Implementation of Unifying mathematical definition of particle method for GPU accelerators

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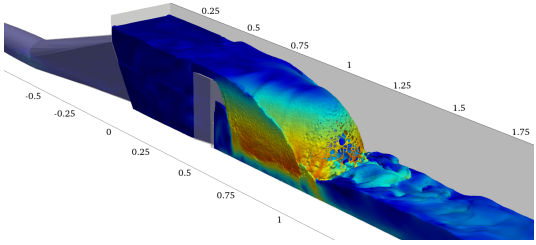
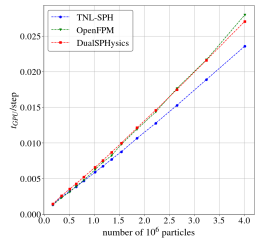
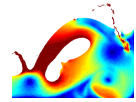
But why?

- We needed **multi-GPUs and distributed computing** for large scale 3D free surface flows in complex geometries
- **Particles are general computational algorithms** - we want general particle framework not only for SPH *(high order particle methods - LABFM, DC-PSE, GFDM, LDD,... image representation, optimization, MD,..)*
- Aim for better abstraction, modularity, generality and clean codebase, while trying to tip the performance







TEMPLATE NUMERICAL LIBRARY

TNL-SPH: Design of TNL particle solver

LAYER 1: TNL - Architecture dependent primitives

Memory management, parallel algorithms,...

LAYER 2: Particles structure

Implementation of particle coordinates, neighbor search, particle distributed communication

LAYER 3: Particles solver

Control of the simulations, connection of particles and model variables

LAYER 4: Numerical schemes

Definition of particle fields and interaction functions

Template Numerical Library (TNL) - unified code for different hardware platforms, written in **C++20**, header only

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- **Usage of lambda functions and parallel algorithms:**

```
const float h = 0.5;

auto v_view = v.getView();
auto func = [ = ] __cuda_callable__( int i ) mutable
{
   v_view[ i ] = i + h;
};
TNL::Algorithms::parallelFor< Device >( 0, v.getSize(), func );
```

Unified memory management, arrays, vectors, flexible parallel reduction, parallel loops, sort,...

- **Expression templates:**

$$\vec{x} = \vec{a} + 2\vec{b} + 3\vec{c}$$

```
x = a + 2 * b + 3 * c;
```

LAYER 1: Flexible reduction, data structures

$$m = \max \left\{ |\vec{a} + \vec{b}| \right\}$$

```
auto a_view = a.getView();
auto b_view = b.getView();
auto fetch = [=] __cuda_callable__ (int i)->float { return abs( a_view[ i ] + b_view[ i ] ); };
auto reduction = [] __cuda_callable__ (float x, float y)->float {
        return max( x, y ); };

result = TNL::Algorithms::reduce< Device >( 0, a.getSize(), fetch, reduction,
std::numeric_limits< float >::lowest() );
```

Or simply using expression templates

```
result = TNL::Max( TNL::Abs( a + b ) );
```

• **TNL provides also data structures oriented towards numerical computing:**
NDarray, matrices, sparse matrices, segments, **unstructured meshes**,...

We add structure for particles (point clouds)

General particle automaton

A **general particle method algorithm** is 7-tuple

$$(P, G, u, f, i, e, \mathring{e})$$

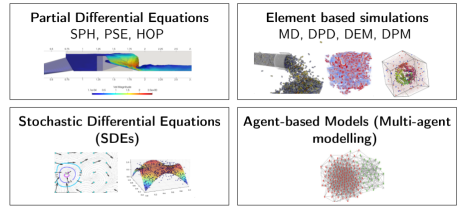
consisting of two data structures

$$P := A_1 \times A_2 \times ... \times A_n \qquad \text{the particle space,}$$
$$G := B_1 \times B_2 \times ... \times B_m \qquad \text{the global variable space}$$

such that $[G \times P^*]$ is the state space of the particle methods and five functions

$$u := [G \times P^*] \times \mathbb{N} \to \mathbb{N}^* \qquad \text{the neighborhood function,}$$
$$f := G \to \{\top, \bot\} \qquad \text{the stopping condition,}$$
$$i := G \times P \times P \to P \times P \qquad \text{the interact function,}$$
$$e := G \times P \to G \times P^* \qquad \text{the evolve function,}$$
$$\mathring{e} := G \to G \qquad \text{the evolve function of global variables}$$

