Implementing Spectral Difference Methods (SDM) for Compressible Euler flow simulations using performance portable library kokkos

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**Motivations:** computational sciences and software engineering

**Short Kokkos overview:** a C++ library for performance portability, a new way of designing portable parallel codes

- Refactoring or designing Hydrodynamics / MHD kernels
- Same performance between old CUDA kernels and new Kokkos Kernels?

**Implementing SDM high-order numerical schemes with Kokkos**

**Performance measurements on multiple architectures:**

- Intel Skylake, ARM ThunderX2: device Kokkos::OpenMP
- Nvidia GPU Pascal P100: device Kokkos::Cuda

**Perspectives / Future applications and developments**

- SDM Integration into our AMR code CanoP
Motivations of this work - 1

- code **RAMSES-GPU**: Magneto-Rotational Instability, MHD turbulence, ...
  - developed in CUDA/C++ for astrophysics applications on regular grid
  - ~ 70k lines of code (out of which ~ 16k in CUDA)
  - developed between **2009 and 2014**!

- Since then both GPU hardware/software have tremendously evolved (in orders of magnitude in memory bandwidth, number of registers per SM, c++11, ...) ⇒ a lot of optimization techniques accumulated over the years are **not so critically important anymore** on today’s GPU.

- Collaborations with domain scientists are hard when required software skills include CUDA.

- **2016-2017** is the right time to refactor code, **sparkle new ways to develop scientific software at a higher abstraction level**

- Can we rewrite an application like RamsesGPU in a new **high-level approach** for better software/science productivity?
Motivations of this work - 2

- **Software engineering**
  - Refactoring existing C++/CUDA code
  - As much as possible **performance portable code**: write the code once, and let the user run it on the available target platform with performance as good as possible.
  - Prefer a **high-level approach** among:
    - **Directive-based**: OpenACC, OpenMP
      ease of use, incremental approach, for large legacy code bases, ...
    - **External smart library** implementing **parallel programming patterns**
      (for, reduce, scan, ...):
      Kokkos, RAJA, agency, arrayFire libraries are such possibilities
      parallel programing patterns as 1\textsuperscript{st} class concepts, architecture adapted data containers, c++ integration / engineering, ...
    - **Other high-level approaches (more experimental)**: SYCL (Khronos Group standard), hpx (heavy use of new c++ standards (11,14,17): std::future, std::launch::async, distributed parallelism, ...)
Motivations of this work - 3

- **Computational science ground** - Computational Fluid Dynamics
  - High-order numerical schemes for compressible hydrodynamics
  - How fast the numerical solution converges to the reference solution when increase space resolution? \(|f - f_r| \leq h^{-N}\)

- From a discussion with Sacha Brun @ CEA, DAp,
  *A compressible high-order unstructured spectral difference code for stratified convection in rotating spherical shells* by Wiang, Liang and Miesch, JCP 2015

- **Spectral Difference Methods** is a high order scheme family \(\approx\) Discontinuous Galerkin
  - Spectral Difference Methods have simpler formulation, (should be) more efficient (esp. high order)
  - Discontinuous Galerkin, more accurate
C++ Kokkos library summary

- Framework for efficient **node-level parallelism (CPU, GPU, ...)**
- Provides
  - **Computationnal parallel patterns** (for, reduce, scan, ...)
  - **Hardware aware memory containers**: e.g. A **multi-dimensionnal data container with hardware adapted memory layout**
- Mostly a header library (C++ metaprograming)
C++ Kokkos library summary

- What do I mean by hardware aware memory containers?
  - Most commonly in a C/C++, multi-dimensionnal array access is done through index linearization (row or column-major in 2D):

  \[ index = i + nx \times j \]

- **Fortran** (column-major format) vs **C/C++** (row-major format) ⇒ memory layout should be hardware-aware configurable

- There is no reason to favour one layout versus the other
  - column-major is better for vectorization on CPU architecture
  - row-major is better for high throughput architecture e.g. GPU (memory coalescence)

- In Kokkos, one should/must avoid this index linearization at the user level, let Kokkos::View do this job (decided at compile-time, hardware adapted)
7-point Heat kernel with Kokkos - 1

- A single high-level parallel programming model for shared memory architectures (CPU, GPU, ...) ⇒ developer more productive
- 3d heat (stencil) kernel - SERIAL

