Modèle et méthode numérique d’ordres élevés pour la dynamique d’un spray polydisperse. Implémentation sur architectures hétérogènes à l’aide du runtime StarPU

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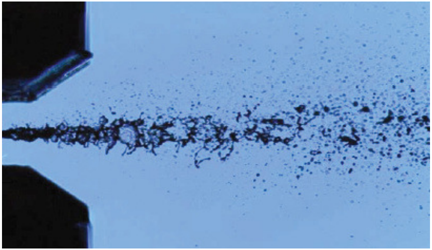
Outline

Context, Model and Numerics

Task-Driven Programming

Results

Context: atomization

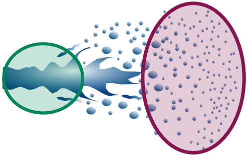


Source: C. Dumouchel, CORIA Rouen.

Source: P. Edwards, Stanford

Separated phases

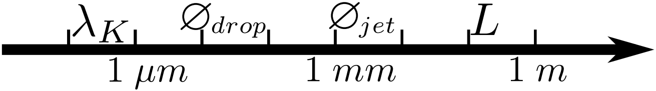
- Smooth interface,
- Instabilities $\lambda \sim 1mm$.
- $Re_\lambda \sim 10^4$, $We_\lambda >> 1$.



Source: J. Réveillon

Disperse phase

- Polydisperse cloud ($d \sim 10\mu m$).
- Drag, collisions, evap., reaction...
- $Re_d < 100, We_d < We_c$



Very large range of scales ($\times 10^6$).

Eulerian moment method

Williams-Boltzmann ([4]) Equation: $f(t, \vec{\mathbf{x}}, \vec{c}, S)$

$$\boxed{\underbrace{\frac{\partial f}{\partial t} + \frac{\partial}{\partial \vec{\mathbf{x}}} \cdot (\vec{c} f)}_{\text{Transport}} + \underbrace{\frac{\partial}{\partial \vec{c}} \cdot \left(\vec{\mathsf{F}} f\right)}_{\text{Acceleration}} + \underbrace{\frac{\partial R_S f}{\partial S}}_{\text{Evap.}} = 0}$$

Velocity Moments [3]

- $\mathcal{M}_m = \int \vec{c}^{\,m} f(t, \vec{\mathbf{x}}, \vec{c}, S) \mathrm{d}\vec{c}$
- Monokinetic: $\psi(\vec{c}, \vec{u}) = \delta(\vec{c} - \vec{u})$

$$\begin{cases} \partial_t n + \partial_{\vec{\mathbf{x}}} \cdot (n\vec{u}) & = \quad K\partial_S n, \\ \partial_t n\vec{u} + \partial_{\vec{\mathbf{x}}} \cdot (n\vec{u} \otimes \vec{u}) & = \quad n\frac{\vec{u}_g - \vec{u}}{\tau_p} + K\partial_S n\vec{u} \end{cases}$$

Fractional Size Moments [2]

- $m_{k/2} = \int_0^{S_{max}} S^{k/2} n(t, \vec{\mathbf{x}}, S) dS$

$$\begin{cases} \Sigma_d \widetilde{G}_d & = & 4\pi \, m_{0/2}, \\ \Sigma_d \widetilde{H}_d & = & 2\sqrt{\pi} \, m_{1/2}, \\ \Sigma_d & = & m_{2/2}, \\ \alpha_d & = & \frac{1}{6\sqrt{\pi}} \, m_{3/2}. \end{cases}$$

Eulerian moment method

Simplifying Hypotheses:

$f(t, \vec{\mathbf{x}}, \vec{c}, S) = n(t, \vec{\mathbf{x}}, S).\psi(\vec{c}, \vec{u})$, **$\vec{\mathbf{F}}$ linear,** $R_S(S) = -K$.

$$\boxed{\frac{\partial f}{\partial t} + \frac{\partial}{\partial \vec{\mathbf{x}}} \cdot (\vec{c} f) = \frac{\partial}{\partial \vec{c}} \cdot \left(\frac{\vec{c} - \vec{u}_g}{\tau_p} f \right) + K \partial_S f}$$

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$$\boxed{\frac{\partial f}{\partial t} + \frac{\partial}{\partial \vec{\mathbf{x}}}\cdot(\vec{c}f) = \frac{\partial}{\partial \vec{c}}\cdot\left(\frac{\vec{c}-\vec{u}_g}{\tau_p}f\right) + K\partial_S f}$$

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System of equations, (Essadki [1, 2])