(J. Pahlke & I. Sbalzarini 2023)



What we understand by particle method:

$$\frac{\mathrm{d}\mathbf{x}_i}{\mathrm{d}t} = \sum_{j \in \mathcal{N}_i} \mathbf{f}_{\mathbf{x}}(\mathbf{x}_i, \mathbf{x}_j, \boldsymbol{\omega}_i, \boldsymbol{\omega}_j),$$

$$\frac{\mathrm{d}\boldsymbol{\omega}_i}{\mathrm{d}t} = \sum_{j \in \mathcal{N}_i} \mathbf{f}_{\boldsymbol{\omega}}(\mathbf{x}_i, \mathbf{x}_j, \boldsymbol{\omega}_i, \boldsymbol{\omega}_j)$$

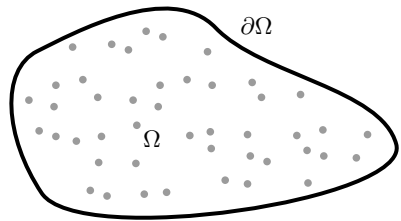
LAYER 2: Representation of particles

Variables:

- n - dim.
- N - count
- $\mathbf{r} \in \mathbb{R}^{N \times n}$

O *grid referential origin*

LAYER 2: Representation of particles



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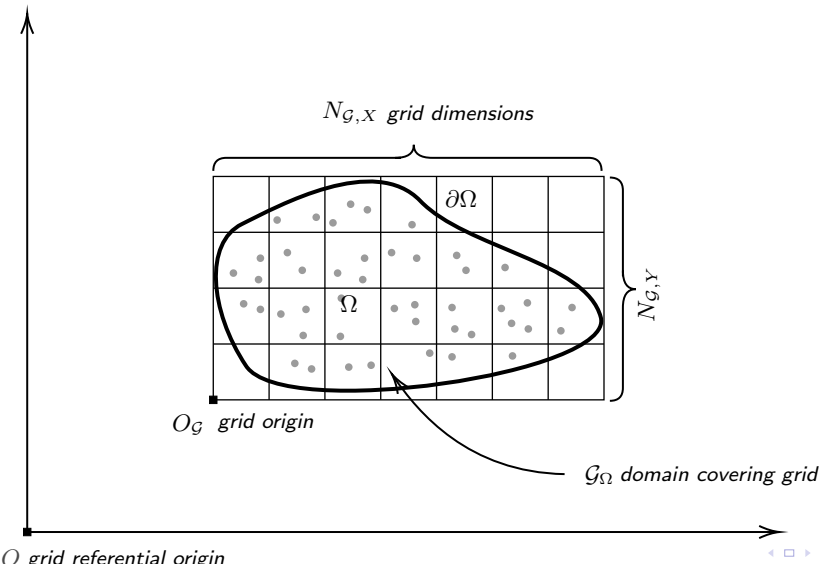
LAYER 2: Representation of particles



Variables:

