Converting DualSPHysics to solve strictly Incompressible SPH

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Outline of Presentation

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- WCSPH vs ISPH
- Why DualSPHysics?
- ISPH on the GPU in DualSPHysics implementation challenges
- Methodology
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  - Implementing open-source linear solver libraries
  - Boundary conditions
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Motivations and project aims

Renewable energy is required!

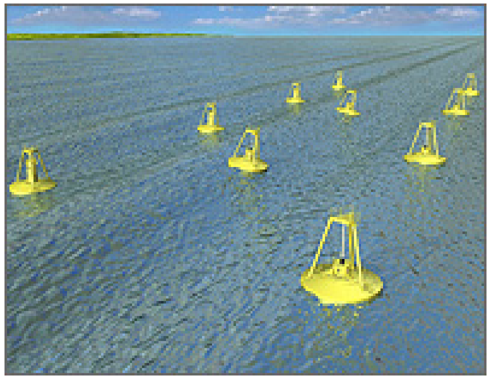
- Recent trends show an increase in offshore development for renewable energies (EWEA, 2016)
- Offshore environments are harsh and difficult to design efficiently and cost effectively

Project aims:

- To create a computational model for solving **incompressible free-surface flows**
- For modelling breaking wave-structure impacts

The European Wind Energy Association (EWEA), *Offshore statistics*. (2016) doi: http://www.ewea.org/statistics/offshore/

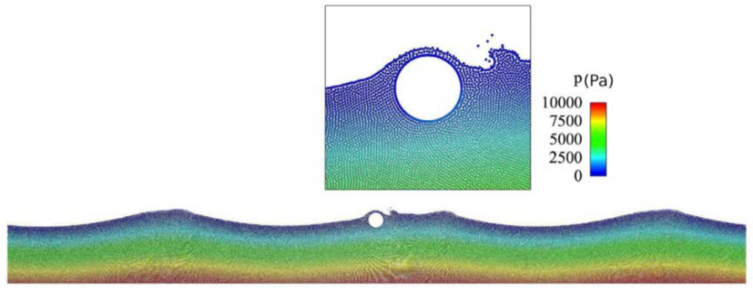
Wind Turbines


Wave Energy Devices

Tidal Stream Turbines

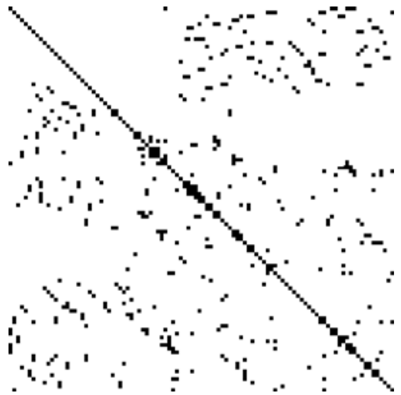
Motivations and project aims

- Incompressible SPH (ISPH) is ideal to model free-surface flows with a smooth, noise-free pressure field.



Wave impact on a circular cylinder (Skillen et al., 2013)

- However, **ISPH has slow computational times.**
    - Due to the need for the **solution of a pressure Poisson equation matrix**, Ax=B



Pressure Poisson equation matrix

- Use of **Graphics Processing Unit (GPU)** to speed things up.

- Hasn't been investigated properly before!

A. Skillen, S. Lind, P. K. Stansby, and B. D. Rogers, *Incompressible smoothed particle hydrodynamics (SPH) with reduced temporal noise and generalised Fickian smoothing applied to body-water slam and efficient wave-body interaction.* Comput. Methods Appl. M. (2013) 265:163-173.

WCSPH vs ISPH

- **Traditional (Weakly-Compressible) SPH uses an artificial equation of state to link density and pressure**, allowing density to vary by 1%.
- **ISPH enforces incompressibility and solves pressure through a pressure Poisson equation (PPE)** in the form of a sparse matrix.

$$p = B\left[\left(\frac{\rho}{\rho_{ref}}\right)^{\gamma} - 1\right]$$

The WCSPH artificial equation of state

$$\nabla.\left(\frac{1}{\rho}\nabla p^{n+1}\right)_i = \frac{1}{\Delta t}\nabla.\mathbf{u}_i^*$$

The ISPH pressure Poisson equation is solved using a system matrix in the form Ax=B

- The **ISPH PPE is the most computationally expensive** part of the algorithm, in terms of **both memory and time.**

ISPH Pressure Poisson Equation

For a 1 million particle simulation, the PPE matrix has (when h/dx=1.3) :

- Approximately 20 million non-zero elements in 2D
- Approximately 100 million non-zero elements in 3D

To be solved every timestep

For this project, the application of a breaking wave–structure impacts will require **several million particles** in a simulation

Why use DualSPHysics?

- DualSPHysics is a WCSPH code BUT there are still **common functions and variables between ISPH and WCSPH** that can be reused: **neighbourlist and particle-reordering, kernel calculations etc.**
- Already highly optimised.
- Implementing in CPU then transferring to GPU is easier than straight to GPU.
- DualSPHysics has a high range of functionality: **floating objects, wavemaker, DEM coupling, multi-phase etc.** Not the biggest concern during implementation but relatively easy to include in the future.

ISPH on the GPU in DualSPHysics implementation challenges

ISPH on the GPU:

- **Memory expensive** method for **memory limited hardware**.
- **Higher resolutions** = Higher matrix condition numbers
  = **Longer PPE solve times**
- **Solving Poisson equations for particle methods on GPUs** is a relatively **new area for research**

Implementation into DualSPHysics:

- Large piece of code - difficult to fully understand the inner workings
  - Challenges in identifying variables to keep/modify/extract
  - Maintaining consistency in the code (parameter values, precision etc.), especially between CPU and GPU.
  - Challenges in adhering to existing DualSPHysics code when adding new code.