Fractional moment model: $f(t, \vec{\mathbf{x}}, \vec{c}, S) = n(t, \vec{\mathbf{x}}, S)\delta(\vec{c} - \vec{u}),\ \tau_p = \theta S$

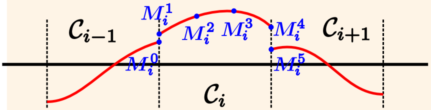
$$
\left\{
\begin{array}{ccccccc}
\partial_t m_{0/2} & + & \partial_{\vec{x}} \cdot \left(m_{0/2}\vec{u}\right) & = & -\mathrm{K}\, n(t, \vec{\mathbf{x}}, S=0), & & \\
\partial_t m_{1/2} & + & \partial_{\vec{x}} \cdot \left(m_{1/2}\vec{u}\right) & = & -\frac{\mathrm{K}}{2}\, m_{-1/2}, & & \\
\partial_t m_{2/2} & + & \partial_{\vec{x}} \cdot \left(m_{2/2}\vec{u}\right) & = & -\mathrm{K}\, m_{0/2}, & & \\
\partial_t m_{3/2} & + & \partial_{\vec{x}} \cdot \left(m_{3/2}\vec{u}\right) & = & -\frac{3\mathrm{K}}{2}\, m_{1/2}, & & \\
 & & & & & & \\
\partial_t \left(m_{2/2}\vec{u}\right) & + & \partial_{\vec{x}} \cdot \left(m_{2/2}\vec{u} \otimes \vec{u}\right) & = & -\mathrm{K}\, m_{0/2}\vec{u} & + & m_{0/2}\frac{\vec{u}_g - \vec{u}}{\theta},
\end{array}
\right.
$$

Operator splitting

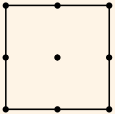
$$
\begin{array}{rcl}
\partial_t \boldsymbol{M} + \partial_{\vec{x}}.\boldsymbol{\mathcal{F}}(\boldsymbol{M}) & = & 0, \\
\mathrm{d}_t \boldsymbol{M} & = & -\boldsymbol{\mathcal{K}}\left[n(t, \vec{\mathbf{x}}, S)\right], \\
\mathrm{d}_t (m_{2/2}\vec{u}) & = & m_{0/2}\frac{\vec{u}_g - \vec{u}}{\theta}.
\end{array}
$$

Advection: Numerical Discretization

Polynomial Discretization



$$M_h(x) = \sum_{i \in \mathcal{M}_h} \sum_{k \in \mathcal{C}_i} M_i^k \varphi_i^k(x)$$

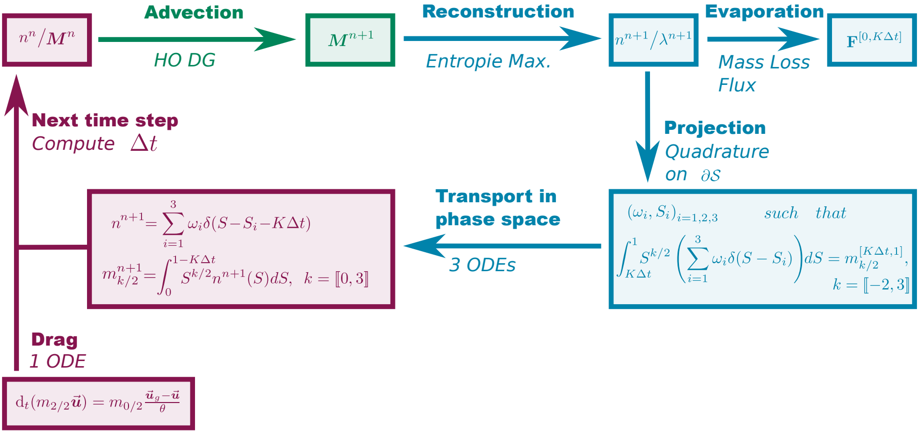


Discontinuous Galerkin Formulation

$$\partial_t M + \partial_x \mathcal{F}(M) = 0 \quad \Rightarrow \quad \int_{\mathcal{C}_i} \left[\partial_t M_h + \partial_x \mathcal{F}(M_h) = 0 \right] \times \varphi_i^l$$

$$\underbrace{|\mathcal{C}_i| \sum_{k \in \mathcal{C}_i} \left(\int_{\mathcal{C}_i} \varphi_i^l \varphi_i^k \right) \partial_t M_i^k}_{\text{Time Evolution}} + \underbrace{\int_{\partial \mathcal{C}_i} \mathcal{F}^*(M_i^{ext}, M_i^{int}, \vec{\mathbf{n}})}_{\text{Numerical Flux (Surface)}} = \underbrace{\int_{\mathcal{C}_i} \mathcal{F}(M_h).\vec{\nabla} \varphi_i^l d\mathbf{x}.}_{\text{Volumic Term}}$$

