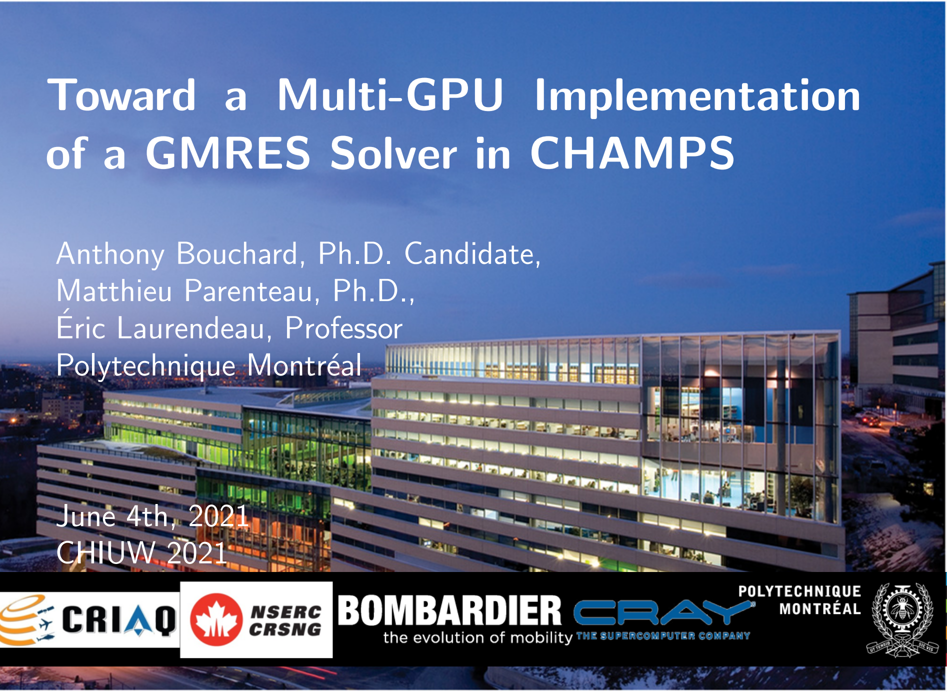

Toward a Multi-GPU Implementation of a GMRES Solver in CHAMPS

Anthony Bouchard, Ph.D. Candidate,
Matthieu Parenteau, Ph.D.,
Éric Laurendeau, Professor
Polytechnique Montréal

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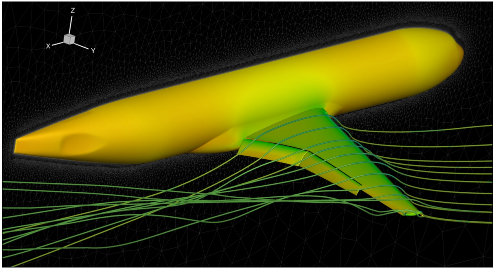
CHAMPS

- 3D Multi-physics CFD code developed by the research team of Professor Éric Laurendeau
- Written in CHAPEL
- (U)RANS flow solver using an unstructured mesh-based second-order cell centered finite volume method



Computed flow solution with CHAMPS around a high-lift configuration aircraft

RANS Equations

CHAMPS solves the Reynolds-Averaged Navier Stokes equations that can be expressed as:

$$\Omega\frac{\partial \boldsymbol{W}_c}{\partial t} = -\boldsymbol{R}(\boldsymbol{W}_c)$$

where $\boldsymbol{W}_c = [\rho, \rho u, \rho w, \rho w, \rho E]$ is the average state vector of the conservative flow variables of a cell, Ω the cell volume and $\boldsymbol{R}$ the residual vector. Using an inexact Newton iteration, the equation becomes

$$\left[\frac{\Omega}{\Delta t}\mathcal{I} + \Omega\frac{\partial \overline{\boldsymbol{R}}}{\partial \boldsymbol{W}_c}\right]^n \Delta \boldsymbol{W}_c^{n+1} = -\boldsymbol{R}(\boldsymbol{W}_c^n)$$

where Δt is the pseudo time step, $\frac{\partial \overline{\boldsymbol{R}}}{\partial \boldsymbol{W}_c}$ is an approximation of the true Jacobian matrix using a first-order discretization of the dissipation fluxes and the Thin Shear Layer (TSL) approximation of the viscous fluxes and $\Delta \boldsymbol{W}_c^{n+1} = \boldsymbol{W}_c^{n+1} - \boldsymbol{W}_c^n$.

