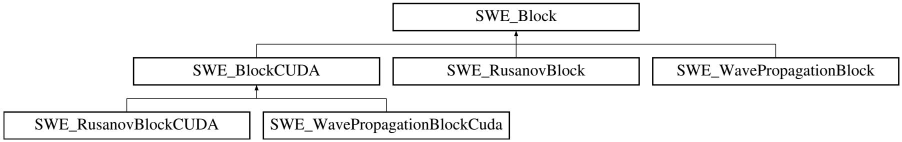
SWE Class Design



abstract class SWE_Block:

- base class to hold data structures (arrays h, hu, hv, b)
- manipulates ghost layers
- methods for initialization, writing output, etc.
- defines interface for main time-stepping loop: computeNumericalFluxes(), updateUnknowns(), . . .

SWE Class Design



derived classes:

- for different model variants: SWE_RusanovBlock, SWE_WavePropagationBlock, . . .
- for different programming models: SWE_BlockCUDA, SWE_BlockArBB, . . .
- override computeNumericalFluxes(), updateUnknowns(), . . .
  $\rightarrow$ methods relevant for parallelization

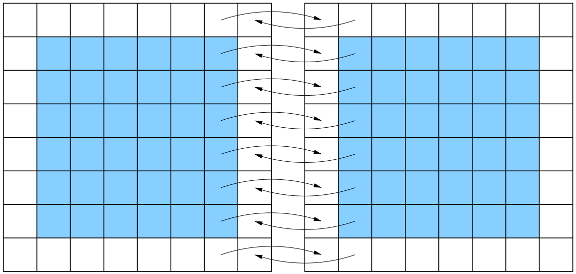
Example: SWE_WavePropagationBlockCUDA

```
class SWE_WavePropagationBlockCuda: public SWE_BlockCUDA {
  /*-- definition of member variables skipped --*/
  public:
    // compute a single time step (net-updates + update of the cells).
    void simulateTimestep( float i_dT );
    // simulate multiple time steps (start and end time as parameters)
    float simulate(float, float);
    // compute the numerical fluxes (net-update formulation here).
    void computeNumericalFluxes();
    // compute the new cell values.
    void updateUnknowns(const float i_deltaT);
};
```

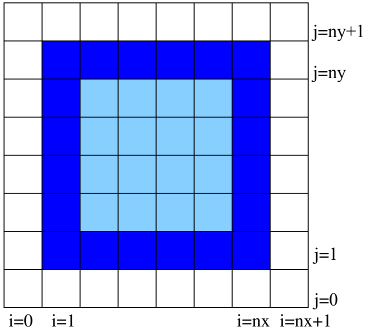
(in file SWE_WavePropagationBlockCuda.hh)

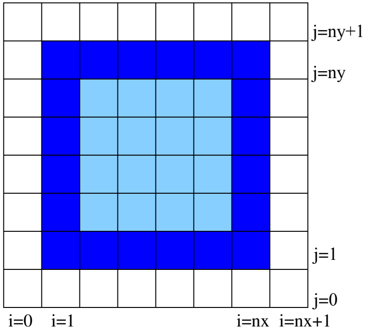
Part IV

SWE Parallelisation



Patches of Cartesian Grid Blocks





Spatial Discretization:

- regular Cartesian meshes; allow multiple patches
- ghost and copy layers to implement boundary conditions, for more complicated domains, and for parallelization

Loop-Based Parallelism within Patches

Computing the Net Updates

- compute net updates on left/right edges:

```
for(int i=1; i < nx+2; i++) in parallel {
  for(int j=1; j < ny+1; j++) in parallel {
    float maxEdgeSpeed;
    fWaveComputeNetUpdates( 9.81,
        h[i-1][j], h[i][j], hu[i-1][j], hu[i][j], /* ... */ );
  }
}
```

- compute net updates on top/bottom edges:

```
for(int i=1; i < nx+1; i++) in parallel {
  for(int j=1; j < ny+2; j++) in parallel {
    fWaveComputeNetUpdates( 9.81,
        h[i][j-1], h[i][j], hv[i][j-1], hv[i][j], /* ... */);
  }
}
```

(function fWaveComputeNetUpdates() defined in file solver/FWaveCuda.h)

Computing the Net Updates

Options for Parallelism

Parallelization of computations:

- compute all vertical edges in parallel
- compute all horizontal edges in parallel
- compute vertical & horizontal edges in parallel (task parallelism)

Parallel access to memory:

- concurrent read to variables h, hu, hv
- exclusive write access to net-update variables on edges

Loop-Based Parallelism within Patches (2)

