Discontinous Galerkin solver design on hybrid computers.

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Outlines

1. Vlasov and hyperbolic systems of conservation laws.
2. Efficient conservation laws solver.
3. Discontinuous Galerkin (DG) solver design.

Vlasov reduction

I) The (x, v) Vlasov equation is an $x-$only hyperbolic system of conservation laws.

Vlasov reduction

We consider the one-dimensional Vlasov-Poisson model

$$\partial_t f + v\partial_x f + E\partial_v f = 0, \tag{1}$$

$$\partial_x E = -1 + \int_v f dv, \tag{2}$$

where $f(x, v, t)$ is the distribution function, $E(x, t)$ is the electric field.
We consider the space-periodic case

$$f(0, v, t) = f(L, v, t), \quad \frac{1}{L}\int_x \int_v f(x, v, 0) = 1,$$

$$\int_{x=0}^{L} E dx = 0.$$

We also suppose that

$$v \in]-\infty; \infty[.$$

Model reduction

We consider a finite number of independent velocity functions $\{\varphi_k(v), k = 1 \cdots P\}$ and expand f on this basis

$$f(x,v,t) \simeq \sum_{j=1}^{P} w^j(x,t)\varphi_j(v)$$
$$= w^j(x,t)\varphi_j(v) \text{ (sum on repeated indices).} \quad (3)$$

The unknown scalar $f(x,v,t)$ is replaced by the unknown vector

$$W(x,t) = \left(w^1(x,t), w^2(x,t), \cdots, w^P(x,t)\right)^T.$$

Armstrong, 1967 [1], Tang & *al.* 1992, 1993 [12, 13], Schumer, Holloway, 1998 [11], le Bourdiec, de Vuyst, Jacquet 2006 [7]...

We introduce the expansion (3) in the Vlasov equation (1), multiply by φ_i and integrate with respect to v. We obtain

$$M\partial_t W + A\partial_x W + B(E)W = 0, \tag{4}$$

where

$$M_{ij} = \int_v \varphi_i \varphi_j, \quad A_{ij} = \int_v v\varphi_i \varphi_j, \quad B(E)_{ij} = E \int_v \varphi_i \partial_v \varphi_j.$$

M is symmetric positive, A is symmetric. The system (4) is thus a hyperbolic system of conservation laws ($M^{-1}A$ has real eigenvalues).

$$\partial_t W + \partial_x F(W) + S(W) = 0.$$

$$F(W) = M^{-1}AW, \quad S(W) = M^{-1}B(E)W.$$

General hyperbolic system

The approach can be extended to gyrokinetic models, higher dimensions, etc. [5]. Hyperbolic system theory is also useful for MHD, Maxwell, fluids, etc.
General case: $W(X,t), \quad X = (x_1, \ldots, x_d)$.

$$\partial_t W + \partial_{x_i} F^i(W) + S(W) = 0.$$

Flux: $n = (n_1 \cdots n_d)$, $F(W,n) = F^i(W) n_i$. Hyperbolicity: the eigenvalues of $D_W F(W,n)$ are real.

II) Comparison of several implementations of a very simple conservation laws solver.

A simple conservation laws solver

Solution $W(x, y, t) \in \mathbb{R}^m$ of Maxwell/fluids/MHD/Vlasov equations $X = (x, y)$. System of conservation laws.

$$\partial_t W + \partial_x F^x(W) + \partial_y F^y(W) = 0.$$

Approximation $W^n_{i,j}$ of $W(i\Delta x, j\Delta y, n\Delta t)$. Finite volume method + Strang splitting

$$\frac{W^*_{i,j} - W^n_{i,j}}{\Delta t} + \frac{F^{x,n}_{i+1/2,j} - F^{x,n}_{i-1/2,j}}{\Delta x} = 0,$$

$$\frac{W^{n+1}_{i,j} - W^*_{i,j}}{\Delta t} + \frac{F^{y,n}_{i,j+1/2} - F^{y,n}_{i,j-1/2}}{\Delta y} = 0.$$

Numerical flux: $F^{x,n}_{i+1/2,j} = F^x_{\text{num}}(W^n_{i,j}, W^n_{i+1,j})$, $F^{y,n}_{i,j+1/2} = F^y_{\text{num}}(W^n_{i,j}, W^n_{i,j+1})$.

CPU Implementation

On large grids ($> 1024 \times 1024$). We compare:

- a naive C implementation without optimization on a CPU single core;
- the same program, but compiled with optimizations;
- the same program with an additional optimization (tiling for optimizing data locality);
- the same program with OpenMP parallelization on a 16-core CPU.

Comparison

Implementation	Time	Speedup
Naive code	30 days	1
Naive code + optim. compil.	146 h	5
Naive code + optim. compil. + tiling	97 h	8
OpenMP version (16 cores)	6.2 h	116

OpenCL

OpenCL model: an accelerator device (GPU or CPU) is made of

- Global memory (typically 2 GB);
- Compute units (typically 30).

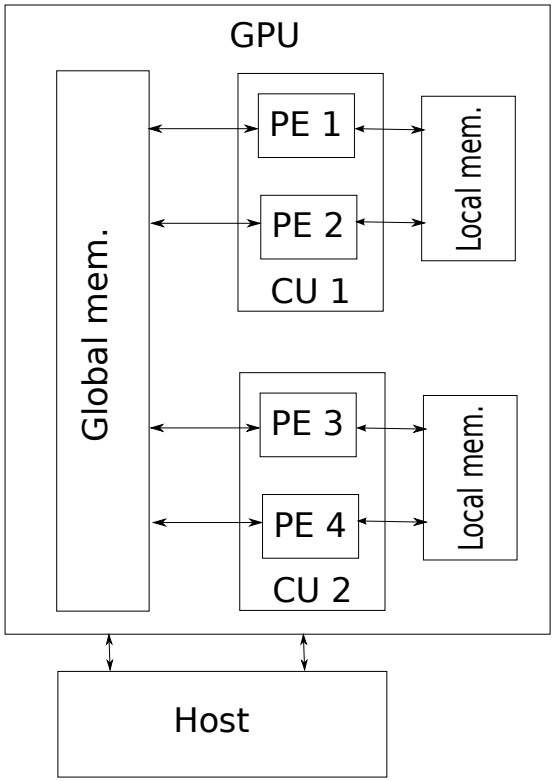
Each compute unit is made of

- Processing elements (typically 8);
- Local memory (typically 32 kb).