GMRES Solver

- Usual linear solvers used in production CFD codes (like SGS) are not well suited for GPUs
- GMRES is well known for its fast convergence when given a suitable initial solution
- Jacobian-free version:
  - Prevents the need to store the true Jacobian matrix and invert it
  - The Jacobian-vector product is calculated using a finite difference approximation, which requires another evaluation of the residuals that is efficient on GPUs
  - The Jacobian-vector product accurately sees the true Jacobian, enhancing the convergence

GMRES Solver (Cont'd)

Usually, in practice, the GMRES algorithm consists of the Arnoldi-Modified Gram-Schmidt orthogonalization method

```
$w_j = Av_j$ [communication point];
for $i = 1, ..., j$ do
    $h_{i,j} = (w_j, v_i)$ [communication point];
    $w_j = w_j - h_{i,j} v_i$;
end
$h_{j+1,j} = \|w_j\|_2$ [communication point];
$v_{j+1} = w_{j+1}/h_{j+1,j}$;
```

and the least square problem $\left\|\beta e_1 - \bar{H}_m y\right\|_2$, for which givens rotation are applied beforehand to the Hessenberg matrix $h_{i,j}$ to obtain a triangular matrix that can be solved efficiently.

GPU Implementation

```
class DistributedVectorGPU_c : Vector_c
{
    /** Number of local elements **/
    const niLocal_ : int;
    /** Local task id **/
    const localTaskId_ : int;
    /** Domain for the local values **/
    const localDomain_ : domain(1) = {0..#niLocal_};

    proc init(ni : int = 0, niLocal : int = 0, localTaskId : int = 0)
    {
        super.init(ni);

        niLocal_ = niLocal;
        localTaskId_ = localTaskId;
    }

    /**
        Computes the norm
    **/
    override proc norm(param comm : bool = true) : real_t
    {
        var res : real;
        local
        {
            if (updateGPU_)
            {
                this.GPUcopy(0);
            }

            res = cublas_Dot(cublasHandle_, niLocal_, d_values_, d_values_); // CUDA function
        }

        if (comm)
        {
            var val = globalReduction.reduceValues(localTaskId_, [res], REDUCE_OPERATION_t.SUM);
            res = val[0];
        }

        return sqrt(res);
    }

```

GPU Implementation (Cont'd)

```
    /**
        Main procedure to solve the linear system

        :arg lhs: The LHS of the linear system to solve
        :arg rhs: The RHS of the linear system to solve
        :arg buildPreconditioner: If the LHS has changed, the preconditioner is updated
      **/
      proc solve(lhs : BSRmatrix_c, rhs : Vector_c, buildPreconditioner : bool = true) : int
      {
        var totalIteration : int = 0;

        var b_norm : real = rhs.norm();

        x_.reset();

        if (buildPreconditioner) then preconditioner_.buildPreconditioner();

        while (totalIteration < maxIterations_)
        {
          ref Q0 = krylovVectors_[0].Q_;
          Q0.set(rhs);

          if (totalIteration > 0)
          {
            x_.exchangeAuxValues(interfaceCommunicator_);
            lhs.dot(x_, workingArray_);
            Q0.addScale(workingArray_,-1.0);
          }

```

GPU Implementation (Cont'd)