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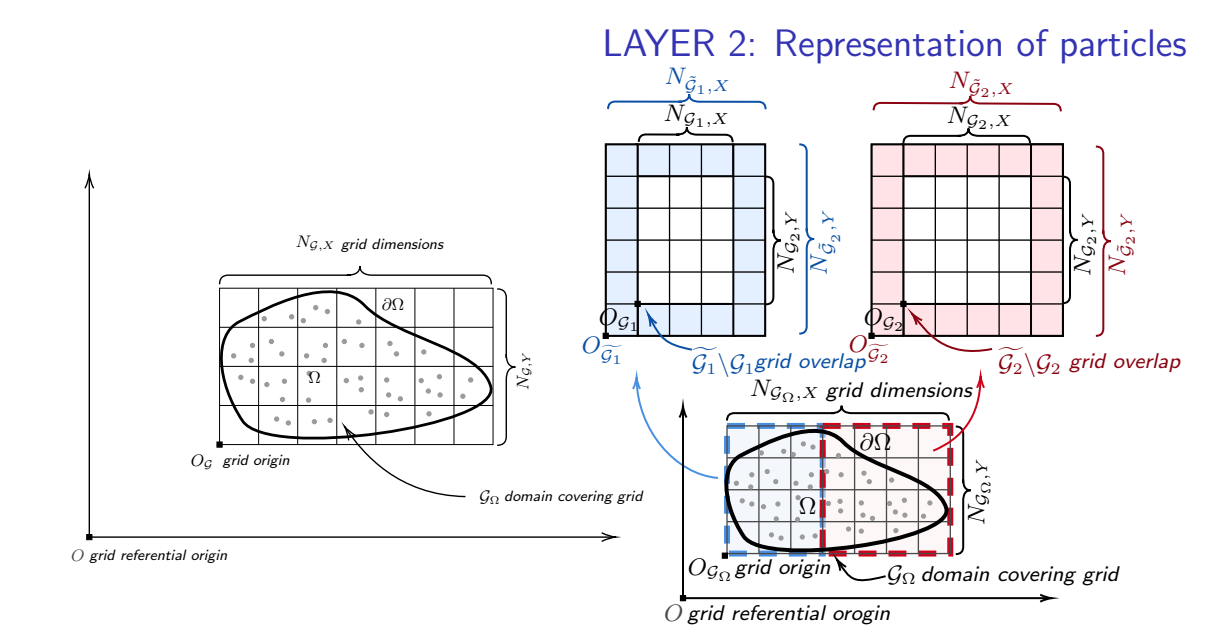
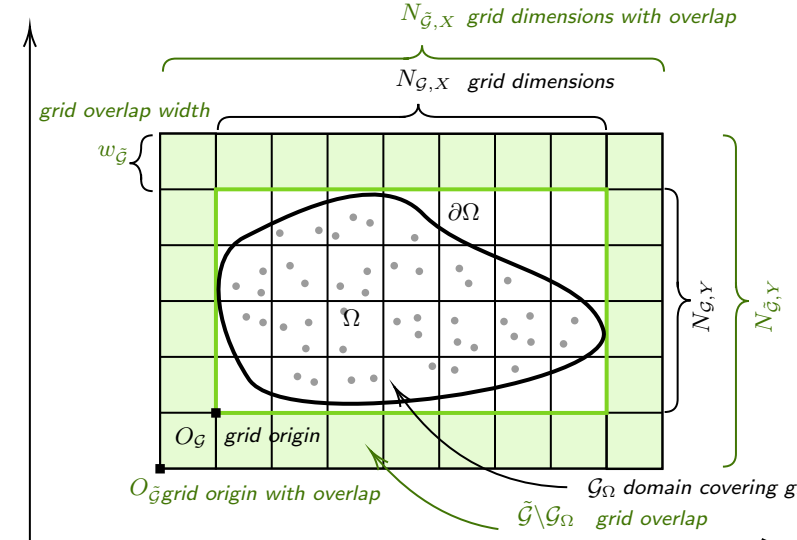
- $\mathbf{r} \in \mathbb{R}^{N \times n}$
- $O_{\mathcal{G}}$
- $N_{\mathcal{G}}$
- r_{cut}

LAYER 2: Representation of particles



LAYER 2: Representation of particles



Variables:

- n - dim.
- N - count
- $\mathbf{r} \in \mathbb{R}^{N \times n}$
- $O_{\mathcal{G}}$
- $N_{\mathcal{G}}$
- r_{cut}
- $w_{\mathcal{G}}$

- **Particles structure:** Structure that handles the points and neighbor search:

```
particles.searchForNeighbors();
```

providing the loops over the particles and neighbors:

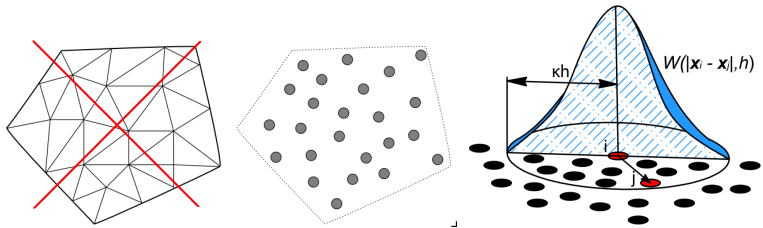
```
// Define operation preformed for every neighbor
auto pairInteraction = [=] __cuda_callable__ ( int i, int j, args.. ) mutable
{
};

// Define operation performed for every particles
auto particleLoop = [=] __cuda_callable__ ( LocalIndexType i ) mutable
{
   ParticlesType::NeighborsLoop::exec( i, r_i, searchToken, pairInteraction, args... );
};
particles.forAll( particleLoop );
```

runs in parallel even for distributed computation!

- **Particles zone:** Provides list of indices of arbitrary selected spatial subdomain.

Smoothed Particle Hydrodynamics - a meshfree particle method based on Lagrangian continuum description



- material particles without mutual topological connections
- approximation of function values $\langle f(\mathbf{x})\rangle$ and its derivatives $\langle \partial^\alpha f(\mathbf{x})\rangle$ are obtained as a weighted summation of surrounding points

$$\langle f(\mathbf{x})\rangle = \sum_{j\in\mathcal{N}_i} f(\mathbf{x}_j)\, w(\mathbf{x}-\mathbf{x}_j,h), \quad \langle \partial^\alpha f(\mathbf{x})\rangle = \sum_{j\in\mathcal{N}_i} f(\mathbf{x}_j)\, w_{\partial^\alpha}(\mathbf{x}-\mathbf{x}_j,h),$$

To solve free surface flows, we use weakly compressible model of fluid (we allow density variations up to 1 %) in Lagrangian description

$$\frac{\mathrm{D}\mathbf{x}_i(t)}{\mathrm{D}t} = \mathbf{v}_i(t) \tag{1}$$

$$\left\langle \frac{\mathrm{D}\rho_i}{\mathrm{D}t} \right\rangle_i (t) = -\rho_i(t) \left\langle \mathrm{div}(\mathbf{v}) \right\rangle_i (t) + \delta_\psi h c_0 \mathcal{D}_i(t) \tag{2}$$

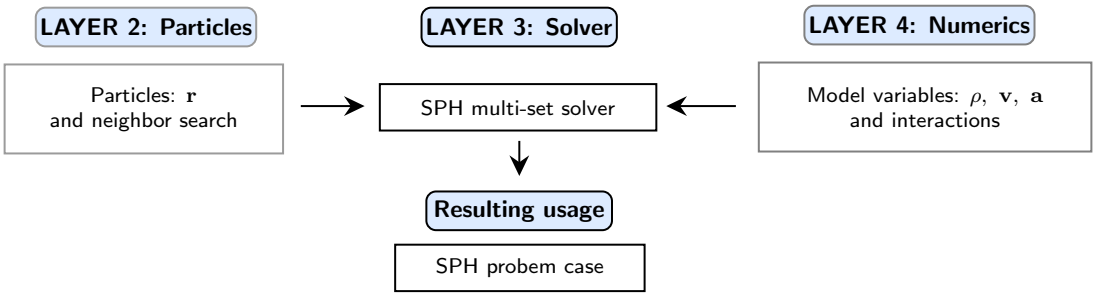
$$\left\langle \frac{\mathrm{D}\mathbf{v}_i}{\mathrm{D}t} \right\rangle_i (t) = -\frac{1}{\rho_i(t)} \left\langle \nabla p \right\rangle_i (t) + \mathcal{V}_i(t) + \mathbf{f}_i \tag{3}$$

$$p_i(t) = p_0 + c_s^2(\rho_i(t) - \rho_0) \tag{4}$$

The spatial differential operators $\langle \mathrm{div}(\mathbf{v}) \rangle$, $\langle \nabla p \rangle$ and viscous terms $\mathcal{V}$ are discretized **Smoothed Particle Hydrodynamics** or **Generalized Meshfree Finite Differences**.