The same program (kernel) can be executed on all the processing elements at the same time.

- All the processing elements have access to the global memory.
- The processing elements have only access to the local memory of their compute unit.
- If two processing elements write at the same location at the same time, only one wins...
- The access to the global memory is slow while the access to the local memory is fast (generally...)

A (virtual) GPU with 2 Compute Units and 4 Processing Elements



OpenCL

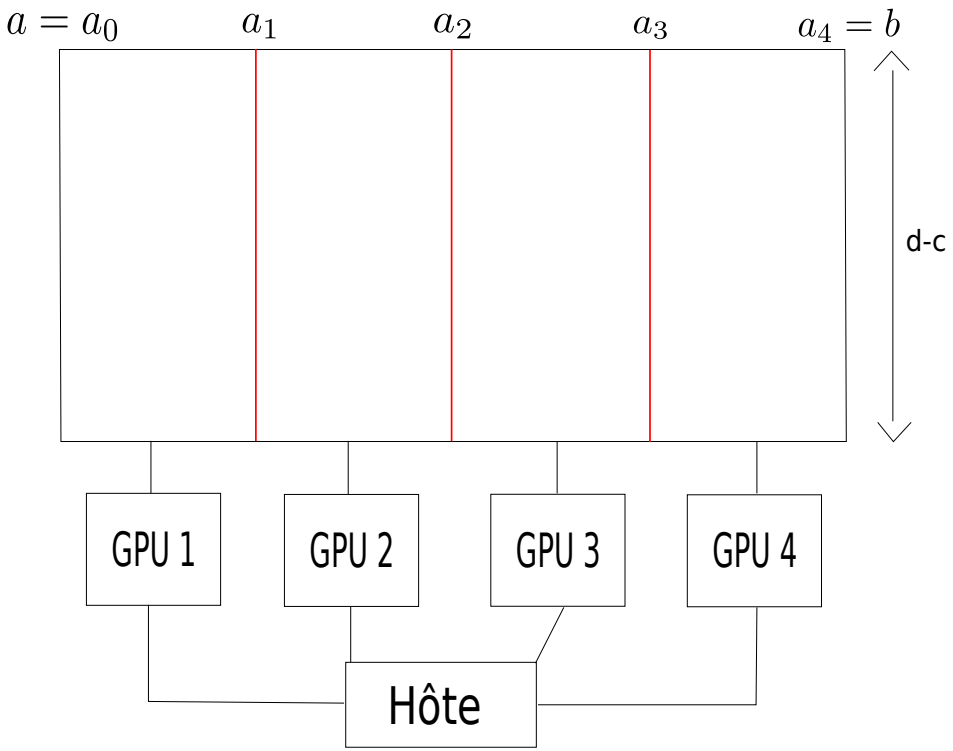
- OpenCL: "Open Computing Language". Library of C functions, called from the host, in order to drive the GPU + C-like language for the kernels. Available since 2009. Specification managed by the Khronos Group (OpenGL).
- Virtually, it allows to have as many compute units (work-groups) and processing elements (work-items) as needed.
- The threads are sent to the GPU thanks to a mechanism of command queues on the real compute units and processing elements. OpenCL manages events and a task graph for asynchronous out-of-order operations.
- Portable: the same program can run on a multicore CPU or a GPU. Drivers exist for: AMD CPU and GPU, Intel CPU and GPU, MIC, ARM, IBM Power7, StarPU, etc.

Implementation of the splitting scheme

We organize the data in a (x, y) grid and for each time step:

- we associate a work-item to each cell of the grid and a work-group to each row.
- we compute the fluxes balance in the x-direction for each cell of each row of the grid.
- we transpose the grid (exchange x and y) with an optimized memory transfer algorithm [10] (see also [9]).
- we compute the fluxes balance in the y-direction for each row of the transposed grid. Memory access are optimal.
- we transpose again the grid.

We apply a subdomain decomposition for multi-GPU computing



Comparison

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OpenMP (CPU Intel 8x2 cores)	6.2 h	116
OpenCL (CPU Intel 6x2 cores)	18 h	40
OpenCL (NVidia Tesla K20)	20 min	2160
OpenCL (AMD Radeon HD 7970)	16 min	2650
OpenCL + MPI (4 x AMD Radeon HD 7970)	5 min	7848

Essential: no test, optimized transposition (10x faster than the naive memory access)

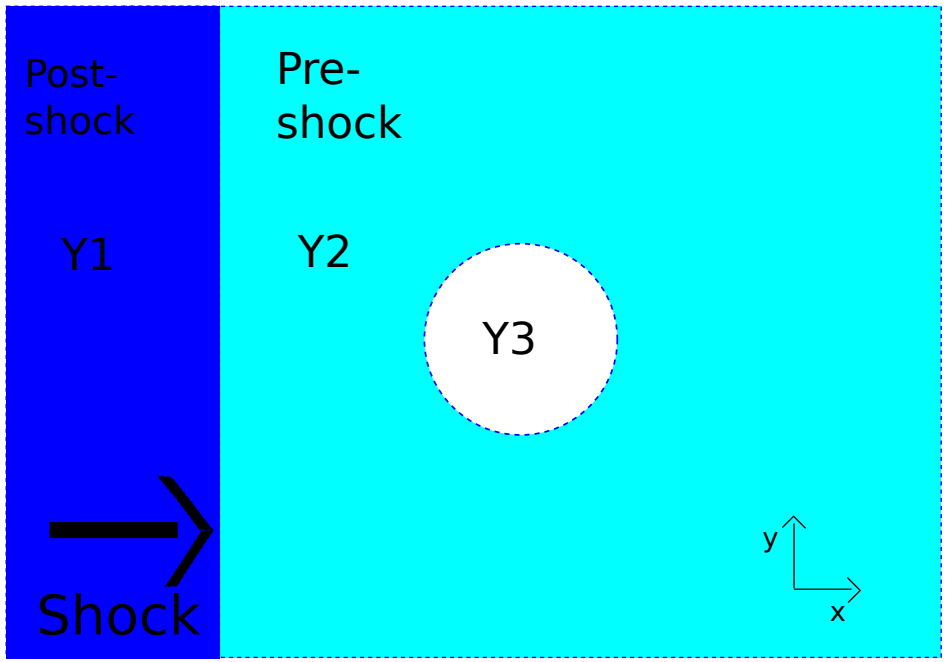
Partial conclusion

Well known conclusions

- GPU computing can be really faster,
- But: no test in OpenCL or CUDA kernels,
- Memory access are essentials.