Global numerical procedure



Outline

Heterogeneous Architechures (Top500)

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Supercomputing Center in Wuxi China	**Sunway TaihuLight** - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
2	National Super Computer Center in Guangzhou China	**Tianhe-2 (MilkyWay-2)** - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
3	DOE/SC/Oak Ridge National Laboratory United States	**Titan** - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
4	DOE/NNSA/LLNL United States	**Sequoia** - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
5	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660

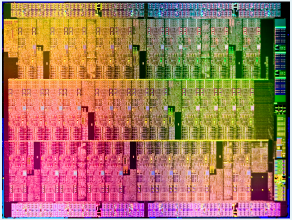
Heterogeneous Architechures

Graphic Cards (GPU)

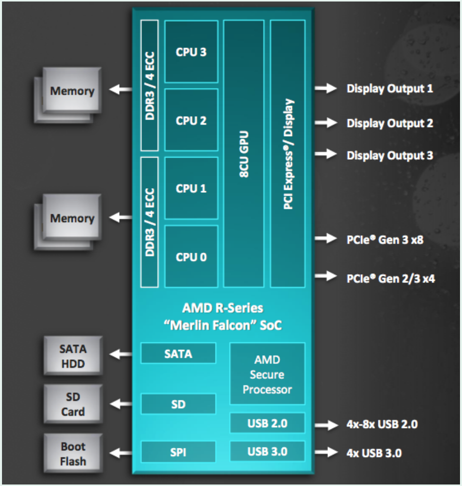
Jaguar Specs (2011)	
Compute Nodes	18,688
Login & I/O Nodes	256
Memory per node	16 GB
# of Opteron cores	224,256
# of NVIDIA K20 "Kepler" accelerators (2013)	N/A
Total System Memory	300 TB
Total System Peak Performance	2.3 Petaflops

Titan Specs (2012)	
Compute Nodes	18,688
Login & I/O Nodes	512
Memory per node	32 GB + 6 GB
# of Opteron cores	299,008
# of NVIDIA K20 "Kepler" accelerators (2013)	18,688
Total System Memory	710 TB
Total System Peak Performance	20+ Petaflops

Many Integrated Core (MIC)



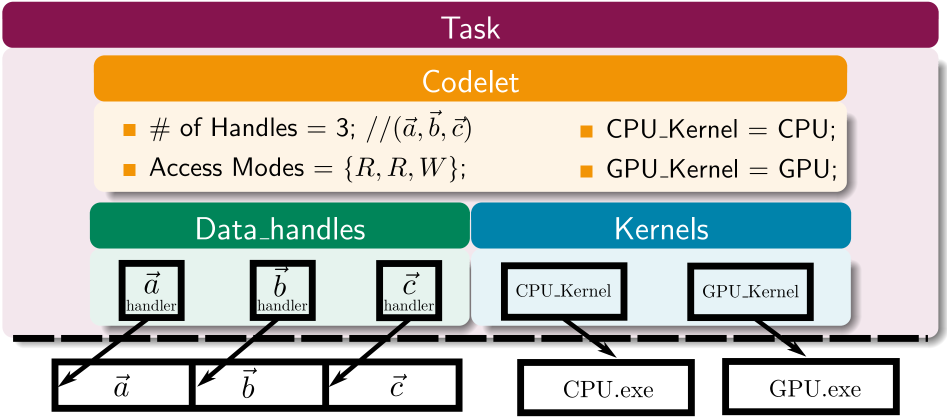
System on Chips (SoC)



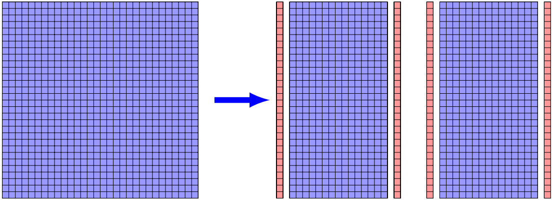
Task-driven Programming: a StarPU Lexicon

$$Task \quad = \quad \underbrace{\color{orange}{Codelet}}_{\text{Task Descriptor}} + \underbrace{\color{teal}{Kernels}}_{\text{Executed Code}} + \underbrace{\color{green}{Data\_handles}}_{\text{Memory Management}}$$

Example: $\vec{c} = \vec{a} + \vec{b}$.