LAYER 3: Particle solver

- Multi-set solver uses **separate particle sets** for fluid, boundary particles and open boundary patches
- **Possibility to build custom time main loop** enhanced with user defined functions



LAYER 4: Numerical solver

Numerical solvers: Defines **variables** of the scheme/model and **interaction functions** *(fluid-fluid, fluid-boundary, boundary-fluid, pre/post interaction functions)*

```
auto fluidFluid = [=] __cuda_callable__ ( LocalIndexType i, LocalIndexType j, /* args i, j,.. */ ) mutable
{
  // load data of neighboring particle
  const VectorType r_j = r_view[ j ]; const VectorType v_j = v_view[ j ]; const RealType rho_j = rho_view[ j ]
  const RealType p_j = EOS::DensityToPressure( rho_j, eosParams );

  const VectorType r_ij = r_i - r_j;
  const RealType drs = l2Norm( r_ij );
  const VectorType v_ij = v_i - v_j;
  const RealType F = KernelFunction::F( drs, h );
  const VectorType gradW = r_ij * F;

  // continuity equation
  const RealType psi = DiffusiveTerm::Psi( rho_i, rho_j, r_ij, drs, diffusiveTermsParams );
  const RealType diffTerm =  psi * ( r_ij, gradW ) * m / rho_j;
  *drho_i += ( v_ij, gradW ) * m - diffTerm;

  // momentum equation
  const RealType p_term = ( p_i + p_j ) / ( rho_i * rho_j );
  const RealType visco =  ViscousTerm::Pi( rho_i, rho_j, drs, ( r_ij, v_ij ), viscousTermTermsParams );
  *a_i += ( -1.0f ) * ( p_term + visco ) * gradW * m;
};
```

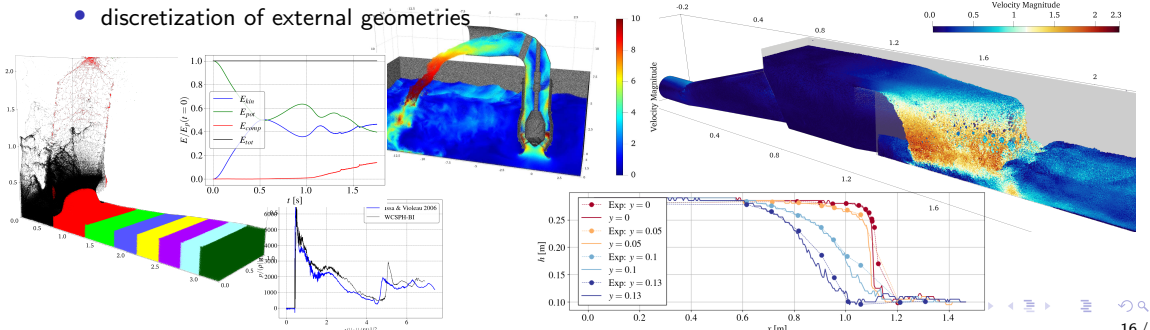
$$\frac{\mathrm{D}\rho_i}{\mathrm{D}t} = \rho_i \sum_{j=1}^{N} (\mathbf{u}_i - \mathbf{u}_j) \cdot \nabla_i W_{ij} V_j + \delta_\psi h c_0 \mathscr{D}$$

$$\frac{\mathrm{D}\mathbf{u}_i}{\mathrm{D}t} = -\frac{1}{\rho_i} \sum_{j=1}^{N} (p_i + p_j) \nabla_i W_{ij} V_j + \frac{1}{\rho_i} \sum_{j=1}^{N} \Pi_{ij} \nabla_i W_{ij} V_j + \mathbf{f}_i$$

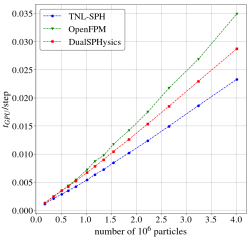
Implemented features

Implementing particular schemes should not be considered as a problem,...