Shock-bubble interaction

Two-phase flow conservation laws system. Density ρ, velocity (u, v), internal energy e, gas mass fraction ϕ.
$W = (\rho, \rho u, \rho v, \rho(e + u^2/2 + v^2/2), \rho\phi)$.

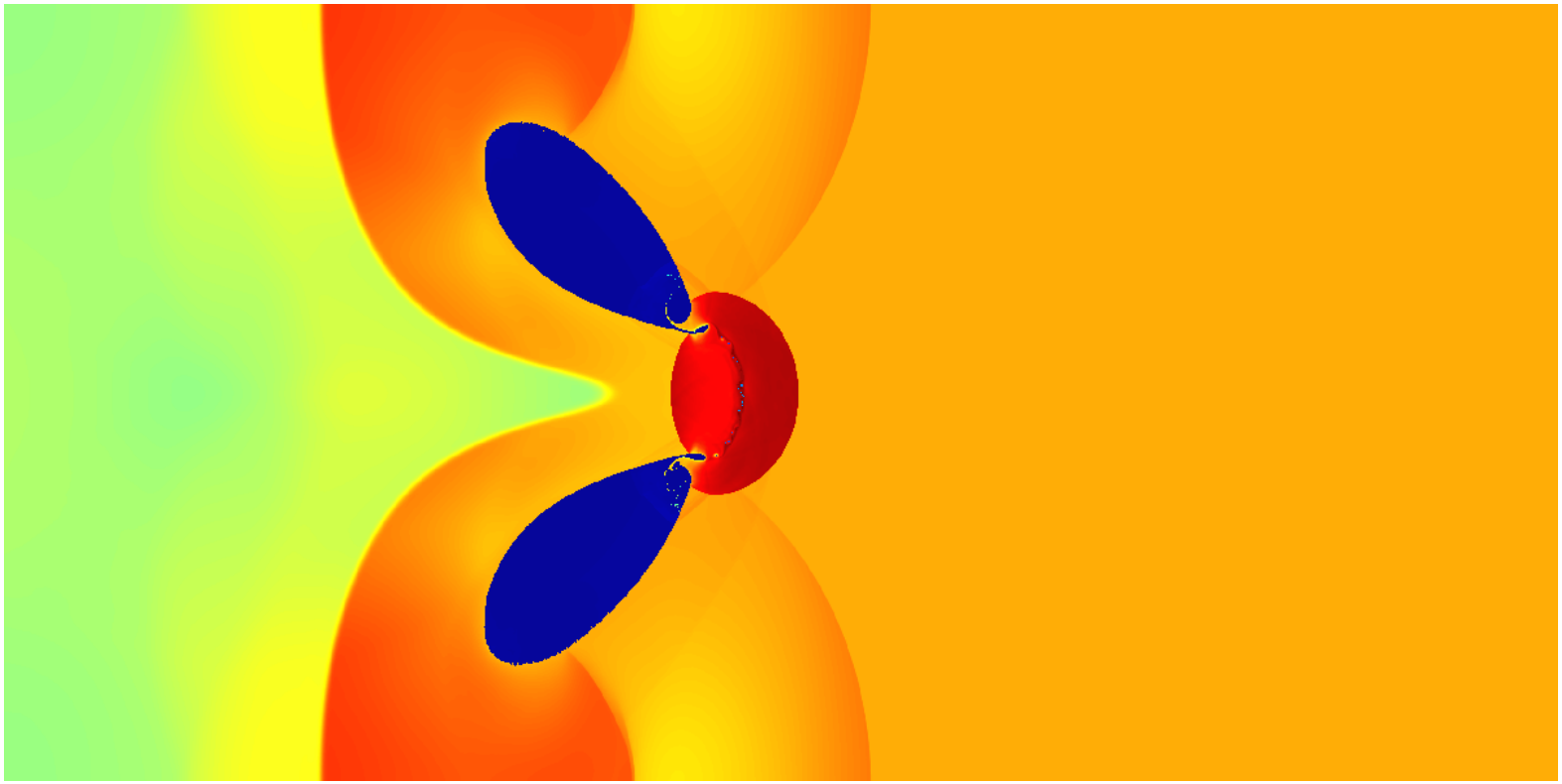


http://www.youtube.com/watch?v=c8hcqihJzbw

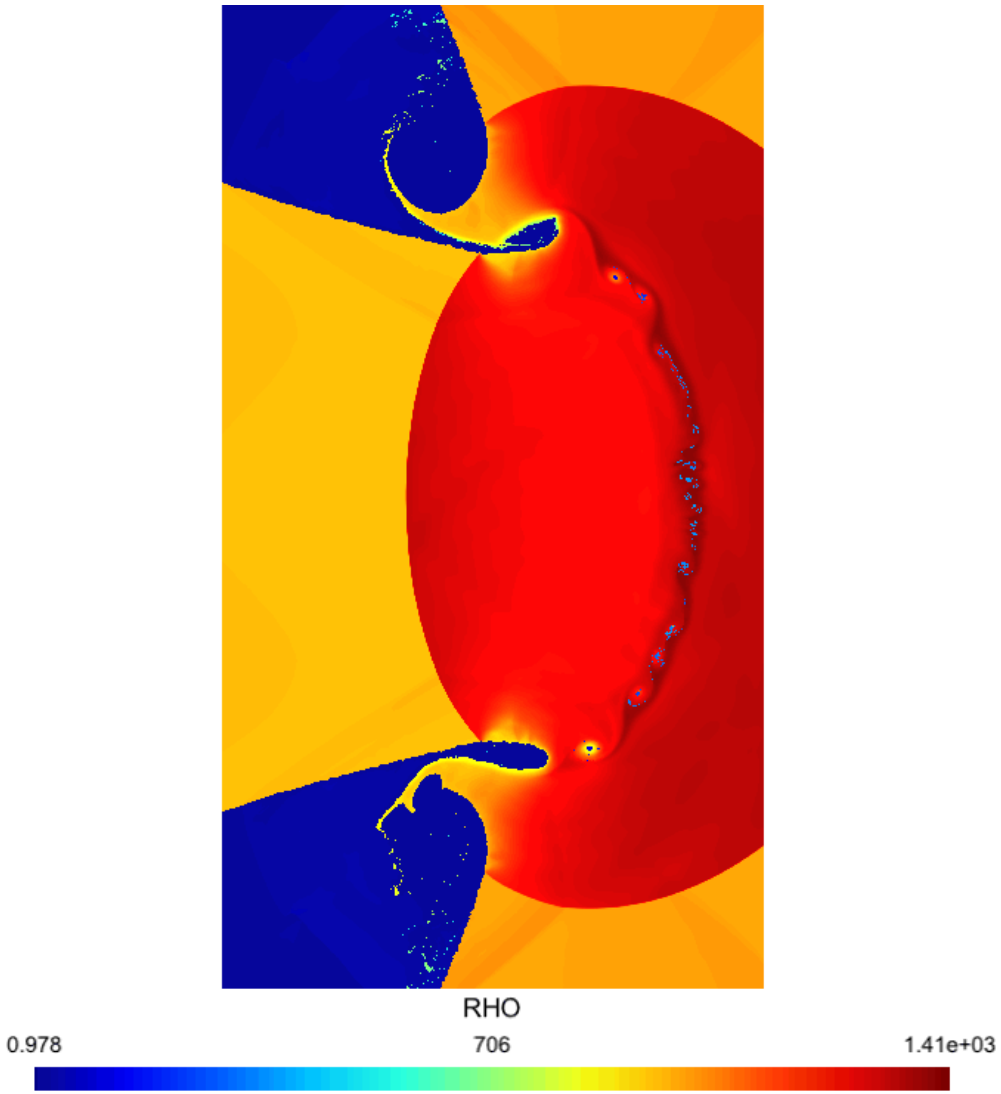
Numerical results

$t_{max} = 0.45$ ms
Grid: 40,000×20,000 (4 billions unknowns for each time step) [6]
GPU time: 30 h (10×NVIDIA K20)