Methodology – Files to change

	CPU	GPU
Arrangement of computation	JSphCpuSingle.cpp JSphCpuSingle.h	JSphGpuSingle.cpp JSphGpuSingle.h
Executing computation	JSphCpu.cpp JSphCpu.h	JSphGpu.ker.cu JSphGpu_ker.h
Adding new variables	JSphCpu.h	JSphGpu.h
Adding new memory	JSphCpu.cpp	JSphGpu.cpp
Adding new parameters	JSph.cpp JSph.h Types.h	JSph.cpp JSph.h Types.h

Methodology – Implementing the ISPH projection step

$$\mathbf{r}_i^* = \mathbf{r}_i^n + \Delta t \mathbf{u}_i^*$$

Initial advection of particles

$$\mathbf{u}_i^* = \mathbf{u}_i^n + \Delta t \sum_j V_j \frac{2\nu \mathbf{r}_{ij}^* . \nabla_i W_{ij}}{\mathbf{r}_{ij}^{*2} + \eta^2} \mathbf{u}_{ij}^n$$

Find intermediate velocity from viscous forces

$$\nabla . \left(\frac{1}{\rho} \nabla p^{n+1} \right)_i = \frac{1}{\Delta t} \nabla . \mathbf{u}_i^*$$

Find pressure from the pressure Poisson equation (PPE)

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^* - \Delta t \left(\frac{\nabla p_i^{n+1}}{\rho} + \mathbf{F}_i^n \right)$$

Correct the velocity with pressure and external forces

$$\mathbf{r}_i^{n+1} = \mathbf{r}_i^n + \Delta t \left(\frac{\mathbf{u}_i^{n+1} + \mathbf{u}_i^n}{2} \right)$$

Correct the position with the new velocity

$$\delta \mathbf{r_s} = -D \nabla C$$

Shift particles to improve distribution

Methodology – Implementing the ISPH projection step

$$\mathbf{r}_i^* = \mathbf{r}_i^n + \Delta t \mathbf{u}_i^*$$

$$\mathbf{u}_i^* = \mathbf{u}_i^n + \Delta t \sum_j V_j \frac{2\nu \mathbf{r}_{ij}^* . \nabla_i W_{ij}}{\mathbf{r}_{ij}^{*2} + \eta^2} \mathbf{u}_{ij}^n$$

$$\nabla . \left(\frac{1}{\rho} \nabla p^{n+1} \right)_i = \frac{1}{\Delta t} \nabla . \mathbf{u}_i^*$$

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^* - \Delta t \left(\frac{\nabla p_i^{n+1}}{\rho} + \mathbf{F}_i^n \right)$$

$$\mathbf{r}_i^{n+1} = \mathbf{r}_i^n + \Delta t \left(\frac{\mathbf{u}_i^{n+1} + \mathbf{u}_i^n}{2} \right)$$

$$\delta \mathbf{r}_s = -D \nabla C$$

DualSPHysics Symplectic step

Predictor

$\frac{d\rho}{dt} \quad \frac{d\mathbf{u}_i}{dt}$	Interaction_Forces()
$\delta \mathbf{r}_s = -D \nabla C$	RunShifting()
(Particle update)	ComputeSymplecticPre()

Corrector

$\frac{d\rho}{dt} \quad \frac{d\mathbf{u}_i}{dt}$	Interaction_Forces()
$\delta \mathbf{r}_s = -D \nabla C$	RunShifting()
(Particle update)	ComputeSymplecticCorr()

Methodology – Implementing the ISPH projection step

Predictor

$$\boxed{\mathbf{r}_i^* = \mathbf{r}_i^n + \Delta t \mathbf{u}_i^*} \longrightarrow \text{Init\_Advection()}$$

$$\frac{d\rho}{dt} \quad \frac{d\mathbf{u}_i}{dt}$$

$$\boxed{\mathbf{u}_i^* = \mathbf{u}_i^n + \boxed{\Delta t \sum_j V_j \frac{2\nu \mathbf{r}_{ij}^*.\nabla_i W_{ij}}{\mathbf{r}_{ij}^{*2} + \eta^2} \mathbf{u}_{ij}^n}} \longrightarrow \text{Interaction\_Forces(ForcesPre)}$$

~~$\delta \mathbf{r}_s = -D\nabla C$ RunShifting()~~

(Particle update) → ComputeSymplecticPre()

$$\boxed{\nabla.\left(\frac{1}{\rho}\nabla p^{n+1}\right)_i = \frac{1}{\Delta t}\nabla.\mathbf{u}_i^*} \longrightarrow \text{SolvePPE()}$$

Corrector

$$\frac{d\rho}{dt} \quad \frac{d\mathbf{u}_i}{dt}$$

$$\boxed{\mathbf{u}_i^{n+1} = \mathbf{u}_i^* - \boxed{\Delta t\left(\frac{\nabla p_i^{n+1}}{\rho} + \mathbf{F}_i^n\right)}} \longrightarrow \text{Interaction\_Forces(ForcesCorr)}$$

~~$\delta \mathbf{r}_s = -D\nabla C$ RunShifting()~~

$$\boxed{\mathbf{r}_i^{n+1} = \mathbf{r}_i^n + \Delta t\left(\frac{\mathbf{u}_i^{n+1} + \mathbf{u}_i^n}{2}\right)}$$

(Particle update) → ComputeSymplecticCorr()

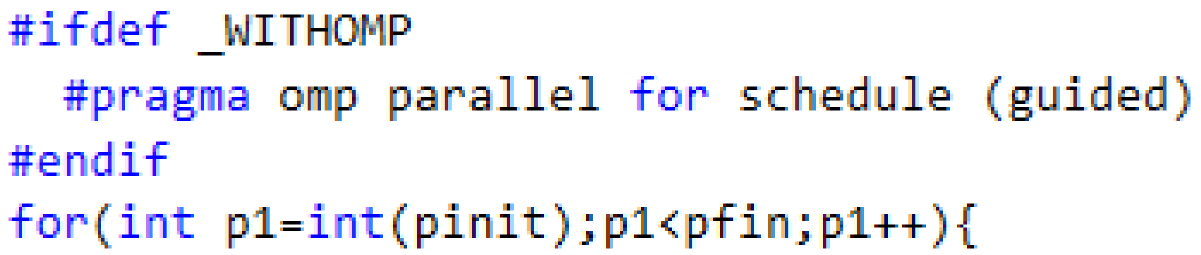
$$\boxed{\delta \mathbf{r}_s = -D\nabla C} \longrightarrow \text{RunShifting()}$$

Methodology – Inserting new computation functions for the PPE setup

- Use existing code as a template and insert necessary equations within

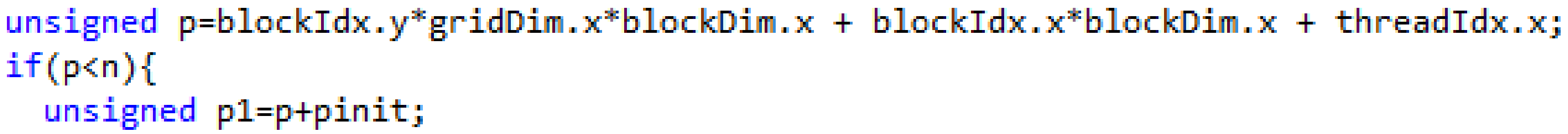
For Example:

<u>CPU – Begin loop through particles</u>



```
#ifdef _WITHOMP
  #pragma omp parallel for schedule (guided)
#endif
for(int p1=int(pinit);p1<pfin;p1++){
```

<u>GPU – Begin loop through particles</u>



```
unsigned p=blockIdx.y*gridDim.x*blockDim.x + blockIdx.x*blockDim.x + threadIdx.x;
if(p<n){
  unsigned p1=p+pinit;
```

Other code that can be reused:

- Calling the neighbour list for each particle
- Calculating the particle interactions for each

Methodology – Implementing a sparse linear solver library for solving the PPE

- Currently using an **open-source sparse matrix solver library** for the CPU and GPU to setup a **preconditioner for the matrix and solve the PPE system.**

- Using an appropriate open-source library to solve the matrix is good:
  - Highly optimised.
  - Saves coding time.
  - Provides different options for preconditioners and linear solvers.

Methodology – Implementing a sparse linear solver library for solving the PPE

- This project is currently using the ViennaCL Library (Rupp, 2010)
  - OpenMP and CUDA availablility

- To include in DualSPHysics, insert the library file path into the properties:
  - **CPU:** C/C++ ->Additional Include Directories
  - **GPU:** JSphGpu_ker.cu
    ->Properties->Custom Build Tool->Command Line

- Insert necessary "#include" library files into where needed, JSphCpu.cpp / JSphGpu_ker.cu etc.
  - **IF using for CPU and GPU, encase "#include" files with "#ifndef _WITHGPU" "#endif" to avoid CPU/GPU conflicts**

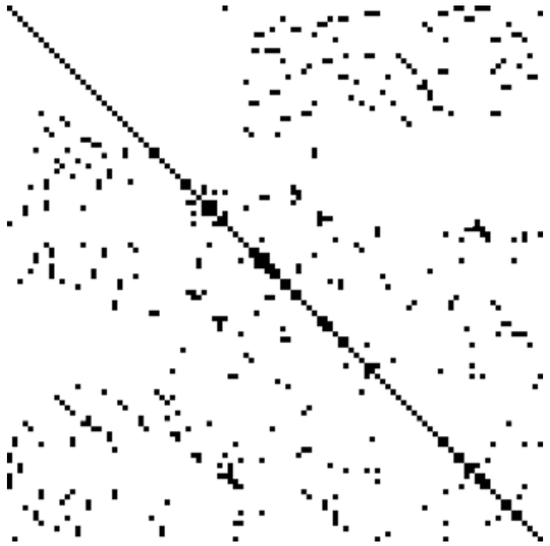
K. Rupp, J. Weinbub, and F. Rudolf. Automatic performance Optimization in ViennaCL for GPUs. In *POOSC '10: Proceedings of the 9th Workshop on parallel/High-Performance Object-Oriented Scientific Computing,* pages 1-6, New York, NY, USA, 2010. ACM.

Methodology – Solving the PPE

- The ISPH PPE is a **non-symmetric sparse matrix**.

- The matrix represents a system in the form, Ax=B.

- Common solvers in ISPH literature used are GMRES and **BiCGSTAB**.



- **High Resolutions =** large condition numbers **= Long solve times**

Methodology – PPE preconditioning

Reducing the solution time: Preconditioning

- Preconditioning lowers the condition number of system so it is faster to solve. For a preconditioner, applied to matrix A :
  - $Ax=b \rightarrow PAP^TPx=b$

- **Preconditioning** the matrix system is **necessary for convergence** of a solution at **high resolutions**.

- In ISPH, the Jacobi preconditioner is typically used.

- Jacobi preconditioning is simple and memory effective.

But…

Methodology – PPE preconditioning

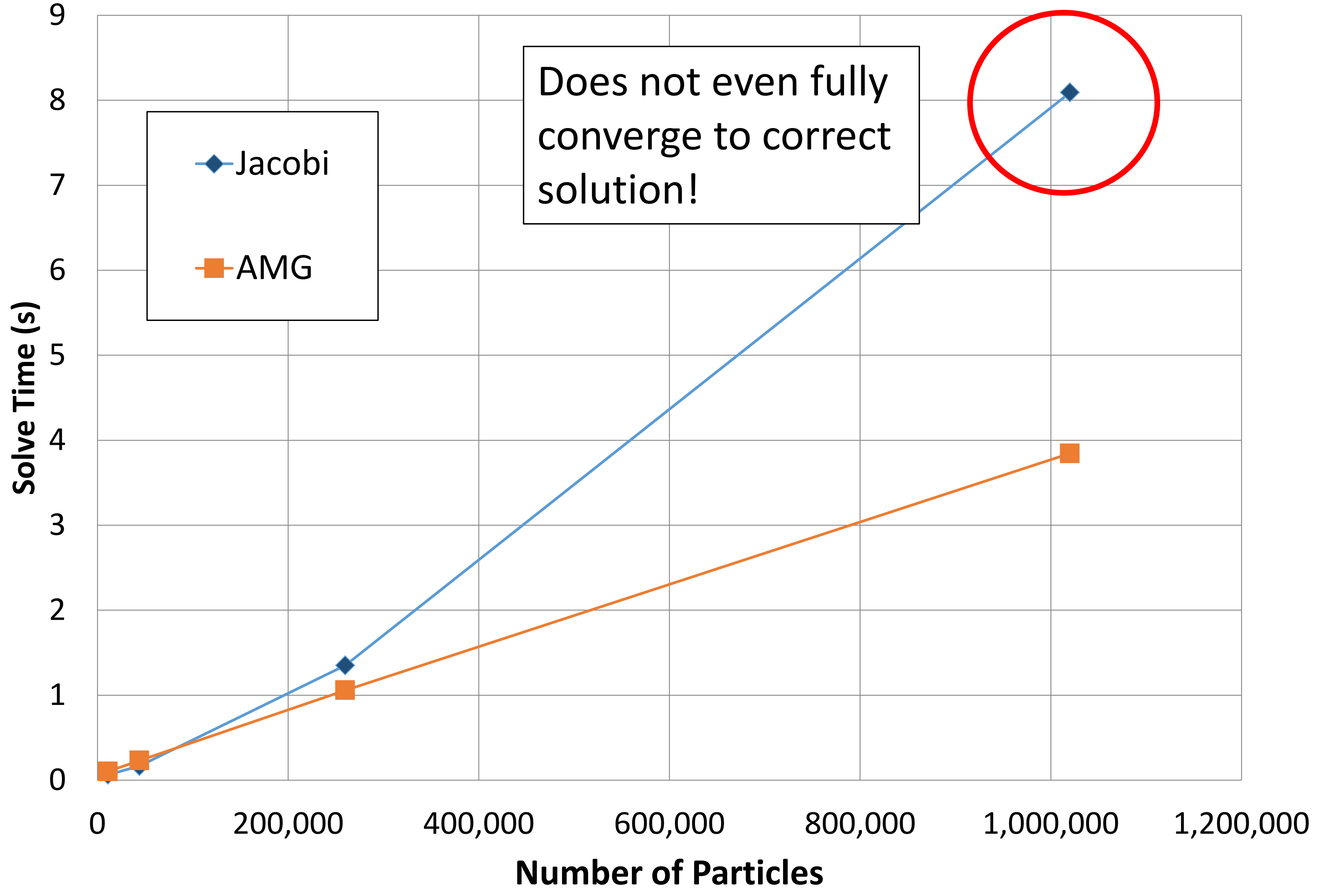
- Guo et al. (2013) has shown the Jacobi does not scale well for high resolutions and may not even converge to a solution.
- Instead he uses an Algebraic Multigrid preconditioner.