// CPU version
for(int i=1; i<nx-1; ++i)
  for(int j=1; j<ny-1; ++j)
    for(int k=1; k<nz-1; ++k) {

      int index = k + j*nz + i*ny*nz

      y[index] = -5*x[index] +
          ( x[index-1] + x[index+1] +
            x[index-nz] + x[index+nz] +
            x[index-nz*ny] + x[index+nz*ny] );

    }
7-point Heat kernel with Kokkos - 2

- A **single high-level parallel programming model for shared memory architectures (CPU, GPU, ...)** ⇒ **developer more productive**
- 3d heat (stencil) kernel - **parallel KOKKOS**

```cpp
// naive Kokkos kernel - for CPU, GPU, ...
Range3d range ( {{0,0,0}}, {{nx,ny,nz}} );

parallel_for(range, KOKKOS_LAMBDA(int i,
                                      int j,
                                      int k) {

    y(i,j,k) = -5*x(i,j,k) +
               ( x(i-1,j ,k  ) + x(i+1,j ,k  ) +
                 x(i  ,j-1,k ) + x(i  ,j+1,k  ) +
                 x(i  ,j   ,k-1) + x(i  ,j   ,k+1) )
});
```
A **single high-level parallel programming model** for shared memory architectures (CPU, GPU, ...) ⇒ **developer more productive**

3d heat (stencil) kernel - **parallel KOKKOS - VECTORIZATION (CPU)**

```cpp
// Kokkos kernel to promote compiler vectorization, e.g. for Intel Skylake
Range2d range ( {{0,0}}, {{nx,ny}} );

// only parallelize the 2 outer loops (i and j)
parallel_for(range, KOKKOS_LAMBDA(int i,
                                  int j) {

    // create 1d subview along z axis - same as a 1d slice in fortran
    auto xij = subview(x,i,j,Kokkos::ALL());
    auto ...

    // only use 1d slices
    // let the compiler vectorize the k-loop
    for (int k=1; k<nz-1; ++k)
        yij(k) = -5*xij(k) +
          ( xij_1(k) + xij_2(k) +
            xij_3(k) + xij_4(k) +
            xij(k-1) + xij(k+1) );
});
```
Spectral difference methods solver - SDM

High-order SDM (Spectral Difference Methods)

- **Euler conservation law:**
  \[
  \frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} + M = 0
  \]

- SDM implementation up to order \( N = 6 \)

- \( N^d \) **solution (DoF) points**
  (Gauss-Chebyshev): \( x_s = \frac{1}{2} \left[ 1 - \cos \left( \frac{2s-1}{2N} \pi \right) \right] \)

- \( N^{d-1}(N+1) \) **flux points per direction**
  (Gauss-Legendre): use the roots of Legendre polynomial of degree \( N - 1 \) + the two end points

- Use **1D (tensor product) Lagrange polynomials** to represent solution.

reference:
Spectral difference method for compressible flow on unstructured grid mixed elements, Liang et al, JCP, vol 228, 2009

- Lagrange interpolation from **solution points** to **flux points** (and opposite flux to solution)

- Interpolation operators \texttt{sol2flux} and \texttt{flux2sol} are implemented via (small size) matrix-vector multiplication
Spectral difference methods solver - SDM

High-order SDM (Spectral Difference Method)

- Euler conservation law:
  \[ \frac{\partial Q}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} + M = 0 \]

- Use 1D (tensor product) Lagrange polynomials to represent solution:
  \[ Q(x, y) = \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} Q_{i,j} l_i(x) l_j(y) \]

  where \( l_i \) is the Lagrange polynomial such that \( l_i(x_j) = \delta_{i,j} \) and \( \delta_{i,j} \) are solution point locations.