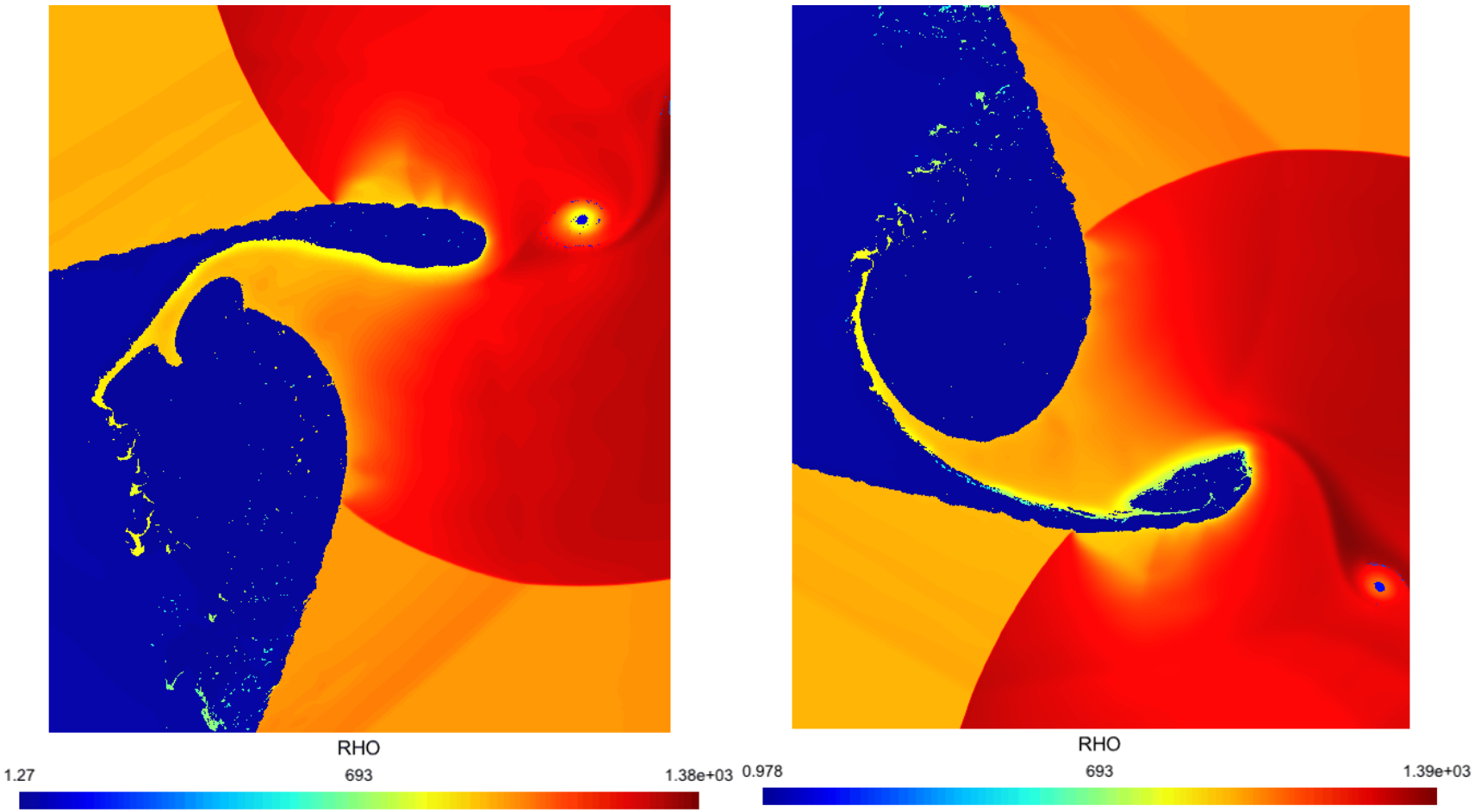
Density



Zoom 1

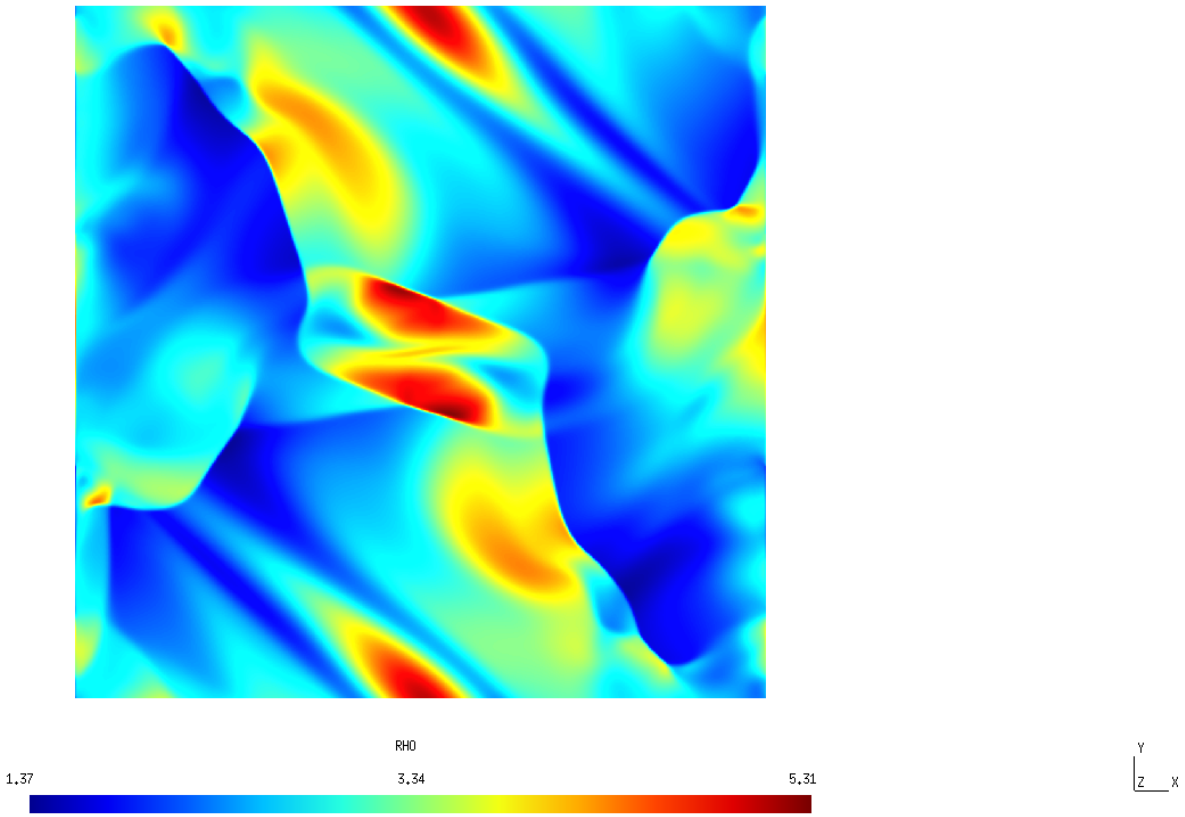


Zoom 2



MagnetoHydroDynamics (MHD)

$W = (\rho, \rho u, \rho v, \rho w, B_x, B_y, B_z, \rho(e + u^2/2 + v^2/2))$. Velocity (u, v, w), magnetic field (B_x, B_y, B_z).
Orszag-Tang vortex (grid size up to 15000×15000) [8].



III) A more versatile approach: the Discontinous Galerkin (DG) method.

DG solver

Generalization of the FV method, DG method in a 3D space, $X = (x, y, z)$. We consider a mesh of the computational domain. In a cell L of the mesh, the field is approximated by polynomial basis functions (sum on repeated indices)

$$W(X,t) = W_L^j(t)\varphi_j^L(X), \quad X \in L.$$

The numerical solution satisfies the DG approximation scheme

$$\forall L, \forall i \quad \int_L \partial_t W \varphi_i^L - \int_L F(W, \nabla \varphi_i^L) + \int_{\partial L} F(W_L, W_R, n_{LR}) \varphi_i^L = 0.$$

- R denotes the neighbor cells along ∂L.
- n_{LR} is the unit normal on ∂L oriented from L to R.
- $F(W_L, W_R, n)$ is the numerical flux (which satisfies $F(W, W, n) = F^x(W)n_x + F^y(W)n_y$).
