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

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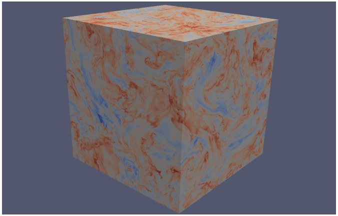
Content

- **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
- **Perpectives / Future applications and developments**
  - **SDM Integration into our AMR code** `CanoP`

Motivations of this work - 1

- code RAMSES-GPU : **Magneto-Rotational Instability, MHD turbulence, ...**
  - developped in CUDA/C++ for **astrophysics applications** on regular grid
  - $\sim$ 70k lines of code (out of which $\sim$ 16k in CUDA)
  - developed between **2009 and 2014** !
- Since then **both GPU hardware/sofware have tremendously evolved** (in orders of magnitude in memory bandwidth, number of registers per SM, c++11, ...) $\Rightarrow$ 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 ?**

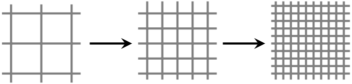


Motivations of this work - 2

- **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^{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

- **Computationnal 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 familly** $\simeq$ **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):

$$index = i + nx * j$$

- **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 througput 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 programing model for shared memory** architectures (CPU, GPU, ...) ⇒ **developper 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 programing model for shared memory** architectures (CPU, GPU, ...) ⇒ **developper more productive**
- 3d heat (stencil) kernel - **parallel KOKKOS**

```
// 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) );
});
```