Updating the Unknowns

- update unknowns from net updates on edges:

```
for(int i=1; i < nx+1; i++) in parallel {
    for(int j=1; j < ny+1; j++) in parallel {
        h[i][j] -= dt/dx * (hNetUpdatesRight[i-1][j-1]
                            + hNetUpdatesLeft[i][j-1] )
                 + dt/dy * (hNetUpdatesAbove[i-1][j-1]
                            + hNetUpdatesBelow[i-1][j] );
        hu[i][j] -= dt/dx * (huNetUpdatesRight[i-1][j-1]
                            + huNetUpdatesLeft[i][j-1] );
        /* ... */
    }
}
```

Updating the Unknowns

Options for Parallelism

Parallelization of computations:

- compute all cells in parallel

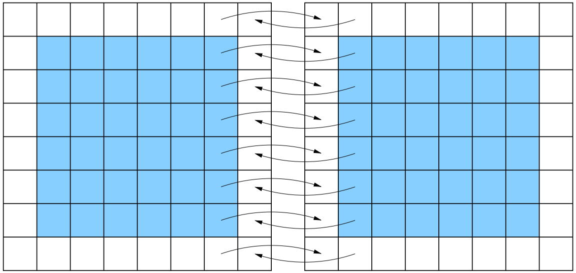
Parallel access to memory:

- concurrent read to net-updates on edges
- exclusive write access to variables h, hu, hv

“Vectorization property”:

- exactly the same code for all cell!

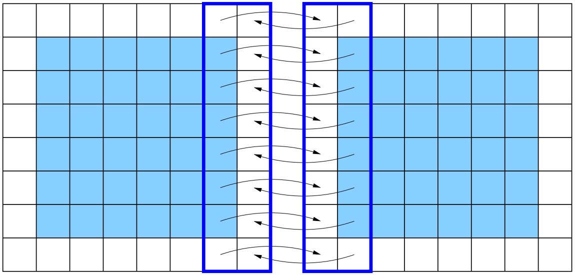
Exchange of Values in Ghost/Copy Layers



Straightforward Approach:

- boundary conditions OUTFLOW, WALL vs. CONNECT or PARALLEL
- disadvantage: method setGhostLayer() needs to be implemented for each derived class

Exchange of Values in Ghost/Copy Layers (2)

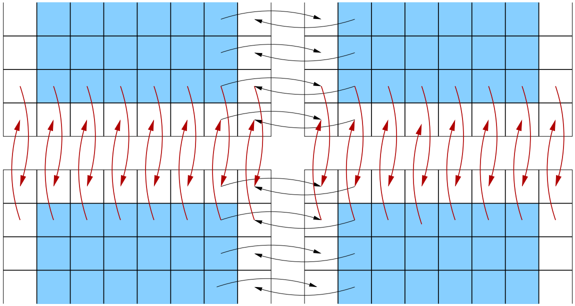


Implemented via Proxy Objects:

- grabGhostLayer() to write into ghost layer
- registerCopyLayer() to read from copy layer
- both methods return a proxy object (class SWE_Block1D) that references one row/column of the grid

Direct-Neighbour vs. "Diagonal" Communication

2-step scheme to exchange data of "diagonal" ghost cells:



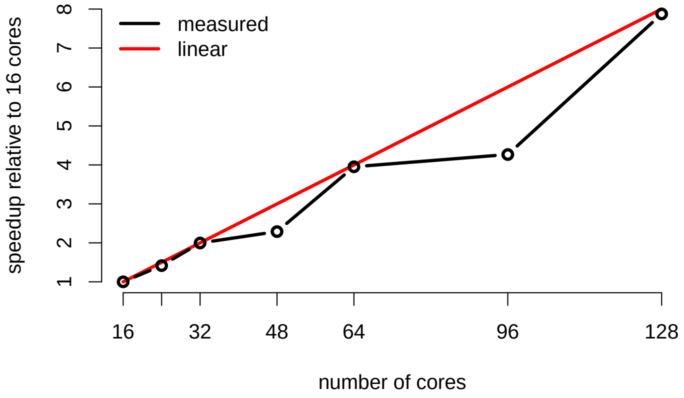
- several "hops" replace diagonal communication
- slight increase of volume of communication (bandwidth), but reduces number of messages (latency)
- similar in 3D (26 neighbours $\rightarrow$ 6 neighbours!)

MPI Parallelization – Exchange of Ghost/Copy Layers

```
SWE_Block1D* leftInflow = splash.grabGhostLayer(BND_LEFT);
SWE_Block1D* leftOutflow = splash.registerCopyLayer(BND_LEFT);

SWE_Block1D* rightInflow = splash.grabGhostLayer(BND_RIGHT);
SWE_Block1D* rightOutflow = splash.registerCopyLayer(BND_RIGHT);

MPI_Sendrecv(leftOutflow->h.elemVector(), 1, MPI_COL, leftRank, 1,
             rightInflow ->h.elemVector(), 1, MPI_COL, rightRank, 1,
             MPI_COMM_WORLD,&status);

MPI_Sendrecv(rightOutflow->h.elemVector(), 1, MPI_COL, rightRank,4,
             leftInflow ->h.elemVector(), 1, MPI_COL, leftRank, 4,
             MPI_COMM_WORLD,&status);
```