- Time integration of a system of ordinary differential equations. Mass matrix $M_{i,j}^L = \int_L \varphi_i^L \varphi_j^L$

DG approach and GPU

advantages:

- varying order, mesh refinement.
- local stencil.
- high order $\Rightarrow$ high amount of local computations.
- many optimizations for hexahedrons meshes.
- MIMD/SIMD parallelism. Subdomains (MPI), elementary computations (OpenMP, CUDA, OpenCL) [3].

possible issues:

- memory access (unstructured mesh).
- branch tests in kernels (physical models, boundary conditions, etc.)
- MPI communications imply GPU$\leftrightarrow$Host memory transfers.

CLAC

CLAC means Conservation Laws Approximation on many Cores. It is a C++ library developed with AxesSim company in Strasbourg. It is actually used for actual electromagnetic simulations.

- "Reasonable" C++: a few templates, almost no inheritance.
- Google coding rules `http://google-styleguide.googlecode.com/svn/trunk/cppguide.xml`
- Git on Inria GForge.
- Doxygen.
- scons.
- Boost: unit tests, graphs.

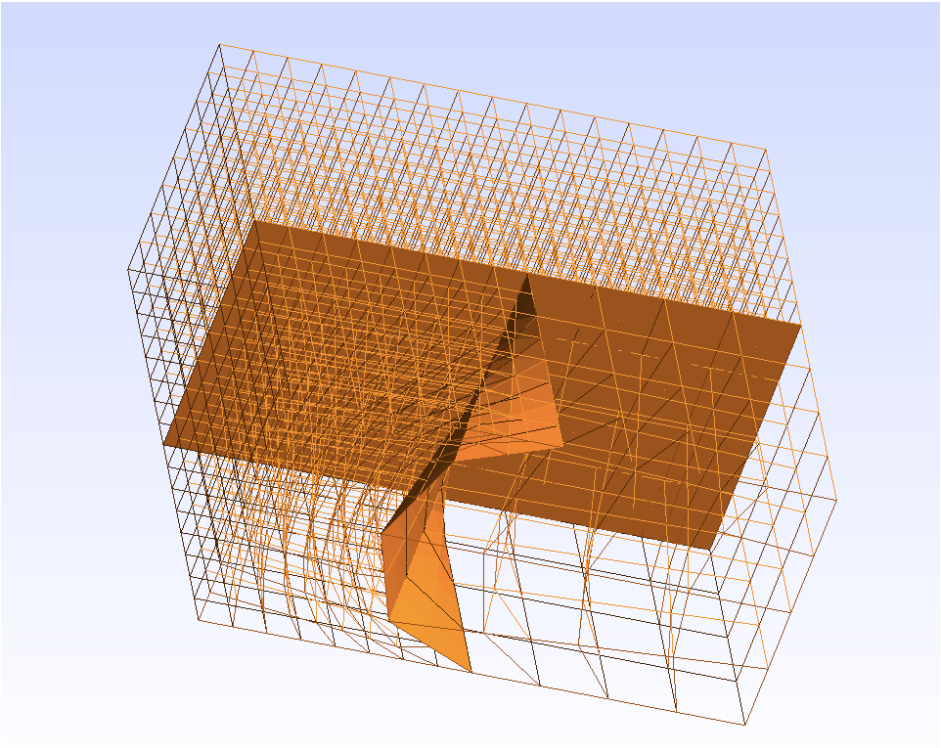
Would be useful: continuous integration...