Solution:

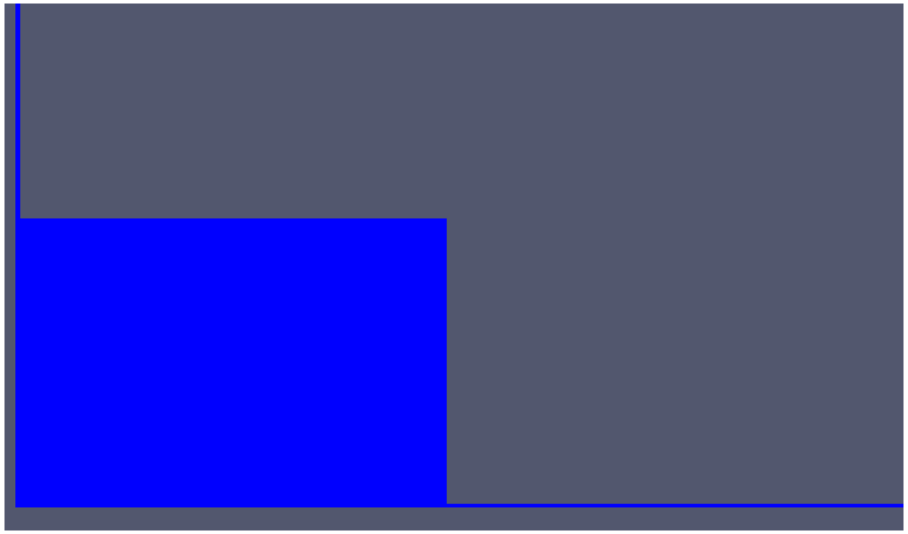
- **The Algebraic Multigrid (AMG) preconditioner** scales much better at higher resolutions and provides a very quick solution time.

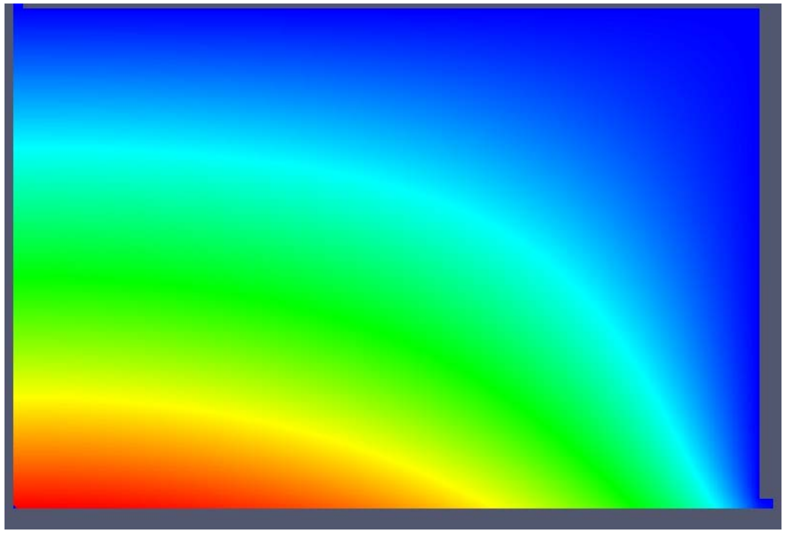
X. Guo, S. J. Lind, B. D. Rogers, P. K. Stansby, and M. Ashworth, *Efficient Massive Parallelisation for Incompressible Smoothed Particle Hydrodynamics with 10^8 Particles,* Proceedings of the 8th international SPHERIC workshop (2013)

