Discontinuous Galerkin solver design on hybrid computers.

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Outlines

2. Efficient conservation laws solver.
3. Discontinuous Galerkin (DG) solver design.
1) The $(x, v)$ Vlasov equation is an $x$–only hyperbolic system of conservation laws.
We consider the one-dimensional Vlasov-Poisson model

\[
\frac{\partial}{\partial t} f + v \frac{\partial}{\partial x} f + E \frac{\partial}{\partial v} f = 0, \tag{1}
\]

\[
\frac{\partial}{\partial x} E = -1 + \int_v f dv, \tag{2}
\]

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

\[
v \in ]-\infty; \infty[.
\]
We consider a finite number of independent velocity functions \( \{ \varphi_k(v), k = 1 \cdots P \} \) and expand \( f \) on this basis

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

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

\[
W(x, t) = \begin{pmatrix} w^1(x, t), w^2(x, t), \cdots, w^P(x, t) \end{pmatrix}^T.
\]

We introduce the expansion (3) in the Vlasov equation (1), multiply by $\varphi_i$ and integrate with respect to $\nu$. We obtain

$$M \partial_t W + A \partial_x W + B(E)W = 0,$$

(4)

where

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

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

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

$$F(W) = M^{-1}AW, \quad S(W) = M^{-1}B(E)W.$$
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: \( n = (n_1 \cdots n_d), \quad F(W, n) = F^i(W)n_i. \) Hyperbolicity: the eigenvalues of \( D_W F(W, n) \) are real.
II) Comparison of several implementations of a very simple conservation laws solver.
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

\[ \frac{W^n_{i,j} - W^n_{i,j}}{\Delta t} + \frac{F^n_{i+1/2,j} - F^n_{i-1/2,j}}{\Delta x} = 0, \]

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

Numerical flux: $F^n_{i+1/2,j} = F_{\text{num}}^x(W^n_{i,j}, W^n_{i+1,j}),$

$F^n_{i,j+1/2} = F_{\text{num}}^y(W^n_{i,j}, W^n_{i,j+1})$. 

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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.
<table>
<thead>
<tr>
<th>Implementation</th>
<th>Time</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Naive code</td>
<td>30 days</td>
<td>1</td>
</tr>
<tr>
<td>Naive code + optim. compil.</td>
<td>146 h</td>
<td>5</td>
</tr>
<tr>
<td>Naive code + optim. compil. + tiling</td>
<td>97 h</td>
<td>8</td>
</tr>
<tr>
<td>OpenMP version (16 cores)</td>
<td>6.2 h</td>
<td>116</td>
</tr>
</tbody>
</table>

Discontinuous Galerkin solver design on hybrid computers.
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

Discontinuous Galerkin solver design on hybrid computers.

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.
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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<td>6.2 h</td>
<td>116</td>
</tr>
<tr>
<td>OpenCL (CPU Intel 6x2 cores)</td>
<td>18 h</td>
<td>40</td>
</tr>
<tr>
<td>OpenCL (NVidia Tesla K20)</td>
<td>20 min</td>
<td>2160</td>
</tr>
<tr>
<td>OpenCL (AMD Radeon HD 7970)</td>
<td>16 min</td>
<td>2650</td>
</tr>
<tr>
<td>OpenCL + MPI (4 x AMD Radeon HD 7970)</td>
<td>5 min</td>
<td>7848</td>
</tr>
</tbody>
</table>

Essential: no test, optimized transposition (10x faster than the naive memory access)
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 $\rho$, velocity $(u, v)$, internal energy $e$, gas mass fraction $\phi$.

$W = (\rho, \rho u, \rho v, \rho(e + u^2/2 + v^2/2), \rho \phi)$. 

http://www.youtube.com/watch?v=c8hcqihJzbw
$t_{\text{max}} = 0.45 \text{ ms}$

Grid: 40,000 $\times$ 20,000 (4 billions unknowns for each time step) [6]

GPU time: 30 h (10 $\times$ NVIDIA K20)
Density

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Discontinuous Galerkin solver design on hybrid computers.
$W = (\rho, \rho u, \rho v, \rho w, B_x, B_y, B_z, \rho(e + u^2/2 + v^2/2))$. Velocity $(u, v, w)$, magnetic field $(B_x, B_y, B_z)$.
Orszag-Tang vortex (grid size up to $15000 \times 15000$) [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)

$$W(X, t) = W_i^L(t) \phi_j^L(X), \quad X \in L.$$ 

The numerical solution satisfies the DG approximation scheme

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

- $R$ denotes the neighbor cells along $\partial L$.
- $n_{LR}$ is the unit normal on $\partial L$ 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 $M_{i,j}^L = \int_{L} \phi_i^L \phi_j^L$. 

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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 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.
googlecode.com/svn/trunk/cppguide.xml
- Git on Inria GFoe.
- Doxygen.
- scons.
- Boost: unit tests, graphs.

Would be useful: continuous integration...
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).
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 $G^L_k$, $G^{\partial L}_k$ and weights $\omega^L_k$, $\omega^{\partial L}_k$ on hexahedrons

$$\int_X h(X) dX \simeq \sum_k \omega^L_k h(G^L_k).$$

Nodal basis function $\varphi^L_i(G^L_k) = \delta_{i,k}$.

- Several optimizations: diagonal mass matrix, complexity $(d + 1)^3 \to 3(d + 1))$, etc. [4]
A single kernel for $\partial L$ 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 $\partial L$ 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.
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.
For the moment, we use Boost Graph.
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 $\approx 2.6$. Asynchronous mode, speedup $\approx 4.15$
\( \mathbf{W} = (E_x, E_y, E_z, H_x, H_y, H_z) \): electric and magnetic field. Maxwell equations.

Plane wave with gaussian profile.
• Aircraft geometry described with 3,337,875 hexaedrons (≈1 billion unknowns per time step). Several PML layers at the boundaries.

• 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.
Waveguide filter

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Waveguide filter

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

$E_z$ at 11.5 GHz, 12 GHz and 12.4 GHz.
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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Philippe Helluy and Jonathan Jung.  
Two-fluid compressible simulations on gpu cluster.  
2014.

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Numerical solution of the vlasov–poisson system using generalized hermite functions.  

Michel Massaro, Philippe Helluy, and Vincent Loechner.  
Numerical simulation for the mhd system in 2d using opencl.  
2013.

David Michéa and Dimitri Komatitsch.  
Accelerating a three-dimensional finite-difference wave propagation code using gpu graphics cards.  

Greg Ruetsch and Paulius Micikevicius.  
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Optimizing matrix transpose in cuda.
*Nvidia CUDA SDK Application Note*, 2009.

Joseph W Schumer and James Paul Holloway.
Vlasov simulations using velocity-scaled hermite representations.

Tao Tang.
The hermite spectral method for gaussian-type functions.

Tao Tang, S McKee, and MW Reeks.
A spectral method for the numerical solutions of a kinetic equation describing the dispersion of small particles in a turbulent flow.