CLAC data structure

- Subdomain decomposition: each domain is associated to a MPI node. Each MPI node is associated to an OpenCL device (CPU or GPU).
- Zone decomposition: each subdomain is split into volume zones and interface zones. A zone possess identical elements (same order, same geometry, same physical model). A computation kernel is compiled for each zone (for avoiding branch tests).
- (Simple) non-conformity between zones is allowed.
- Geometry and interpolation are separated (possibility to replace memory access by computations).

CLAC data structure

Example of a domain made of two subdomains, three volume zones and three interface zones. the mesh is non-conforming.
Subdomain 0: only one big refined volume zone. Two interface zones.
Subdomain 1: two small volume zones (coarse and refined). Three interface zones.



Nodal interpolation

- Numerical integration: Gauss-Legendre integration points G_k^L, $G_k^{\partial L}$ and weights ω_k^L, $\omega_k^{\partial L}$ on hexahedrons

$$\int_L h(X)dX \simeq \sum_k \omega_k^L h(G_k^L).$$

  Nodal basis function $\varphi_i^L(G_k^L) = \delta_{i,k}$.
- Several optimizations: diagonal mass matrix, complexity $(d+1)^3 \rightarrow 3(d+1)$), etc. [4]

Implementation details

- A single kernel for ∂L and L integration steps. Intermediate results stored in the cache of the compute unit. One processor per Gauss point. The number of Gauss points is different on ∂L and $L \Rightarrow$ some processors are idling in the volume integration step.
- A function class (pointer to the actual function + headers and sources: needed for the OpenCL compilation at runtime). We generally hide memory access into function calls.
- Customized kernels are assembled and compiled for each zone.

CLAC task graph

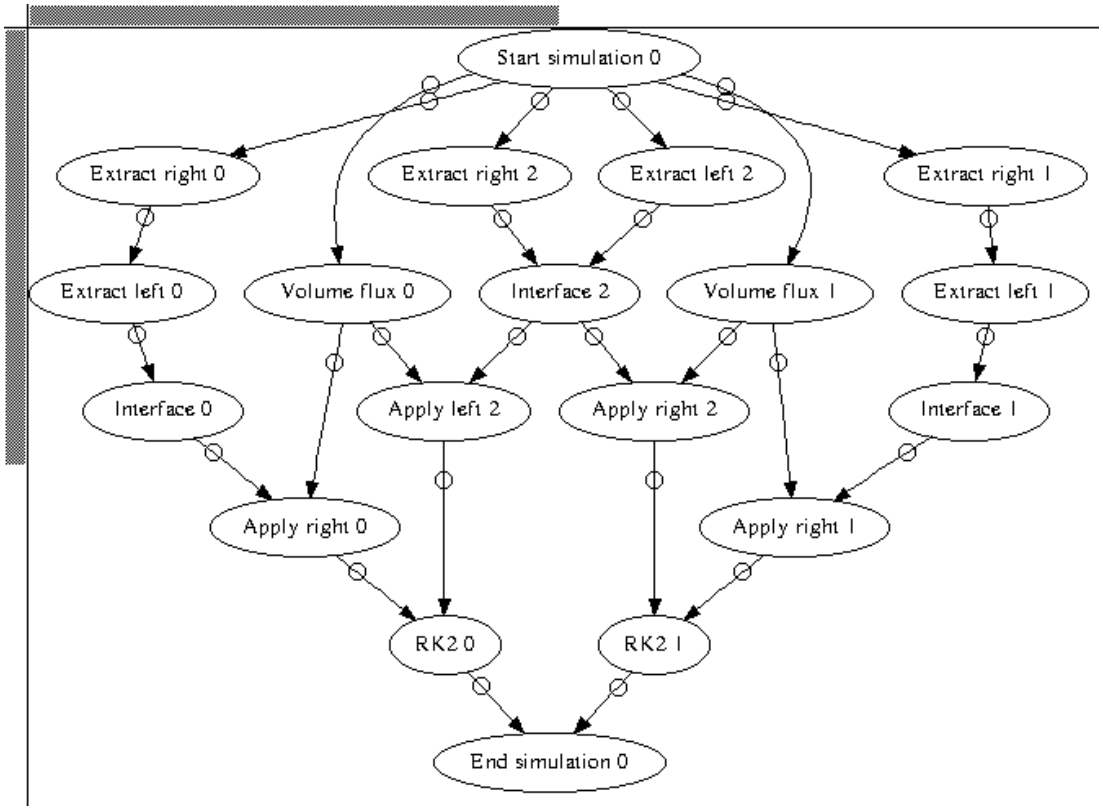
Important kernels:

- Volume zone: internal fluxes and sources assembly ("Volume flux").
- Interface zone: field extraction from right and left volume zones ("Extract left", "Extract right"). The extraction may imply MPI communications.
- Interface zone: flux computations ("Interface").
- Interface zone: boundary fluxes assembly on the left and right volume zones ("Apply right" or "Apply left").
- Volume zones: RK2 integration step ("RK2").

GPU-host transfers occur only in the extraction task at an interface between two subdomains.

Task dependency graph

For the moment, we use Boost Graph.



