A High-Order Discontinuous Galerkin Solver with Dynamic Adaptive Mesh Refinement to Simulate Cloud Formation Processes

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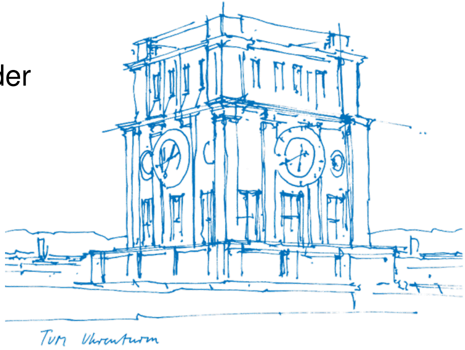


The ExaHyPE-Engine[1]

Goals

A PDE ‘engine’ (‘engine’ as in ‘game engine’).
Provides numerics/mesh for user-defined applications.
Allow **smaller** teams to realize **large-scale** simulations of hyperbolic PDEs.

Capabilities

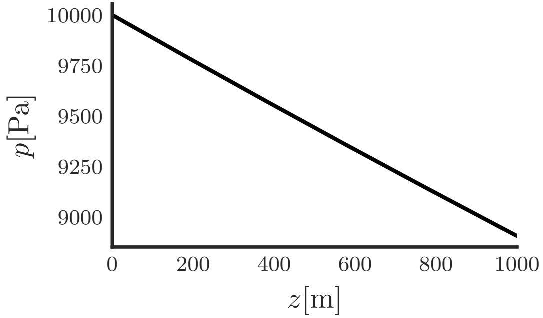
- Numerics: ADER-DG (optimized) & Finite Volume
- Dynamic Adaptive Mesh Refinement (AMR)
- Hybrid MPI + Intel TBB Parallelization

Available (**open-source**) at `exahype.eu`

[1] A. Reinarz et al. ‘ExaHyPE: An Engine for Parallel Dynamically Adaptive Simulations of Wave Problems’. In: *arXiv e-prints* (May 2019).

Two Bubbles: Hydrostatic Equilibrium[2]

- Air is in hydrostatic equilibrium: Gravitational force and pressure-gradient force are **exactly balanced**.
- Constant potential temperature (temperature normalized by pressure) with larger, warm bubble and small, cold bubble on top.



Background pressure in equilibrium

[2] A. Robert. 'Bubble Convection Experiments with a Semi-implicit Formulation of the Euler Equations'. In: *Journal of the Atmospheric Sciences* 50.13 (July 1993).

Two Bubbles: Simulation

The ADER-DG Approach[3]

Solve **hyperbolic conservation laws** of the form

$$\frac{\partial}{\partial_t}\boldsymbol{Q} + \nabla \cdot \boldsymbol{F}(\boldsymbol{Q}) = \boldsymbol{S}(\boldsymbol{x}, t, \boldsymbol{Q}) \tag{1}$$

with $\boldsymbol{Q}$ vector of conserved variables, $\boldsymbol{x}$ position, t time, $\nabla \cdot \boldsymbol{F}(\boldsymbol{Q})$ divergence of flux and $\boldsymbol{S}(\boldsymbol{x}, t, \boldsymbol{Q})$ source term.

Discontinuous Galerkin (DG) divides domain into disjoint elements, approximates solutions by piecewise-polynomials. Elements are connected by solving the Riemann problem.

ADER-Approach uses space-time polynomials for time integration instead of Runge-Kutta procedures.

[3] M. Dumbser et al. 'A unified framework for the construction of one-step finite volume and discontinuous Galerkin schemes on unstructured meshes'. In: *Journal of Computational Physics* 227.18 (Sept. 2008).

The Navier-Stokes Equations

$$\frac{\partial}{\partial t}\underbrace{\begin{pmatrix}\rho\\ \rho\boldsymbol{v}\\ \rho E\end{pmatrix}}_{\boldsymbol{Q}} + \nabla\cdot\underbrace{\begin{pmatrix}\rho\boldsymbol{v}\\ \boldsymbol{v}\otimes\rho\boldsymbol{v} + \boldsymbol{I}p + \boldsymbol{\sigma}(\boldsymbol{Q},\nabla\boldsymbol{Q})\\ \boldsymbol{v}\cdot(\boldsymbol{I}\rho E + \boldsymbol{I}p + \boldsymbol{\sigma}(\boldsymbol{Q},\nabla\boldsymbol{Q})) - \kappa\nabla T\end{pmatrix}}_{\boldsymbol{F}(\boldsymbol{Q},\nabla\boldsymbol{Q})} = \underbrace{\begin{pmatrix}S_\rho\\ -\boldsymbol{k}\rho g\\ S_{\rho E}\end{pmatrix}}_{\boldsymbol{S}(\boldsymbol{Q},\boldsymbol{x},t)} \tag{2}$$

With ρ density of fluid, $\rho\boldsymbol{v}$ velocity density, ρE energy density, and $\boldsymbol{k}$ unit vector in z-direction.

Pressure with gravitational term $p(\boldsymbol{Q}, z)$, stress tensor $\boldsymbol{\sigma}$, heat diffusion $\kappa\nabla T$ with temperature T.

Trick: cancel out constant background pressure in flux and source.