GPU Still Water Preconditioner Total Solve Times

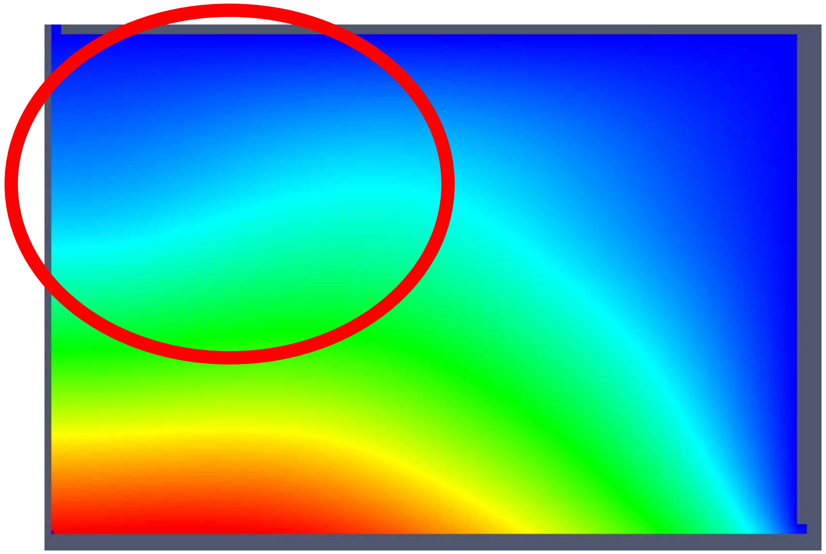


Methodology – PPE preconditioning

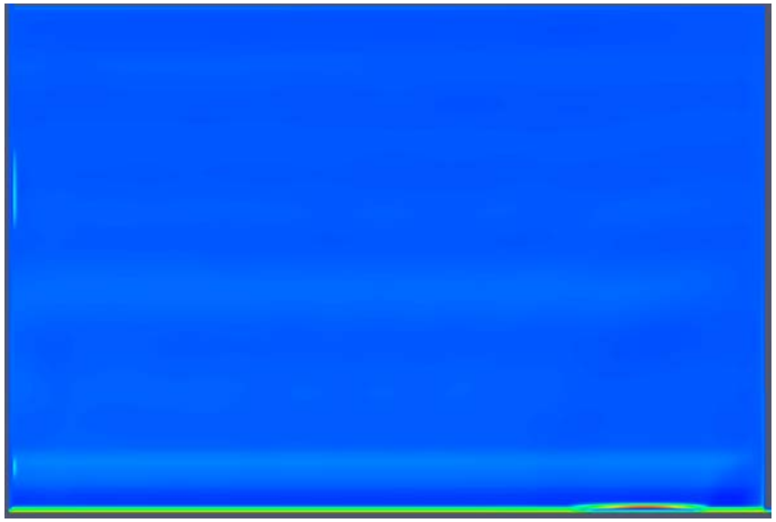




AMG: 1,577,091 particles



Jacobi: 270,891 particles



Jacobi: 1,577,091 particles

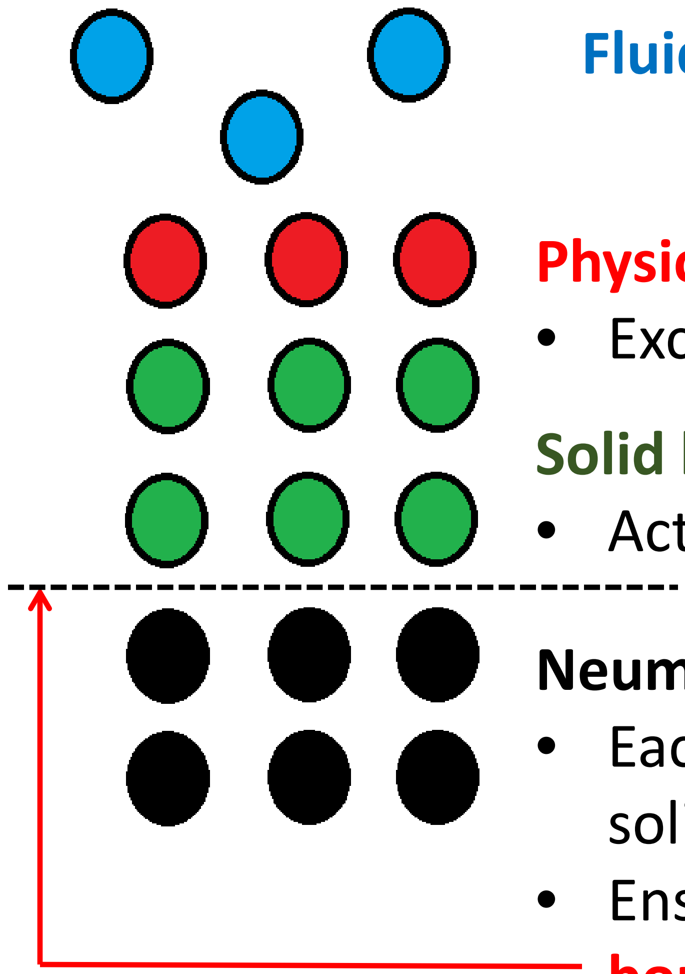
Methodology – Boundary conditions

- Taking advantage of the existing fixed dummy particle generation in GenCase and DualSPHysics.

- Dummy particles are:
  - Simple for parallel implementation
  - Can deal with complex geometries

- However, still need to be modified for the ISPH to include Neumann boundary conditions for the PPE matrix.

Methodology – Boundary conditions



Fluid Domain

Physical boundary particles

- Excluded from boundary velocity interpolation

Solid boundary particles

- Act as normal fixed particles

Neumann boundary particles

- Each Neumann particle pressure = closest solid boundary particle pressure + dp/dn
- Ensures exact “mirroring” across **Neumann boundary line**

Research Challenges

- Getting the ISPH formulation right! No ISPH literature using a combination of:
    - Wendland Kernel
    - Dummy boundary particles
    - Kinematic viscosity as low as $10^{-6}m^2/s$
- Implementing linear solver libraries – some more demanding than others, mixed level of documentation
    - Invested 6 months into finding out why the parallel MIS2-AMG preconditioner for the GPU failed to consistently work with ISPH, which has now been corrected.
- CPU code to GPU code not always straightforward – some differences in implementation
- Making sure CPU and GPU code give the same/similar results – mixed precision issues (maintaining consistency)

Research Challenges

Researching ISPH on the GPU has opened up many other new and exciting possible avenues of research:

- The on going development of ISPH in general
- ISPH for higher resolutions and the challenges associated with it
- The **solution of the ISPH PPE** at **high resolutions**:
  - **In particular, on the GPU**
  - **Preconditioning** Poisson equation matrices for **particle methods**.
    - **In particular, on the GPU**