- 1 CUDA thread per dimension of array
- cuBLAS library is used for complex vector operations
- Each zone is assigned to a task and distributed to the available *Locales*
- Each task is assigned to an asynchronous CUDA stream
- Communication is done on the CPU side, copying a buffer array from the GPU to the CPU and back to the GPU once the exchange is done

Multi-GPU Implementation

$$
\begin{array}{r}
\text{task: 0}\left\{\begin{array}{c}\\\end{array}\right.\\
\\
\text{task: 1}\left\{\begin{array}{c}\\\end{array}\right.\\
\\
\text{task: 2}\left\{\begin{array}{c}\\\end{array}\right.
\end{array}
\begin{bmatrix}
\color{red}2 & \color{red}0 & | & \color{blue}4 & \color{blue}0 & | & \color{blue}4 & \color{blue}1\\
\color{red}0 & \color{red}3 & | & \color{blue}5 & \color{blue}6 & | & \color{blue}0 & \color{blue}8\\
- & - & - & - & - & - & - & -\\
\color{blue}0 & \color{blue}2 & | & \color{red}5 & \color{red}0 & | & \color{blue}8 & \color{blue}1\\
\color{blue}1 & \color{blue}0 & | & \color{red}0 & \color{red}1 & | & \color{blue}6 & \color{blue}0\\
- & - & - & - & - & - & - & -\\
\color{blue}0 & \color{blue}4 & | & \color{blue}7 & \color{blue}0 & | & \color{red}1 & \color{red}1\\
\color{blue}1 & \color{blue}2 & | & \color{blue}0 & \color{blue}6 & | & \color{red}0 & \color{red}3
\end{bmatrix}
\times
\begin{Bmatrix}
\color{red}1\\
\color{red}3\\
-\\
\color{red}2\\
\color{red}5\\
-\\
\color{red}4\\
\color{red}9
\end{Bmatrix}
$$

Illustration of a distributed matrix and vector for multiple GPUs (one task per GPU)

Multi-GPU Implementation (Cont'd)

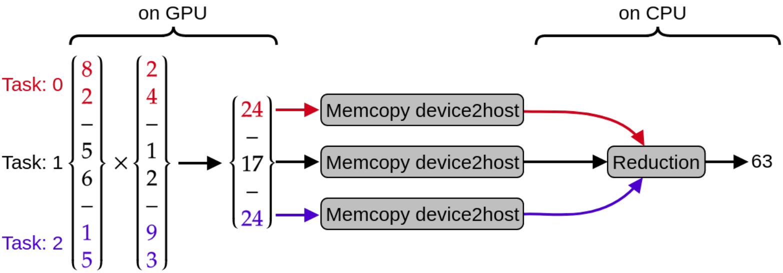
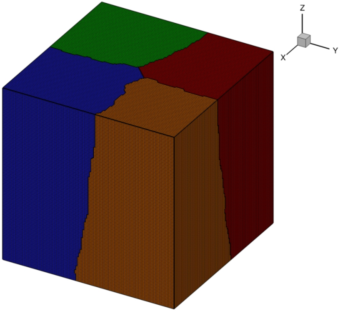


Illustration of a parallel dot product with multiple GPUs (one task per GPU)

Results

Cartesian Grid:

- 2M elements
- 4 zones
- Euler equations solved for 5 unknowns (10M total)
- Cases are run on Béluga

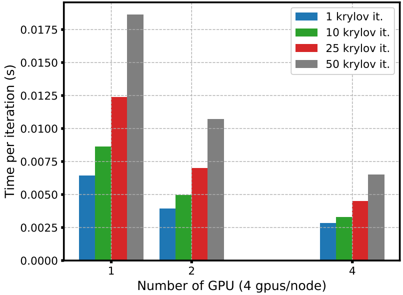


Cluster Hardware

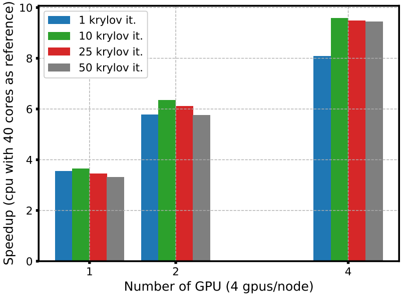
Summary of the CPUs and GPUs on one Beluga node