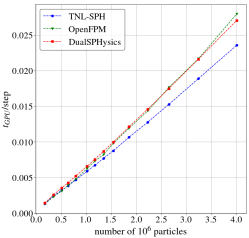
- WCSPH (diffusive terms, various boundary conditions: DBC, MDBC, **boundary integrals**)
- Unconditionally stable SPH scheme *(Cercos-Pita, 2024)*
- RSPH, **SHTC-SPH** - unified framework for solid and fluids
- various integration schemes (Verlet, symplectic Verlet, RK45, implicit midpoint)
- open boundary conditions (inlet, outlets)
- discretization of external geometries



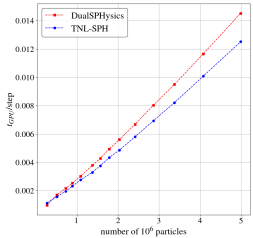
Benchmarks



NVIDIA A40



NVIDIA A100



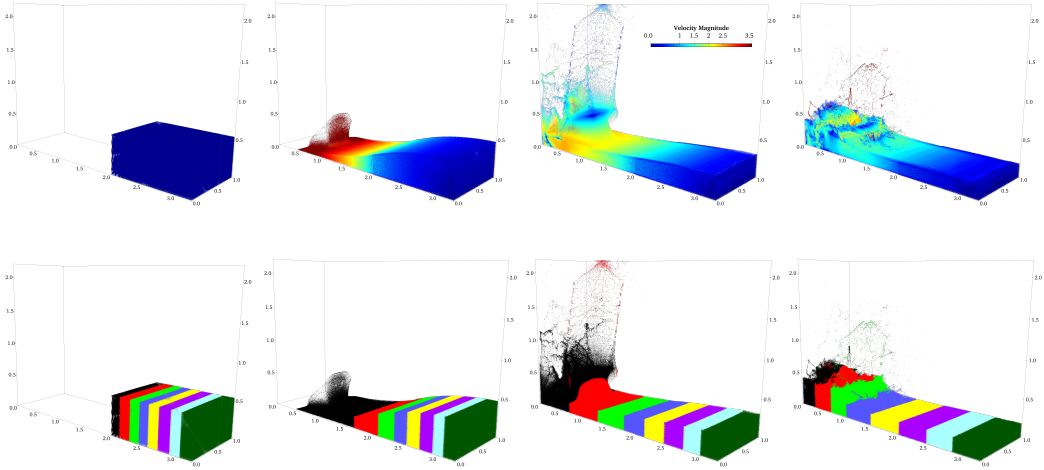
NVIDIA H100

	TNL-SPH		DualSPHysics		OpenFPM	
GPU	t_{step} [s]	MPUPS	t_{step} [s]	MPUPS	t_{step} [s]	MPUPS
A40	0,023	172,3	0,029	139,6	0,035	114,9
A100	0,024	170,2	0,027	148,2	0,028	143,4
H100	0,013	320,5	0,015	276,2		

Test case: SPHERIC testcase 2: 3D dam break, δ-WCSPH scheme with Molteni-DT, artificial viscosity, DBC, Verlet scheme, $\Delta t = const.$, resolutions $\Delta x = [0.02, 0.006]$, **table shows data for** $\Delta x = 0.006$

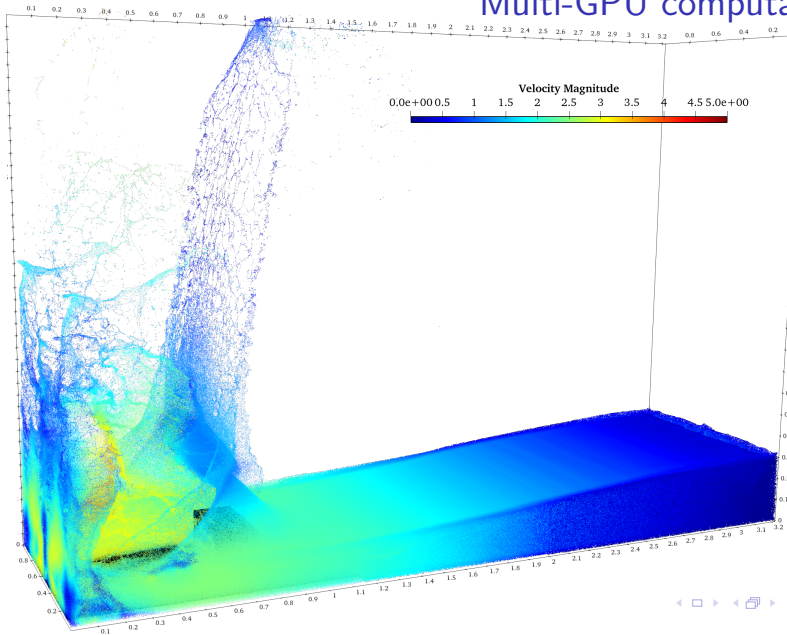
Benchmark setups for all solvers: `https://github.com/tomashalada/sph-benchmarks/`