Despite the on going challenges, the **rewards are high**

Results

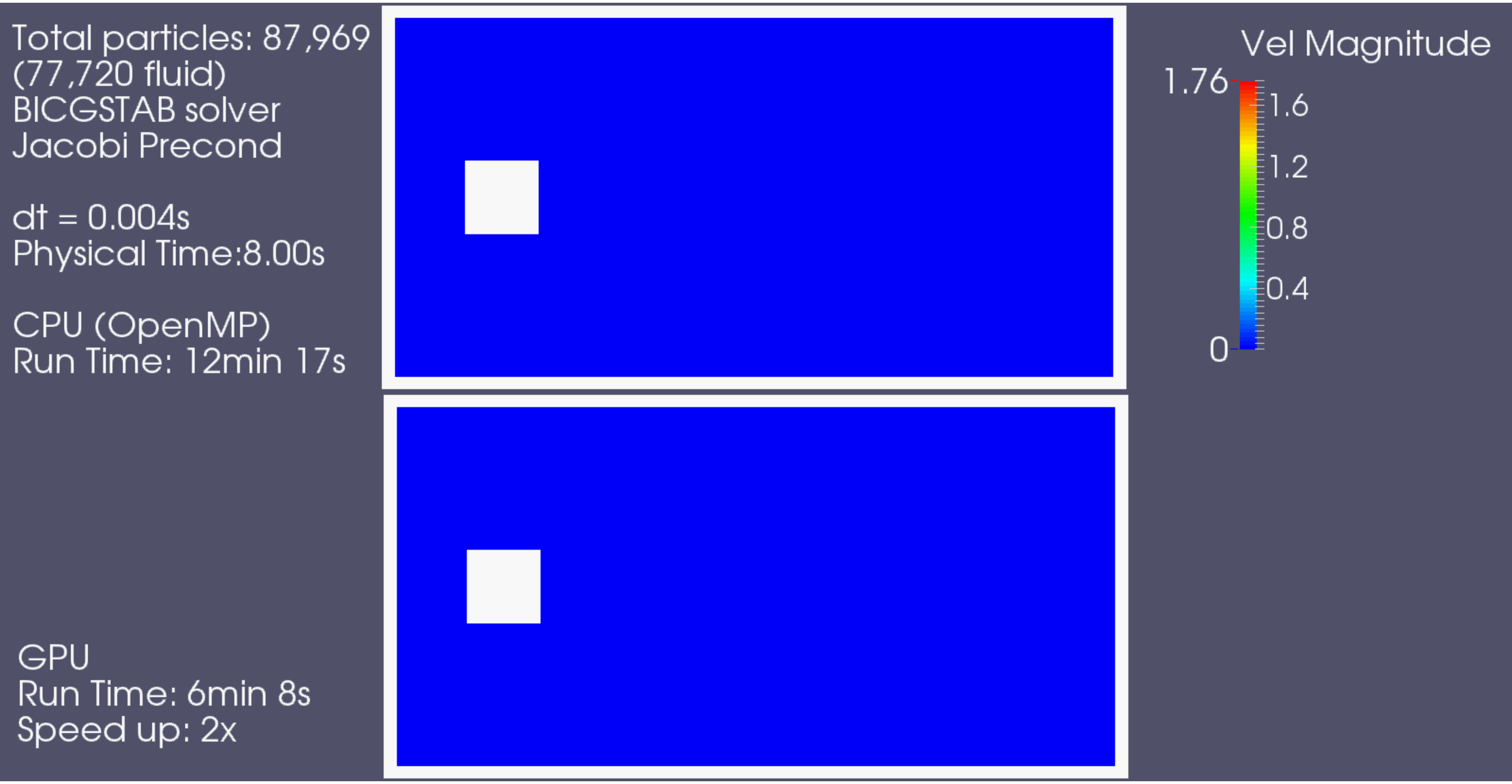
CPU
Intel i-7 4790 processor
Clockspeed: 3.6 GHz
Cores: 4
Threads: 8
OpenMP enabled

GPU
Nvidia GeForce GTX 980
Clockspeed: 1.126 GHz
CUDA Cores: 2048

- Wendland kernel: h=1.8dp

ViennaCL Library:
- Linear solver: BiCGStab, tolerance = 10^{-5}

SPHERIC Benchmark Test Case 6 Moving Box, Re=150



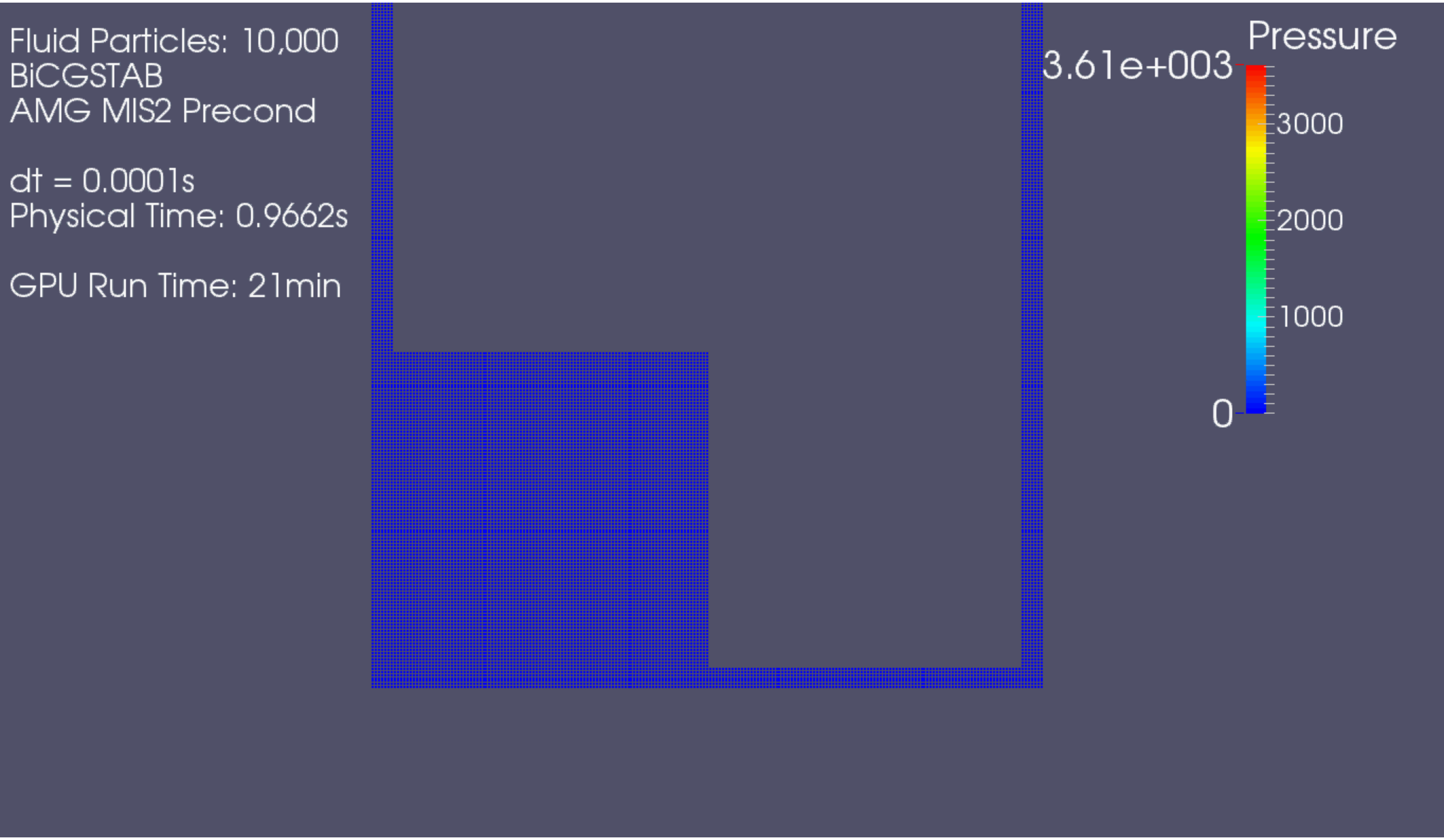
Total particles: 87,969
(77,720 fluid)
BICGSTAB solver
Jacobi Precond