Description of the Tasks



Time Stepping

- `InitialCondition`
- `StoreU0`
- `CheckTimeStep`
- `RKUpdate`

Advection Update

- `Interpolate`
- `InnerResiduals`
- `Projection`
- `BorderResiduals`

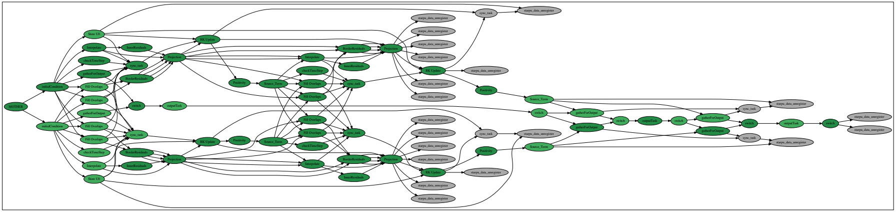
Other

- `FillOverlaps`
- `Drag`
- `Evaporation`
- `Positivity`

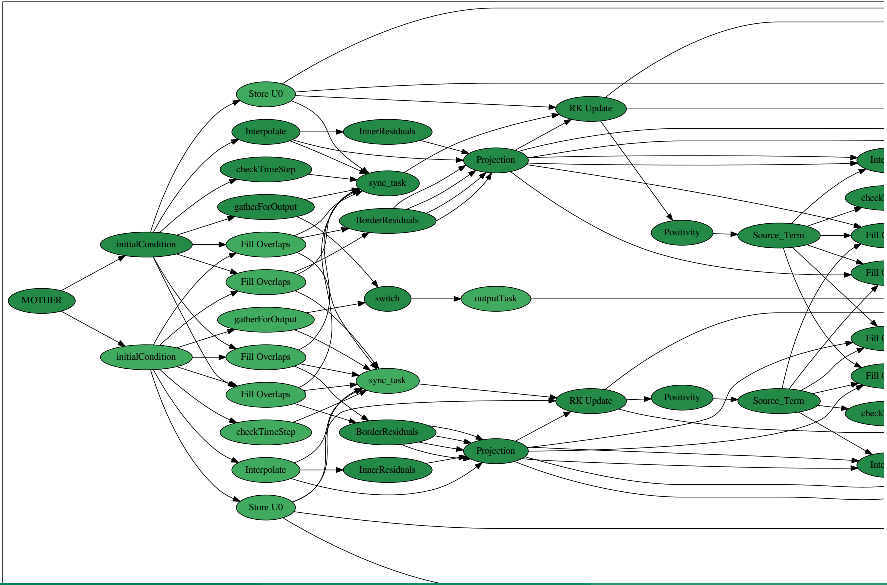
Input/Output

- `gatherForOutput`
- `OutputTask`