Multi-GPU computations

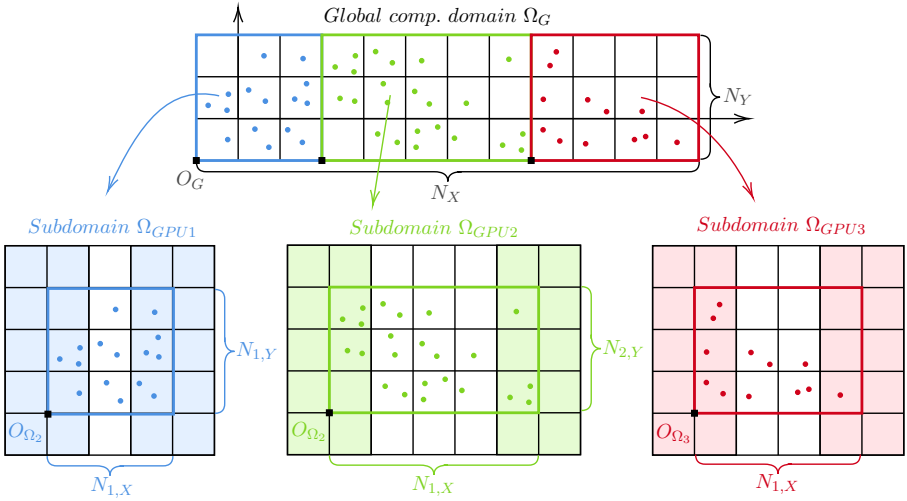


Support of multi-GPUs and distributed computations using MPI, with 1D, 2D or 3D domain decomposition and subdomains load balancing.

Multi-GPU computations - detail



Domain decomposition



Multi-GPU computations - benchmarks

Strong scaling:

N_{GPUs}	GPUPS	t_{step} [s]	*Speedup*	*Eff*
1	0,297	0,346	1,00	1,00
2	0,585	0,176	1,97	0,99
4	1,157	0,089	3,90	0,97
8	2,154	0,048	7,26	0,91

Weak scaling:

N_{GPUs}	$N_{\text{ptcs}}(10^6)$	GPUPS	t_{step} [s]	*Speedup*	*Eff*
1	15,2	0,335	0,045	1,00	1,00
2	28,5	0,622	0,046	1,98	0,99
4	53,8	1,147	0,047	3,87	0,97
8	102,8	2,136	0,048	7,54	0,94

Test case: SPHERIC test case 2: 3D dam break, δ-WCSPH scheme with Molteni-DT, artificial viscosity, DBC, Verlet scheme, **weak scaling** 20×10^6 **particles per GPU, strong scaling** 10^8 **particles**, NVIDIA H100 cards

- *Iterating by particles*: The limiting factor is the memory access - to many neighborhood particles with too much data to read
- *Iterating by pairs*: The limiting factor is writing to memory - too much data to write

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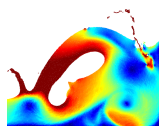
TNL-SPH: Open source, modular, header only, and pretty fast SPH solver oriented towards industrial hydrodynamics



TEMPLATE NUMERICAL LIBRARY

TODO: Remeshed particles, adaptive cell lists.

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