dt = 0.004s
Physical Time:8.00s

CPU (OpenMP)
Run Time: 12min 17s

GPU
Run Time: 6min 8s
Speed up: 2x

Dambreak



Fluid Particles: 10,000
BiCGSTAB
AMG MIS2 Precond

dt = 0.0001s
Physical Time: 0.9662s

GPU Run Time: 21min

Conclusions and future work

<u>Project aim:</u> to develop a solver for incompressible free-surface flows capable of modelling breaking wave-structure impacts

- To achieve the project aim, a novel method of implementing ISPH on the GPU is being used, DualSPHysics is the vehicle used to create the model.

- The main idea for converting DualSPHysics is to use as much as possible of what is already available.
  - This is also applies for the use of an open-source linear solver library for the PPE.

- Current work already shows a significant improvement in speed and resolution capability from current ISPH literature.

- Lots of new research can be made with an accelerated ISPH.

Conclusions and future work

Future work:

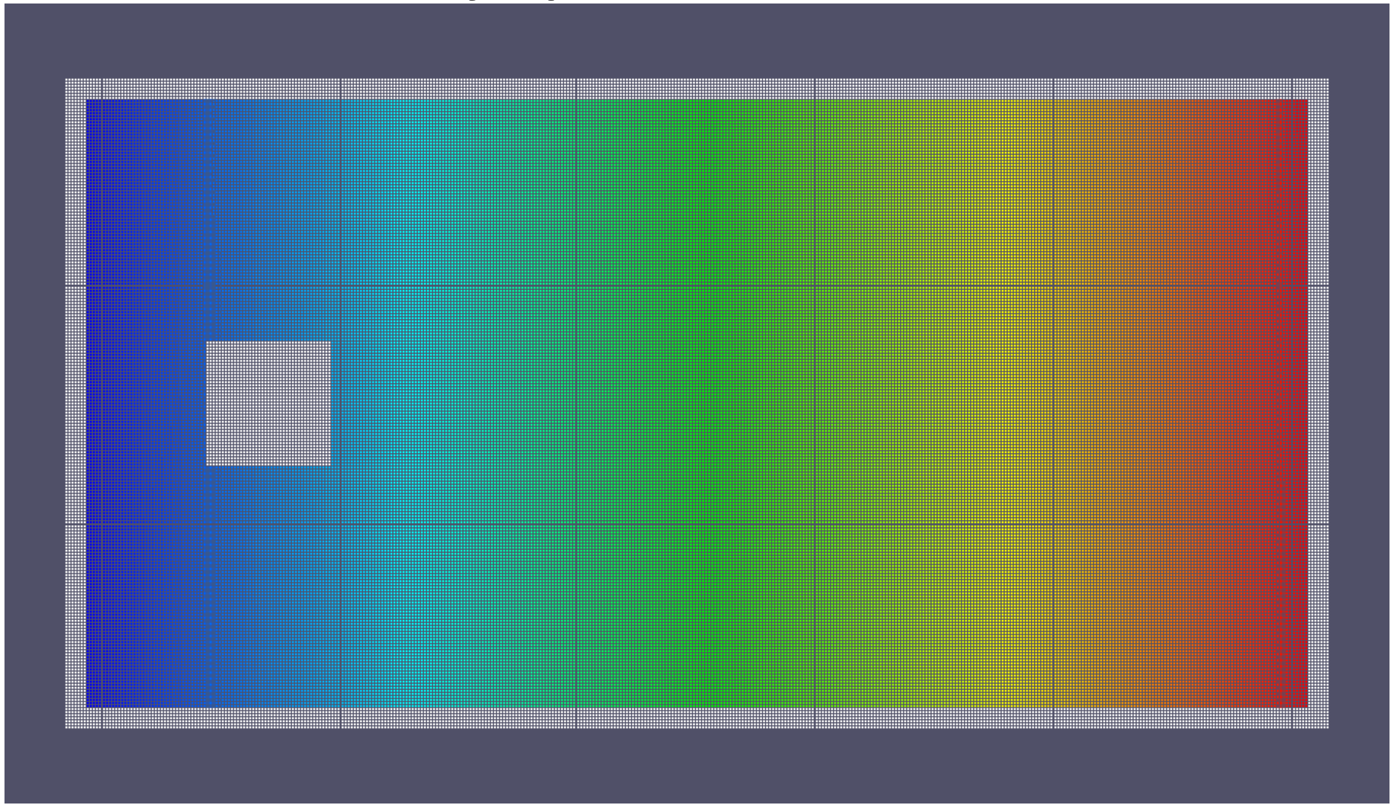
- Fix bugs
    - Currently on about the “10th last bug”…

- The model needs to be extended to 3D.

- More rigorous analysis and accuracy testing needs to be done to fully validate the model.

Thank you

Any questions?



Acknowledgements

- All of the DualSPHysics team
    - In particular: Dr Georgios Fourtakas, Dr Athansios Mokos, Dr Jose Dominguez, and Dr Stephen Longshaw
- The developer of the ViennaCL library Karli Rupp

Methodology – Inserting new computation functions for the PPE setup

CPU – Call p1 neighbours

```
int cxini,cxfin,yini,yfin,zini,zfin;
GetInteractionCells(dcell[p1],hdiv,nc,cellzero,cxini,cxfin,yini,yfin,zini,zfin);


for(int z=zini;z<zfin;z++){
  const int zmod=(nc.w)*z+cellinitial;
  for(int y=yini;y<yfin;y++){
    int ymod=zmod+nc.x*y;
    const unsigned pini=beginendcell[cxini+ymod];
    const unsigned pfin=beginendcell[cxfin+ymod];
```