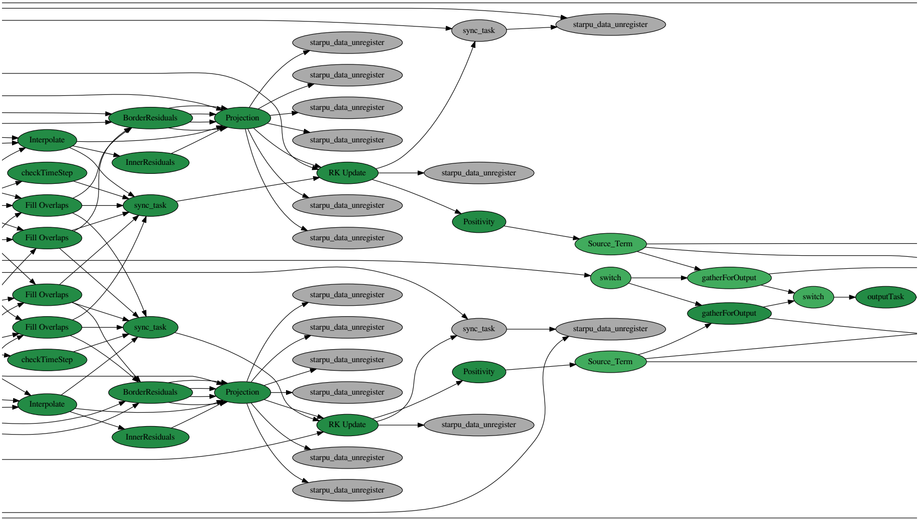
DG-$\mathbb{P}^1$ task diagram



DG-$\mathbb{P}^1$ task diagram

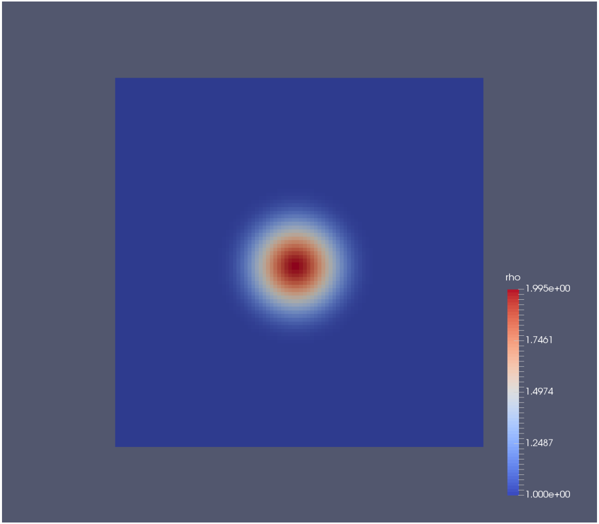


DG-$\mathbb{P}^1$ task diagram

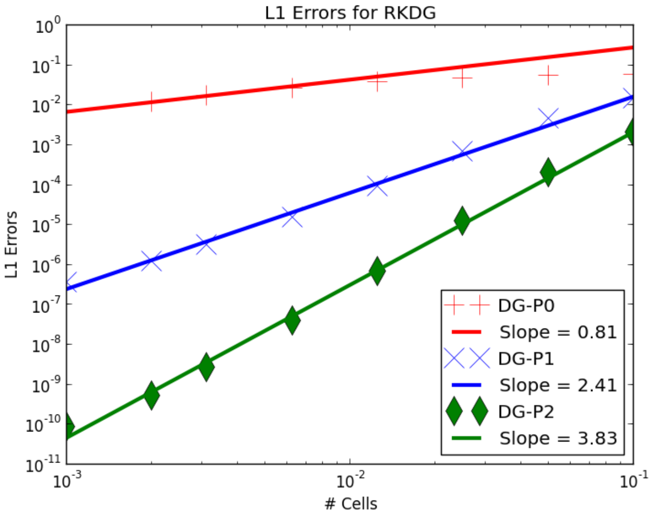


Outline

Simple Advection

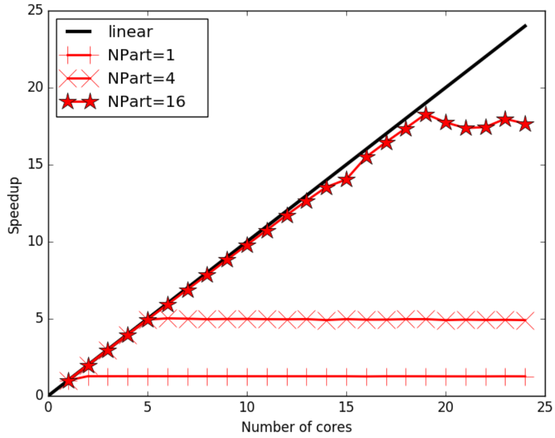


Numerical Convergence



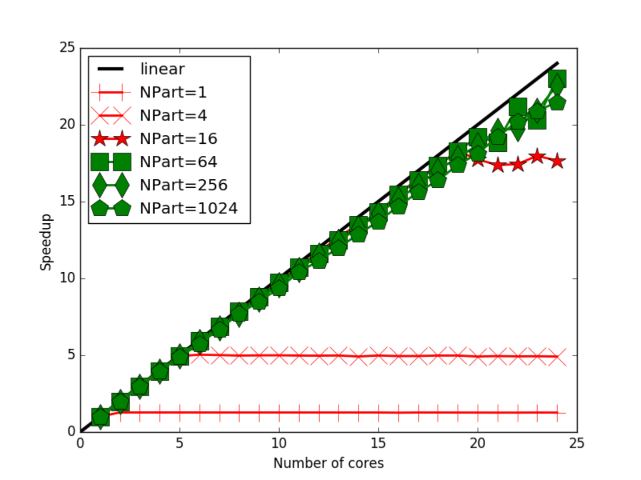
Parrallel efficiency

Number of Tasks Limited Cases