  **step1:** Lagrange interpolation from solution points to flux points.
Spectral difference methods solver - SDM

High-order SDM (Spectral Difference Method)

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- **step2**: 
  - solve Riemann problem at end points
  - evaluate fluxes at **flux points**
  - interpolate fluxes at **solution points**
Spectral difference methods solver - SDM

High-order SDM (Spectral Difference Methods) ingredients

- **MPI + Kokkos parallelization** (Intel CPU, Nvidia GPU, ARM CPU, ...)
- **SSP (strong stability preserving) Runge-Kutta**
- **No artificial viscosity for stability.**
- **TVD limiter:**
  

- **Positivity preserving:** adapt ideas from DG to SDM

High-order numerical scheme comparison - SDM

SDM degree 2 - device Kokkos : : Cuda

SDM degree 4 - device Kokkos : : Cuda

resolution: 200$^2$, 400$^2$, 800$^2$

Performed on system ouessant (Nvidia GPU P100) at IDRIS/GENCI, France.
High-order numerical scheme comparison - SDM

- **SDM degree 2** vs **SDM degree 4** for Compressible Euler, TVD_RK3
- **same # DoFs**: $400^2$ degree 2 $\leftrightarrow$ $200^2$ degree 4
- **⚠️ high-order** ⇒ **CFL constraint more restrictive**
- **Time to solution (1 GPU, Pascal P100):**

<table>
<thead>
<tr>
<th>nb cells</th>
<th>#DoFs</th>
<th>degree</th>
<th>time (seconds)</th>
<th>speed (Dofs/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SDM 200$^2$</td>
<td>$400^2$</td>
<td>2</td>
<td>5</td>
<td>57</td>
</tr>
<tr>
<td>SDM 200$^2$</td>
<td>$800^2$</td>
<td>4</td>
<td>25</td>
<td>101</td>
</tr>
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<td>SDM 400$^2$</td>
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<tr>
<td>SDM 400$^2$</td>
<td>$1600^2$</td>
<td>4</td>
<td>156</td>
<td>127</td>
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<tr>
<td>SDM 800$^2$</td>
<td>$1600^2$</td>
<td>2</td>
<td>155</td>
<td>111</td>
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<td>SDM 800$^2$</td>
<td>$3200^2$</td>
<td>4</td>
<td>1150</td>
<td>138</td>
</tr>
</tbody>
</table>

- **SDM implementation is more efficient for high degree** (ratio compute/bandwidth higher ⇒ better for GPU)
Spectral Difference Method convergence

- Use the **isentropic vortex advection** test (**exact solution of compressible Euler flow**): periodic boundary conditions, vortex should return to the initial conditions at $t = 10.0$

\[
T = T_0 - \frac{(\gamma - 1) \times \beta^2}{8\gamma\pi^2} e^{1-r^2}
\]

\[
\rho = \rho_0 \frac{T^{\frac{1.0}{\gamma-1}}}{T_0}
\]

\[
\rho u = \rho \left( u_0 - (y - y_0) \frac{\beta}{2\pi} e^{0.5*(1.0-r^2)} \right)
\]

\[
\rho v = \rho \left( v_0 + (x - x_0) \frac{\beta}{2\pi} e^{0.5*(1.0-r^2)} \right)
\]

\[
\rho e = \frac{\rho T}{\gamma - 1} + \frac{1}{2} \rho (u^2 + v^2)
\]

reference:
https://www.cfd-online.com/Wiki/2-D_vortex_in_isentropic_flow
Spectral Difference Method convergence

L1 convergence of several spectral difference method schemes

- $h^{-2}$
- $h^{-3}$
- $h^{-4}$
- $h^{-5}$
- $h^{-6}$
2D SDM schemes - Intel Skylake vs Nvidia P100

- Test on skylake (dual socket) performed on alfven at CEA/IRFU.
- Skylake compiler is INTEL icpc 18.0
- Time integration is RK3
- **Pascal P100** is \( \sim x2.5 \) faster than Skylake (20 cores - dual socket - 2018)
- 2018 Skylake performs better than Nvidia K80
2D SDM - Intel Skylake vs ARM TX2 vs Nvidia P100

Introduction
High-order Spectral Difference schemes
Kokkos SDM versus RamsesGPU performances

2D SDM Performance

- Test on Skylake (dual socket) performed on a1fven at CEA/IRFU.
- Test on ARMv8TX2 (dual socket) performed on GENCI prototype @ CEA/DAM
- Test on P100 performed on GENCI prototype ouessant @ IDRIS
- Skylake compiler is GNU g++ 7.3
- ARMv8TX2 compiler is GNU g++ 7.1
- Time integration is RK3
**Effet of numerical viscosity:** illustration using same number of #Dof for the Kelvin-Helmholtz setup:

- SDM, degree3, $512^2$
- SDM, degree6, $256^2$
Spectral difference methods - numerical viscosity

- **Effet of numerical viscosity:** illustration using same number of #Dof for the Kelvin-Helmholtz setup:
  - SDM, degree3, $512^2$
  - MUSCL, Finite Volume, degree2, $1536^2$
Spectral difference methods - Jet test - High Mach flow

SDM scheme, Mach=27, comparison between order 3 and 4
CanoP - a parallel adaptive mesh refinement framework

- **What is CanoP?** *An applicative layer on top of* p4est *(distributed mesh management library)*

- CanoP *wraps the core* p4est *functionalities in a set of a few C++ class*

- CanoP *provides a template application framework:* new users don’t need to have a deep knowledge of how p4est works
  - parallel IO (HDF5+XDMF),
  - input parameter file management (LUA),
  - Init, border condition factory,
  - refine/coarsen indicator factory
List of solvers available in CanoP

- **Some pedagogical schemes** (for training new users):
  - finite volume scalar advection, **A. Fikl**
  - scalar viscous/inviscid Burgers equation, **Q. Wargnier, R. DiBattista, PK**
- **bifluid**: a two-phase flow model (**F. Drui, A. Fikl**, A. Larat; S. Kokh, M. Massot)
- **ramses**: monophasic Euler with 2nd order MUSCL-Hancock numerical scheme, for astrophysics applications, **PK**, poisson solver (**O. Iffrig, PK**), adaptive time stepping (**O. Iffrig**)
  - study angular momentum transport in accretion disk: **N. Brucy / W. Verdier** M1 intership, 2018, P. Hennebelle, O. Iffrig, PK)
- **Spray**: droplet evaporation modeling with a kinetic approach, **M. Essadki, PhD thesis**, M. Massot, S. De Chaisemartin
- **BN**: two-phase flow with Baer-Nunziato model (**F. Chen, PhD student**, A. Allou, JD Parisse, S. Kokh, PK)
- **MHD-KT**: WIP - magneto-hydrodynamics (MHD) with Kurganov-Tadmor discretization, multi-component plasma, solar physics, magnetic reconnection problem (**Q. Wargnier, PhD student**, M. Massot, PK)
- **ramsesRT**: WIP - Euler equations with radiative transfer (**H. Bloch, PhD student**, MDLS, 2018, P. Tremblin, M. Gonzalez, A. Audit)
CanoP: Two-phase flow solver

Experiment:

Simulations with canoP

Credit F. Drui (Phd, MDLS and ECP)
CanoP : self-gravitating accretion disk

Application to protoplanetary disk, N. Brucy, W. Verdier, Ml
intership with P. Hennebelle, O. Iffrig, PK
Gained expertise at designing / refactoring C++/CUDA applications using Kokkos
- much better global software design: separation of concerns
- high-level concept (no CUDA), focus on parallel computing pattern (for, reduce, scan, ...)
- data array access closely look like Fortran syntax
- C++11 + template: a key to generic cleaner code

Developed new high-order num schemes: SDM
Conclusion

- **Futur developments: towards multi-architecture AMR with Kokkos**
- Adapt SDM scheme to spherical geometry via coordinate transformation + mesh refinement *(CanoP)*
  \[ \partial_t Q + \partial_x F + \partial_y G + \partial_z H + M = 0 \Rightarrow \partial_t \tilde{Q} + \partial_\xi \tilde{F} + \partial_\eta \tilde{G} + \partial_\zeta \tilde{H} + \tilde{M} = 0 \]
  
- Implement SDM schemes for MHD
- **WIP: CanoP + Kokkos integration,** make it available to all solvers
- Towards **global solar dynamo and surface physics** with Sacha Brun *(CEA)*
2D SDM schemes - IBM Power8 vs Nvidia P100

- Time integration is RK3
- On average, Pascal P100 is $\times 2.8$ to $\times 3.0$ faster than Kepler K80 (single GPU), no special optimization, just rebuild with architecture flags.
- Pascal P100 is $\sim x5.8$ faster than Power8 - HT8
- by activating 8-way hyperthreading, Power8 version is 15 to 20% faster
- Performed on system ouessant at IDRIS/GENCI.