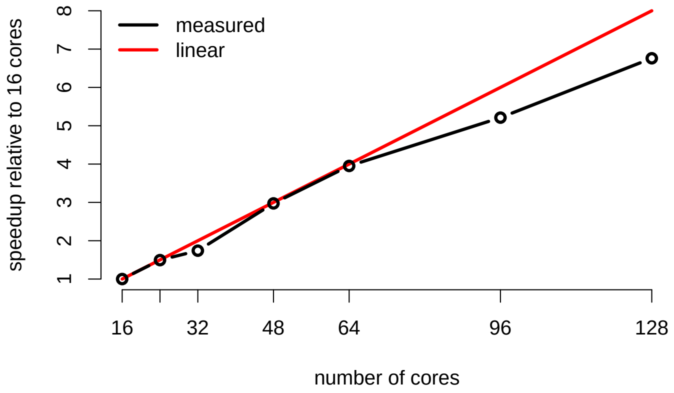
(cmp. file examples/swe_mpi.cpp)

MPI – Some Speedups



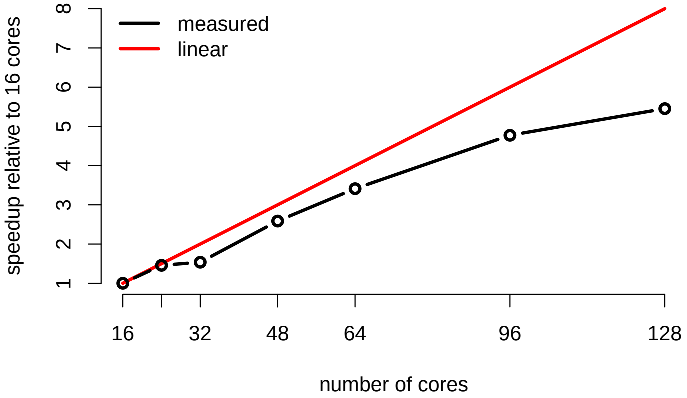
- 1 MPI process per core
- (expensive) augmented Riemann solvers

Speedups for MPI/OpenMP



- 1 MPI process per node, 8 OpenMP threads (1 per core)
- straightforward OpenMP parallelization of for-loops

Speedups for MPI/OpenMP



- 1 MPI process per node, 8 OpenMP threads (1 per core)
- hybrid f-Wave/aug. Riemann solver $\rightarrow$ poor load balancing

Teaching Parallel Programming with SWE

SWE in Lectures, Tutorials, Lab Courses:

- non-trivial example, but model & implementation easy to grasp
- allows different parallel programming models (MPI, OpenMP, CUDA, Intel TBB/ArBB, OpenCL, . . .)
- prepared for hybrid parallelisation

Some Extensions:

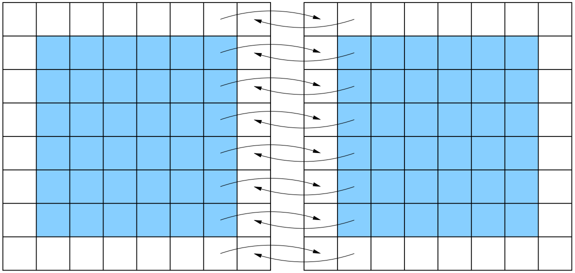
- ASAGI - parallel server for geoinformation (S. Rettenberger, Master's thesis)
- OpenGL real-time visualisation of results (T. Schnabel, student project; extended by S. Rettenberger)

$\rightarrow$ **http://www5.in.tum.de/SWE/**

$\rightarrow$ **https://github.com/TUM-I5**

Part V

Workshop – SWE Parallelisation



MPI Communication Between Patches

Extend sequential SWE program `swe_serial.cpp`**:**

- goal: one patch (SWE_Block per MPI process
- establish assignment of patches to MPI ranks (“who is my neighbour?”)
- implement exchange between ghost & copy cells (preferably via proxy objects)
- parallelize adaptive time step control
- produce speed-up graphs (strong and weak scaling)

Possible extensions: (for the ambitious . . .)

- compare blocking vs. non-blocking communication
- try overlapping communication and computation
- allow multiple patches per MPI process

Loop Parallelism in SWE Using OpenMP

What should be done before starting with OpenMP?

- determine most time-consuming parts of your code ($\rightarrow$ week 2)
- use option "guided auto-parallelism" of Intel compiler ($\rightarrow$ welcome to try, but does not give many hints for SWE)

Extend MPI-parallel SWE program towards MPI+OpenMP:

- what are the most time-consuming loops in SWE?
- ToDo: loop parallelism for these loops using **#pragma** ...
- test performance of OpenMP vs. MPI implementation

Possible extensions: (for the ambitious . . .)

- parallelize adaptive time step control (reduction)
- multiple-patch version: try OpenMP on patches