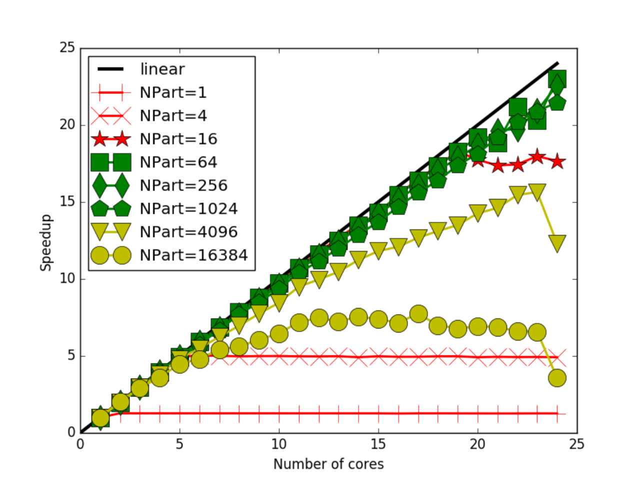
Parrallel efficiency

Correct Scalling



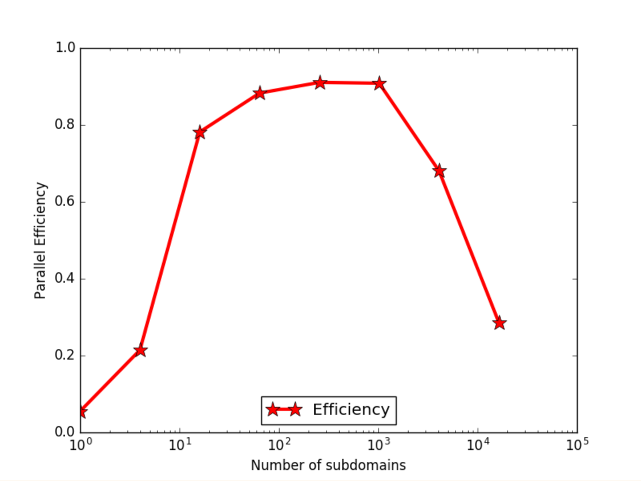
Parrallel efficiency

Task Over-head Limitation



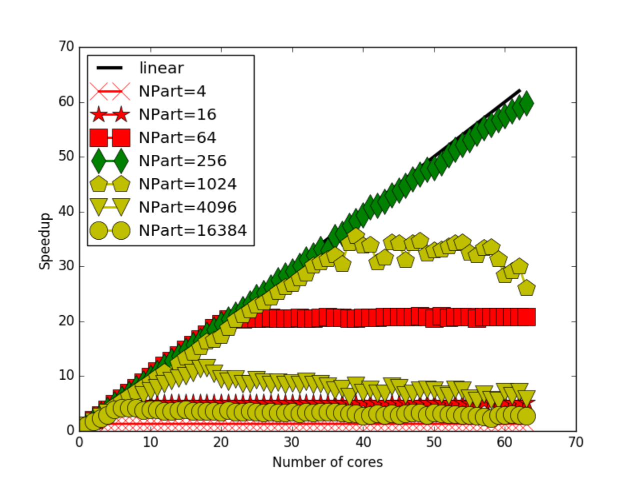
Parrallel efficiency

Efficiency



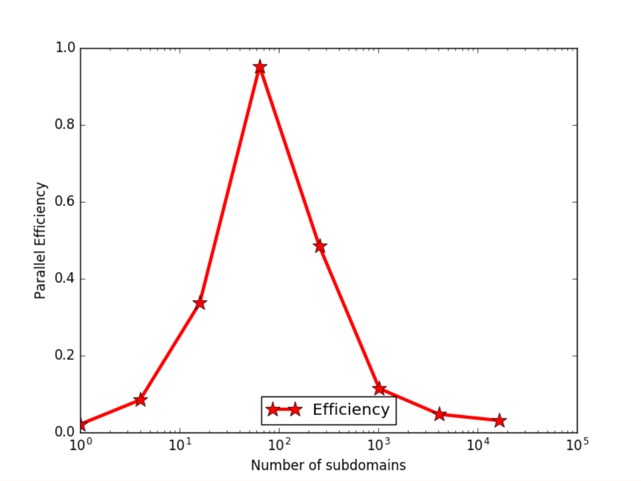
Parrallel efficiency

Knights Landing Xeon Phi, 64 procs

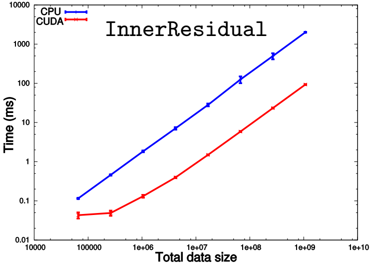