7-point Heat kernel with Kokkos - 3

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

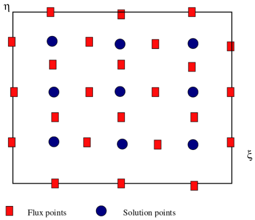
```
// Kokkos kernel to promote compiler vectorization, e.g. for Intel Skylake
Range2d range ( {{0,0}}, {{nx,ny}} );

// 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 `sol2flux` and `flux2sol` are implemented via (small size) matrix-vector multiplication

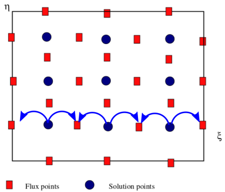
Spectral difference methods solver - SDM

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:

$$Q(x,y) = \sum_{i=0}^{i=N-1} \sum_{j=0}^{j=N-1} Q_{i,j} l_i(x) l_j(y)$$

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)

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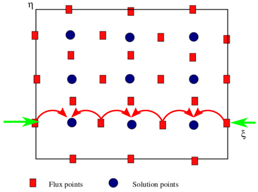
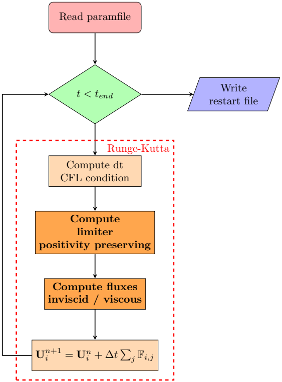


- **step2:**
  - solve Riemann problem at end points
  - evaluate fluxes at **flux points**
  - interpolate fluxes at **solution points**

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 articial viscosity for stability.**
- **TVD limiter:** A Spectral Difference Method for the Euler and Navier-Stokes Equations on Unstructured Meshes, by Wang et al., J. Sci. Comp., 2007
- **Positivity preserving:** adapt ideas from DG to SDM On positivity-preserving high order discontinuous Galerkin schemes for compressible Euler equations on rectangular meshes, Zhang et al, JCP 2010, vol. 229, Issue 23.

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** ⇔ 200^2 **degree 4**
- ⚠ **high-order** ⇒ **CFL constraint more restrictive**
- Time to solution (1 GPU, Pascal P100):

nb cells	#DoFs	degree	time(seconds)	speed (Dofs/s)
SDM 200^2	400^2	2	5	57
SDM 200^2	800^2	4	25	101
SDM 400^2	800^2	2	23	93
SDM 400^2	1600^2	4	156	127
SDM 800^2	1600^2	2	155	111
SDM 800^2	3200^2	4	1150	138

- **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 returns to the initial conditions at $t = 10.0$

$$T = T_0 - \frac{(\gamma - 1) * \beta^2}{8\gamma\pi^2} e^{1-r^2}$$

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

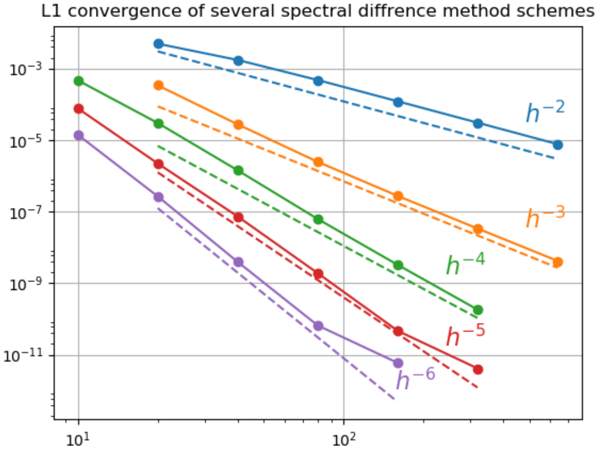
$$\rho u = \rho \left(u_0 - (y - y_0) \frac{\beta}{2\pi} e^{0.5*(1.0-r^2)} \right)$$

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

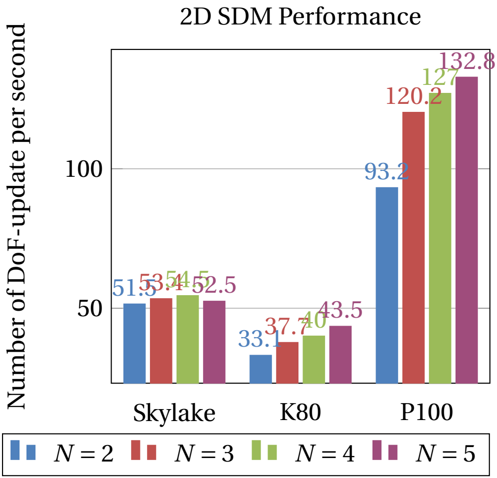
$$\rho e = \frac{\rho T}{\gamma - 1} + \frac{1}{2} \rho (u^2 + v^2)$$

reference:
https://www.cfd-online.com/Wiki/2-D_vortex_in_isentropic_flow

Spectral Difference Method convergence

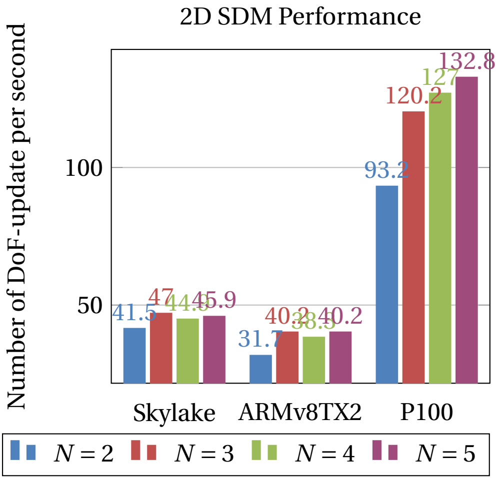


2D SDM schemes - Intel Skylake vs Nvidia P100



- 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 ∼ $x2.5$ faster than **Skylake** (20 cores - dual socket - 2018)
- 2018 Skylake performs better than Nvidia K80

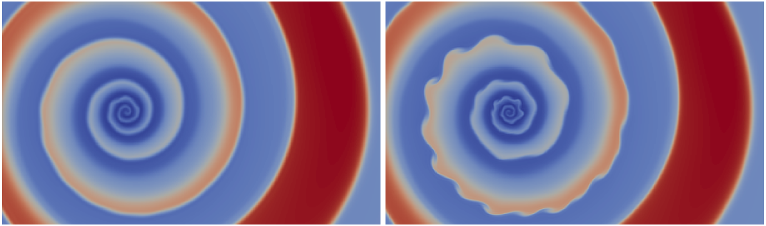
2D SDM - Intel Skylake vs ARM TX2 vs Nvidia P100



- Test on skylake (dual socket) performed on `alfven` 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