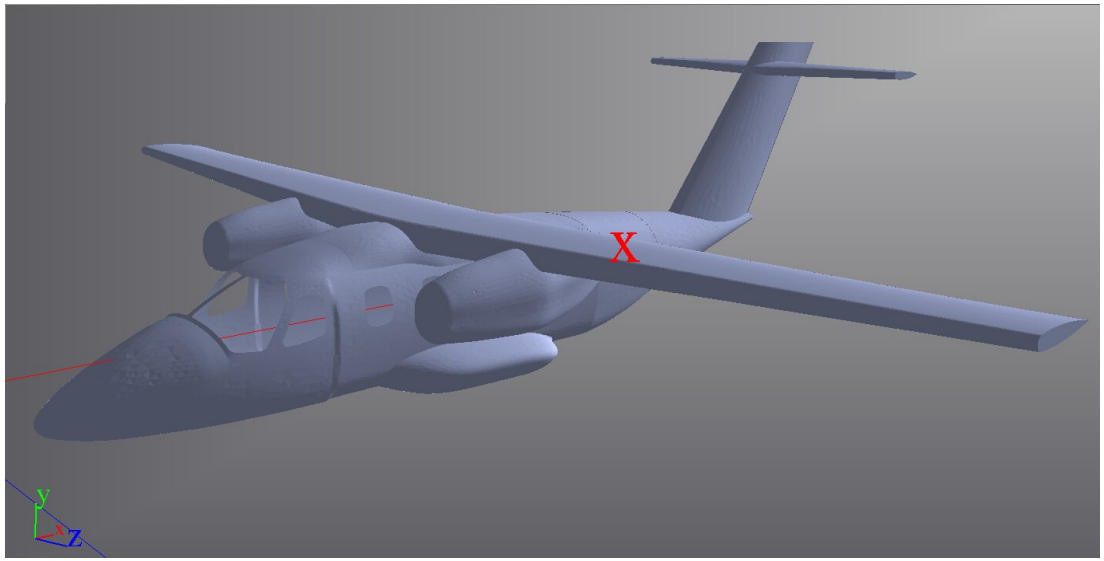
MPI/OpenCL events management

Problem: how to express the dependency between MPI and OpenCL operations ?

- We decided to rely only on the OpenCL events management.
- The beginning of a task depends on the completions of a list of OpenCL events. The task is itself associated to an OpenCL event.
- At an interface zone between two subdomains, an extraction task contains a GPU to host memory transfer, a MPI send/receive communication and a host to GPU transfer.
- we create an OpenCL user event, and launch a MPI blocking sendrecv in a thread. At the end of the communication, in the thread, the OpenCL event is marked as completed. Using threads avoids blocking the main program flow.
- Efficiency: test on 4 NVidia GTX 780. Synchronous mode, speedup$\simeq$2.6. Asynchrounous mode, speedup $\simeq 4.15$

Aircraft

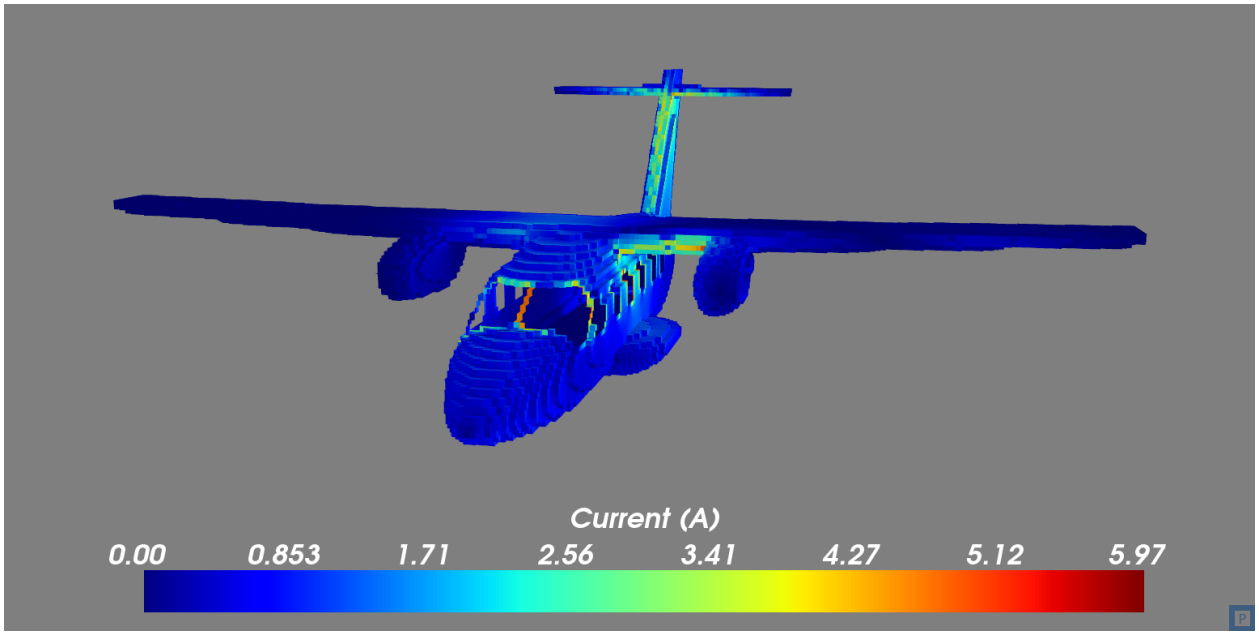
$W = (E_x, E_y, E_z, H_x, H_y, H_z)$: electric and magnetic field. Maxwell equations.
Plane wave with gaussian profile.