	Intel Xeon Gold 6148 Skylake	**NVidia V100SXM2**
Number of CPUs/GPUs	2	4
Clocks	2.4 GHz	1.53GHz
Number of cores/SMs per CPU/GPU	20 cores, 40 threads	80 SMs, 32 DP CUDA cores/SM
DP Peak TFLOPS per CPU/GPU	0.704	7.8
Peak memory bandwidth	128 GB/s	900 GB/s
Power per CPU/GPU	150 W	300 W

Speedup

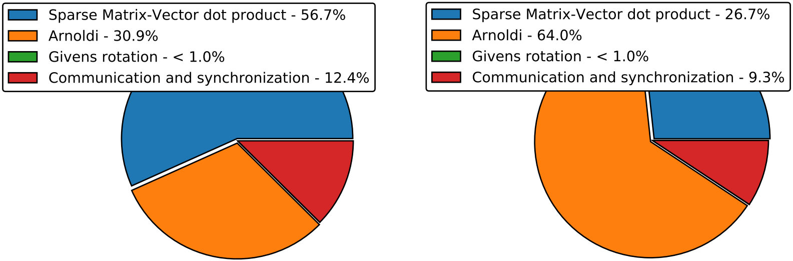


Real time per iteration in seconds for the GMRES algorithm on the GPU for different number of Krylov iterations



Speedup of the GPU version of GMRES compared to 2 CPUs

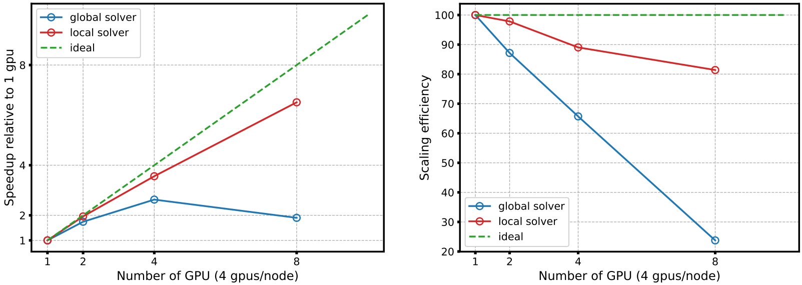
Time Distribution on a Single Node



(a) (b)

Comparison of the time distribution for (a) 10 Krylov iterations and (b) 50 Krylov iterations with 2 CPUs and GPUs

Strong Scaling

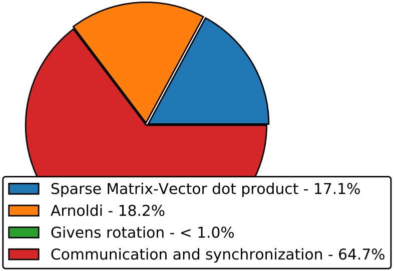


(a)

(b)

Strong scaling analysis of the GPU version of GMRES showing (a) the speedup and (b) the efficiency up to 8 GPUs

Time Distribution over 2 Compute Nodes



Time distribution with 8 GPUs distributed over two compute nodes for 10 Krylov iterations

Conclusion and Future Work

Conclusions:

- The speedup is close to the ratio of memory bandwidth without communication
- The Arnoldi orthogonalization is more and more costly when increasing the number of Krylov iterations
- The use of network atomics prevents efficient scaling on infiniband system

Future Work:

- Work with Cray on a fix for the synchronization problem on infiniband systems
- Port the preconditioners, the JFNK solver and the rest of the flow solver (& turbulence model) over GPU
- Compute end-to-end convergence speedups of the RANS solver

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Thank you for your attention!

Questions?