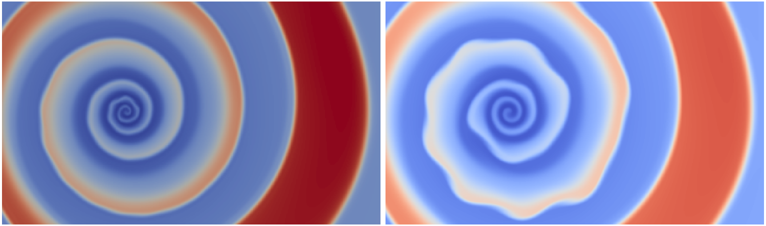
Spectral difference methods - numerical viscosity

- **Effet of numerical viscosity:** illustration using same number of #Dof for the Kelvin-Helmholtz setup:
  - SDM, degree3, 512^2
  - SDM, degree6, 256^2



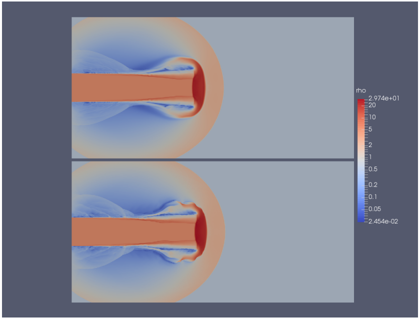
Spectral difference methods - numerical viscosity

- **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



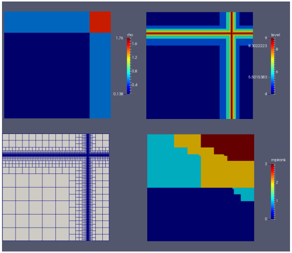
Spectral difference methods - Jet test - High Mach flow

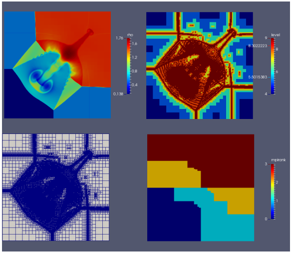
SDM scheme, Mach=27, comparison between order 3 and 4



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 conditon factory,
  - refine/coarsen indicator factory



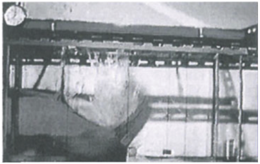


List of solvers available in CanoP

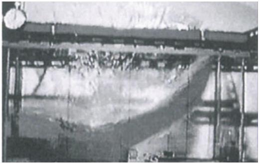
- **Some pedagogical schemes** (for training new users):
  - finite volume scalar advection, **A. Fikl**
  - scalar viscous/invicid Burgers equation, **Q. Wargnier, R. DiBattista, PK**
- **bifluid**: a two-phase flow model (**F. Drui, A. Fikl**, A. Larat; S. Kokh, M. Massot)
- **ramses**: monophasic 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:



0.2s



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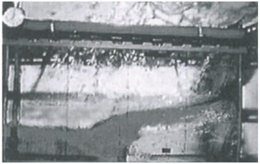

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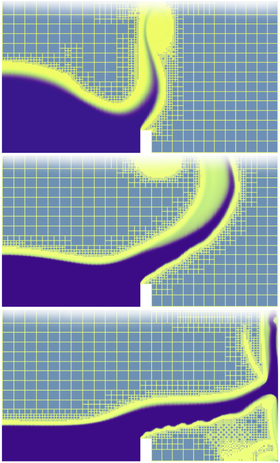
Credit F. Golay

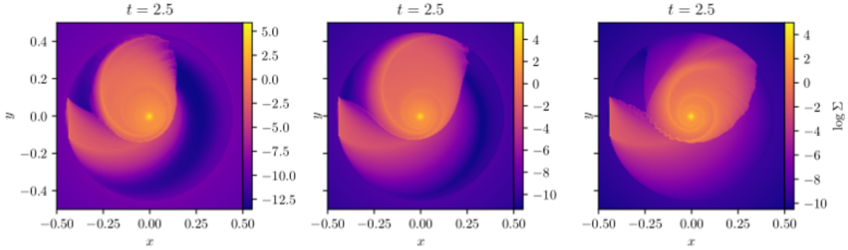
Simulations with canoP



Credit F. Drui (Phd, MDLS and ECP)

CanoP : self-gravitating accretion disk

Application to protoplanetary disk, N. Brucy, W. Verdier, M1 intership with P. Hennebelle, O. Iffrig, PK

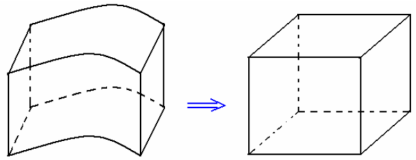


Conclusion

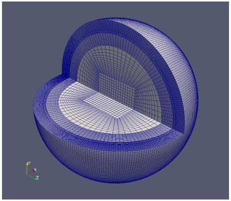
- **Gained expertise at designing / refactoring C++/CUDA applications using Kokkos**
  - much better global software design : **separation of concerns**
  - high-level concept (no CUDA), focus on **parallel computing pattern** (`for, reduce, scan, ...`)
  - data array access closely look like Fortran syntax
  - C++11 + template: a key to generic cleaner code
- **Developped new high-order num schemes: SDM**

Conclusion

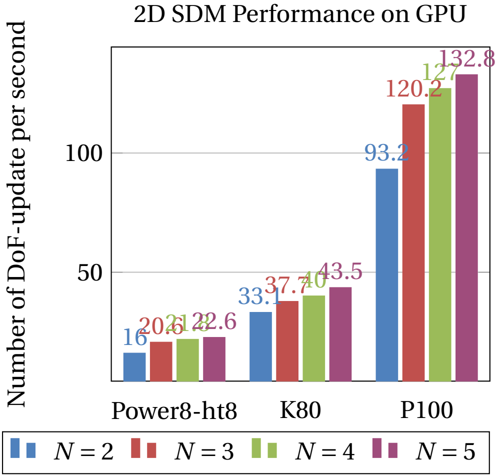
- **Futur developments: towards multi-architecture AMR with Kokkos**
- **adapt SDM scheme to spherical geometry via coordinate transformation + mesh refinement** (`CanoP`)
  $\partial_t Q + \partial_x F + \partial_y G + \partial_z H + M = 0 \Rightarrow \partial_t \tilde{Q} + \partial_\xi \tilde{F} + \partial_\eta \tilde{G} + \partial_\zeta \tilde{H} + \tilde{M} = 0$



- 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 ~ $x5.8$ faster than **Power8 - HT8**
- by activating 8-way hyperthreading, Power8 version is 15 to 20% faster
- Performed on system `ouessant` at **IDRIS/GENCI**.