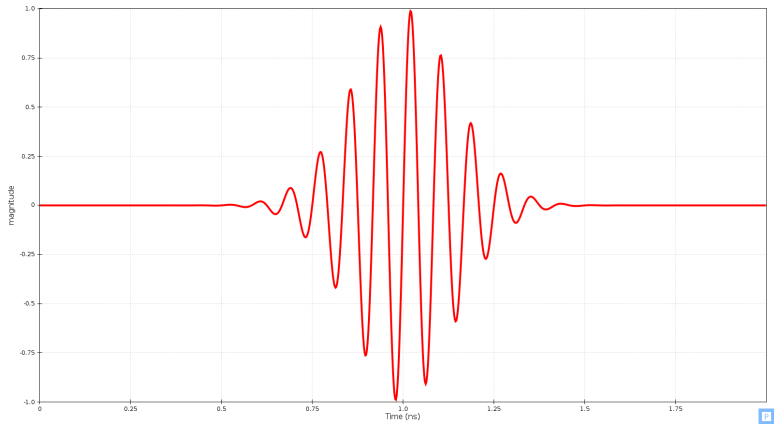
Aircraft

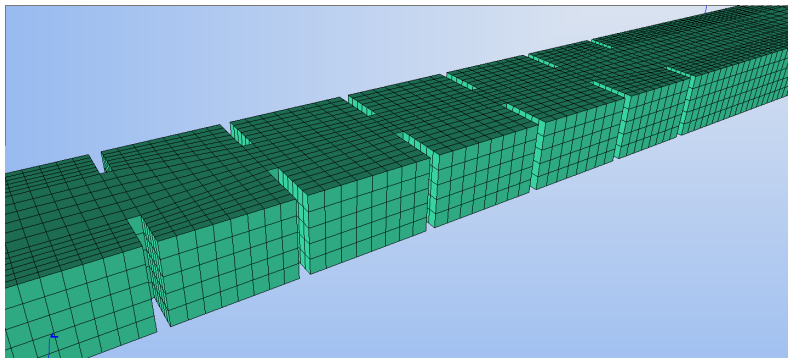
- Aircraft geometry described with $3,337,875$ hexaedrons ($\simeq$1 billion unknowns per time step). Several PML layers at the boudaries.
- We use 8 GPUs to perform the computation. The simulation does not fit into a single GPU memory. 400 Gflops.
- In this test case we spend about 30% of the computation time in the memory transfers between the CPU and the GPU and about 20% in the MPI communications. We expect much better speedups with the asynchronous task graph.

Aircraft



Waveguide filter



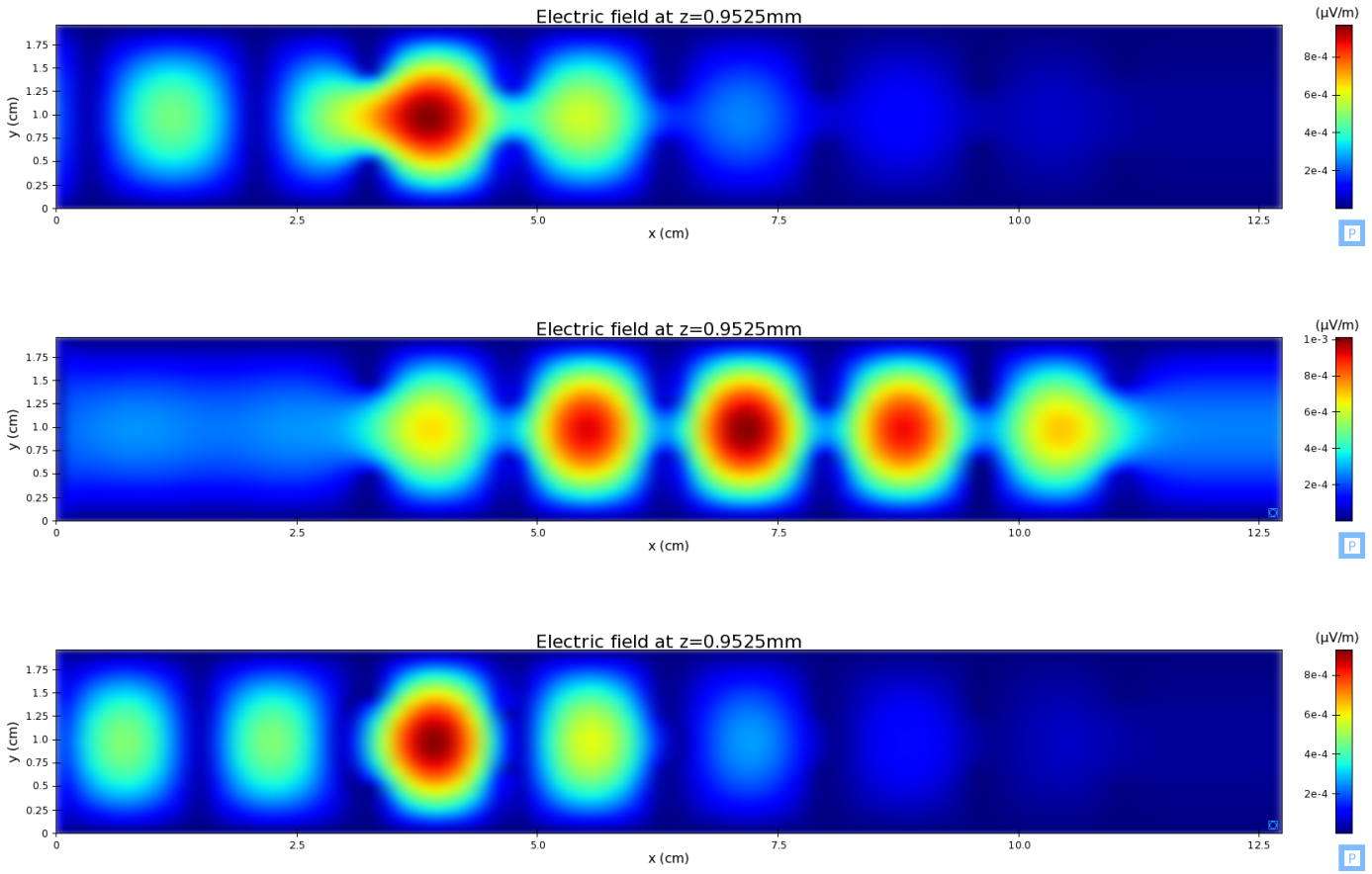


Waveguide filter

- 8370 cells, 3 millions unknowns (second order nodal interpolation).
- 10 cPML layers on two sides.
- dt = 1.36e-13s et dx = 8.14316e-04m. tmax = 25e-9s. 184076 iterations. 19.5mm$\times$9.525mm.
- GPU time 4092s on one NVIDIA GTX 680.

Waveguide filter

Ez at 11.5 GHz, 12 GHz and 12.4 GHz.



Conclusion

- CLAC: asynchronous hybrid DG solver based on OpenCL and MPI.
- It works...
- Work in progress: Gauss-Lobatto integration, memory transfer optimization (zone transpositions), etc. Summer CEMRACS project
  `http://smai.emath.fr/cemracs/cemracs14/lessiv.pdf`
- Task graph: we are reaching our position of incompetence. StarPU, SOCL ?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