Exclude 'cellinitial' for boundary neighbours

CPU – Call p2 neighbours

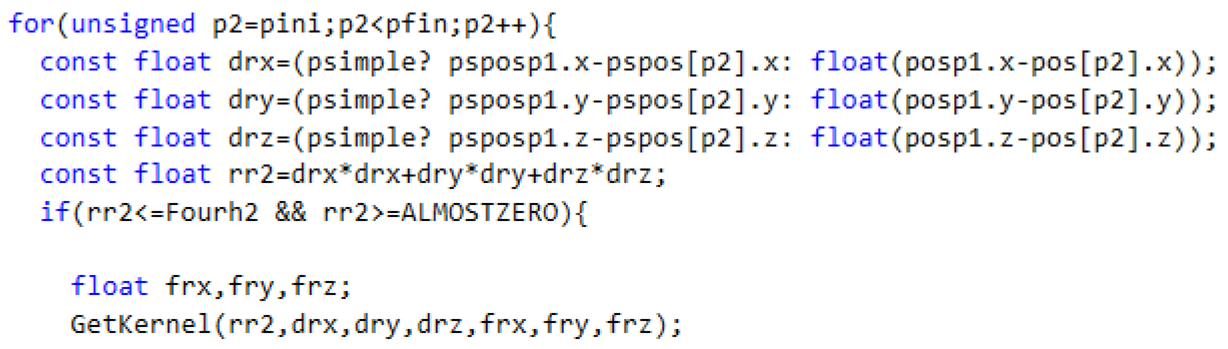
```
for(int z=zini;z<zfin;z++){
  int zmod=(nc.w)*z+cellfluid;
  for(int y=yini;y<yfin;y++){
    int ymod=zmod+nc.x*y;
    unsigned pini,pfin=0;
    for(int x=cxini;x<cxfin;x++){
      int2 cbeg=begincell[x+ymod];
      if(cbeg.y){
        if(!pfin)pini=cbeg.x;
        pfin=cbeg.y;
      }
    }
    if(pfin){
```

Exclude 'cellinitial' for boundary neighbours

//Insert __DEVICE__ function for particle interaction equation here

Methodology – Inserting new computation functions (for the PPE setup)

<u>CPU – p1 interact with p2</u>

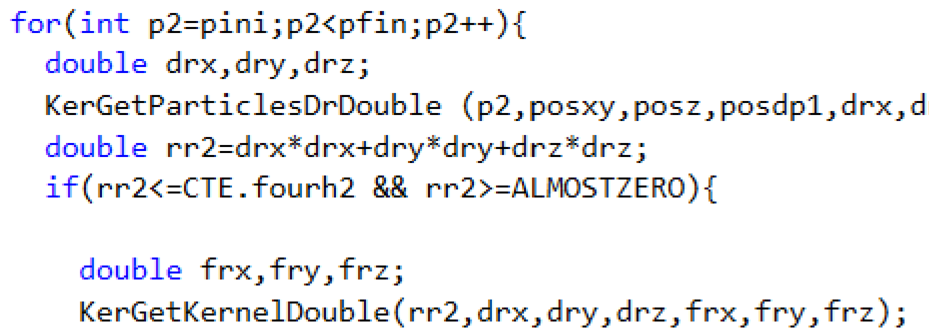


```
for(unsigned p2=pini;p2<pfin;p2++){
  const float drx=(psimple? psposp1.x-pspos[p2].x: float(posp1.x-pos[p2].x));
  const float dry=(psimple? psposp1.y-pspos[p2].y: float(posp1.y-pos[p2].y));
  const float drz=(psimple? psposp1.z-pspos[p2].z: float(posp1.z-pos[p2].z));
  const float rr2=drx*drx+dry*dry+drz*drz;
  if(rr2<=Fourh2 && rr2>=ALMOSTZERO){

    float frx,fry,frz;
    GetKernel(rr2,drx,dry,drz,frx,fry,frz);
```

//Insert equations here

<u>GPU – p1 interact with p2</u>

//Call device function for particle interaction here {



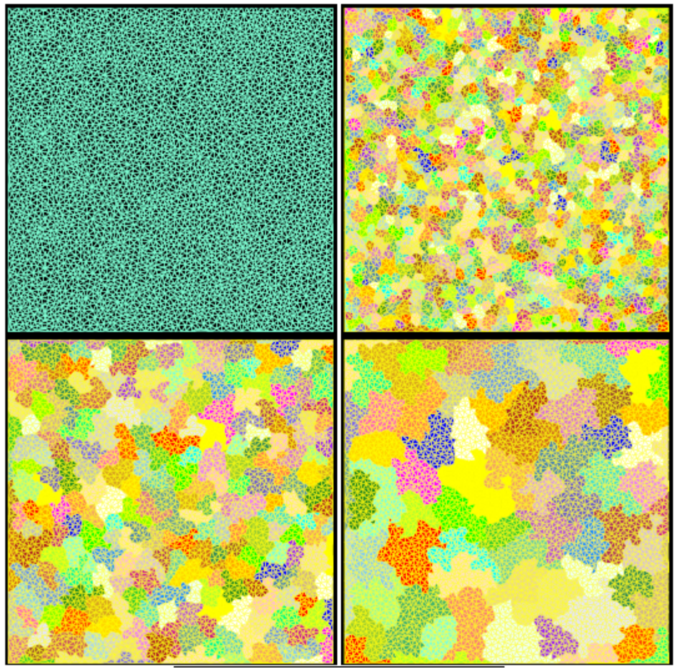
```
for(int p2=pini;p2<pfin;p2++){
  double drx,dry,drz;
  KerGetParticlesDrDouble (p2,posxy,posz,posdp1,drx,dry,drz);
  double rr2=drx*drx+dry*dry+drz*drz;
  if(rr2<=CTE.fourh2 && rr2>=ALMOSTZERO){

    double frx,fry,frz;
    KerGetKernelDouble(rr2,drx,dry,drz,frx,fry,frz);
```

//Insert equations here

Algebraic Multigrid (AMG)

A quick Algebraic Multigrid (AMG) overview:

- The preconditioner breaks the matrix down into different "levels" of fineness, the original matrix is the "finest level"
- The different levels will reduce errors of high and low frequencies in the result
- This produces a much faster convergence rate compared to other preconditioners
- This method is also highly scalable unlike the Jacobi



The AMG creates different levels of a matrix (Sumant et al., 2009)

P. S. Sumant, A. C. Cangellaris, and N. R. Aluru. A node-based agglomeration AMG solver for linear elasticity in thin bodies. Coummunications in Numerical Methods in Engineering, 25:219-236, 2009.