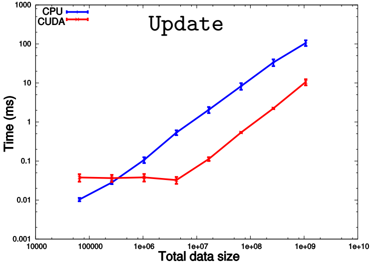
Parrallel efficiency

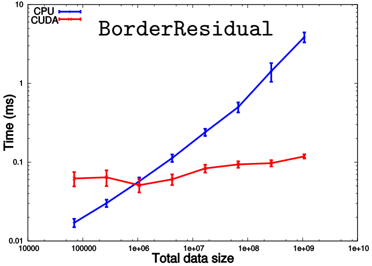
Efficiency

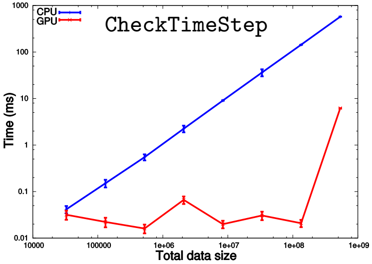


GPU: Some tasks are faster. . .

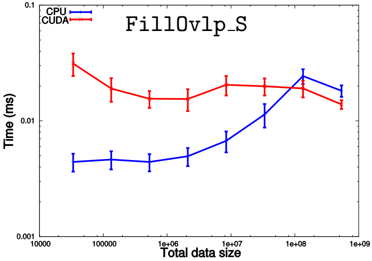


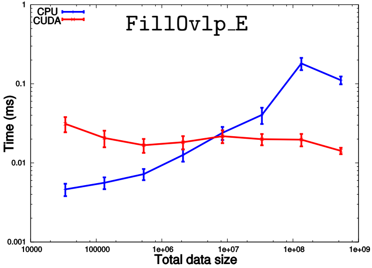


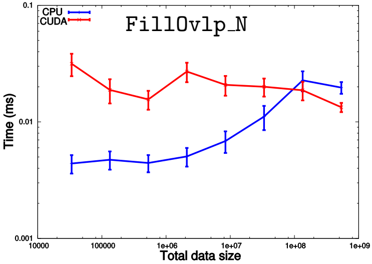


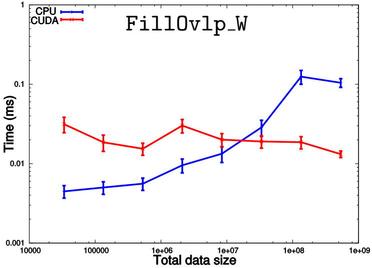


GPU: Some tasks are not!

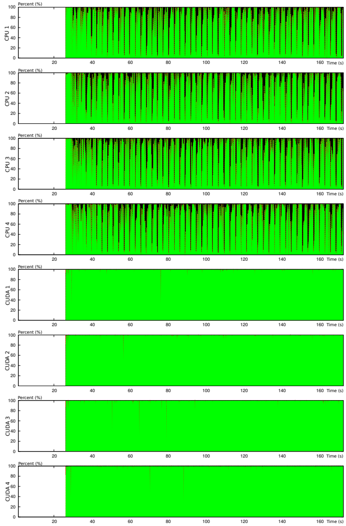




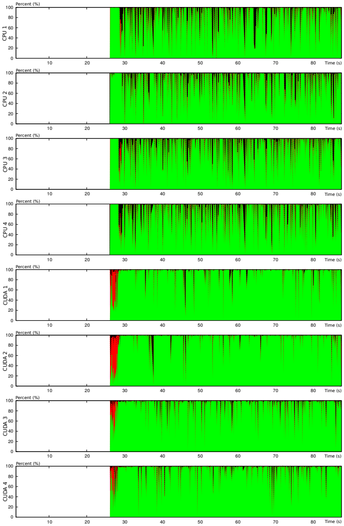




Scheduler Choice

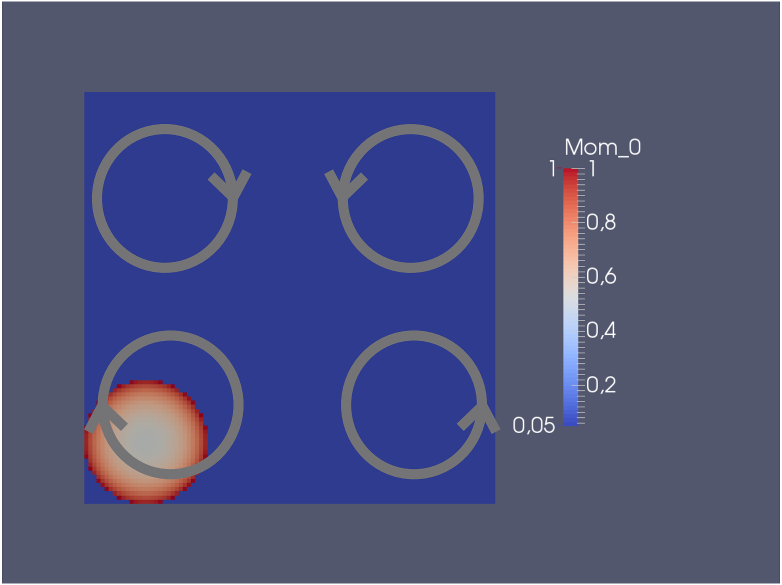


`eager` scheduler. Final time = 146s

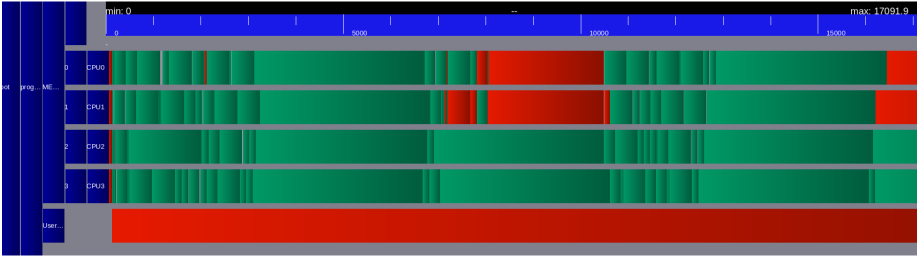


`dmda` scheduler. Final time = 61s

Evaporating spray: Taylor-Green vortex

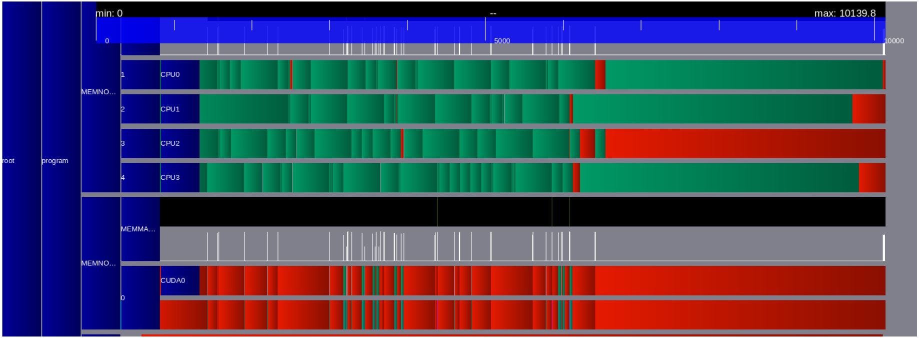


GPU Gain (6 domains, 4 CPUs, 2 GPUs)



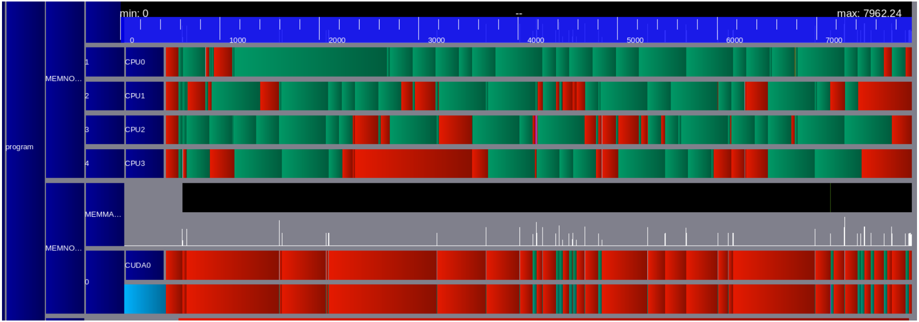
Gant Diagram on CPUs only. Final time = 17.09s.

GPU Gain (6 domains, 4 CPUs, 2 GPUs)



Some tasks are given to the GPUs. Final time = 10.13s.

GPU Gain (6 domains, 4 CPUs, 2 GPUs)



Better choice of scheduler. Final time = 7.96s.

Future Work

- MPI Extension
- Arbitrary High Order DG
- Look at other frameworks (Kokkos, DAGuE, ORCCA, . . .)
- Integration within Aerosol

Acknowledgment

- IFPEn
- EDMH
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- Plafrim
- Université Aix-Marseille
- CEMRACS 2016 organizing commitee

References

[1] M. Essadki, S. de Chaisemartin, M. Massot, F. Laurent, A. Larat, and S. Jay.
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