Problem: Not hyperbolic

ExaHyPE (thus far) solves equations of the form (e.g. Euler):

$$\mathrm{P}\frac{\partial \boldsymbol{Q}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{Q}) + \sum_{i=1}^{d} \mathrm{B}_i(\mathrm{Q})\frac{\partial \boldsymbol{Q}}{\partial x_i} = \boldsymbol{S}(\boldsymbol{x}, t, \boldsymbol{Q}) \tag{3}$$

We have:

$$\mathrm{P}\frac{\partial \boldsymbol{Q}}{\partial t} + \nabla \cdot \boldsymbol{F}(\boldsymbol{Q}, \nabla \boldsymbol{Q}) + \sum_{i=1}^{d} \mathrm{B}_i(\mathrm{Q})\frac{\partial \boldsymbol{Q}}{\partial x_i} = \boldsymbol{S}(\boldsymbol{x}, t, \boldsymbol{Q}) \tag{4}$$

Solution: Modify numerical flux (Riemann solver), time step size (CFL-condition) and boundary conditions to **allow diffusive terms**[4].
No explicit discretization of gradient $\nabla \boldsymbol{Q}$.

[4] M. Dumbser. 'Arbitrary high order PNPM schemes on unstructured meshes for the compressible Navier–Stokes equations'. In: *Computers & Fluids* 39.1 (Jan. 2010); G. Gassner, F. Lörcher and C.-D. Munz. 'A Discontinuous Galerkin Scheme based on a Space-Time Expansion II. Viscous Flow Equations in Multi Dimensions'. In: *Journal of Scientific Computing* 34.3 (2008).

Adaptive Mesh Refinement: Indicator

Total Variation

$\boldsymbol{f}(\boldsymbol{x}) : \mathbb{R}^{N_\text{vars}} \to \mathbb{R}$ maps solution to indicator variable (here: potential temperature).
Total variation of $\boldsymbol{f}$ for a cell C:

$$\text{TV}\left[f(\boldsymbol{x})\right] = \| \int_C \left| \nabla f\left(\boldsymbol{x}\right) \right| \mathrm{d}\boldsymbol{x} \, \|_1 \tag{5}$$

Intuition

- **Large** total variation $\mapsto$ interesting
- **Small** total variation $\mapsto$ boring

'Edge detection' of numerical solution

Adaptive Mesh Refinement: Feature Detection

Chebyshev's inequality

$$\mathbb{P}(|X - \mu| \geq c\sigma) \leq {}^{1}/_{c^2} \tag{6}$$

Mean μ, standard deviation σ, constant c
Better bounds exist with further assumptions on distribution.

Intuition

Not all variables are sufficiently special.
Feature detection

Adaptive Mesh Refinement: Global Criterion

Criterion

$$\text{evaluate-refinement}(\boldsymbol{Q}, \mu, \sigma) = \begin{cases} \text{refine} & \text{if } \operatorname{TV}\left(\boldsymbol{f}(\boldsymbol{Q})\right) \geq \mu + T_{\text{refine}}\sigma \\ \text{delete} & \text{if } \operatorname{TV}\left(\boldsymbol{f}(\boldsymbol{Q})\right) < \mu + T_{\text{delete}}\sigma \\ \text{keep} & \text{otherwise} \end{cases} \tag{7}$$

Choose T_{refine} and T_{delete} according to cost-accuracy trade-off.
Computation of mean μ, standard deviation σ with **stable**, pairwise reduction[5].

[5] T. F. Chan, G. H. Golub and R. J. LeVeque. 'Updating Formulae and a Pairwise Algorithm for Computing Sample Variances'. In: *COMPSTAT 1982 5th Symposium held at Toulouse 1982*. 1982.

AMR vs. Fully Refined Grid

Settings

AMR Mesh with sizes from $1000/81\,\mathrm{m} \approx 12.35\,\mathrm{m}$ to $1000/9\,\mathrm{m} \approx 111.11\,\mathrm{m}$.
Two levels of dynamic AMR.
$T_{\text{refine}} = 2.5$ and $T_{\text{delete}} = -0.5$.

Reference $81 \times 81 = 6561$ cells.

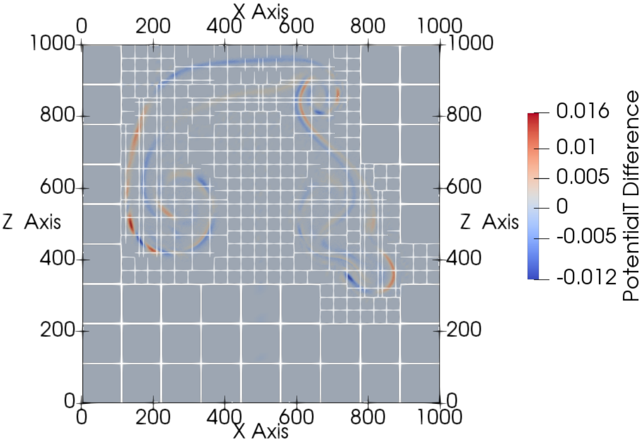
Both polynomial order 6. Viscosity $\mu = 0.01$. Simulate until $t_{\text{end}} = 600\,\mathrm{s}$.

Results

AMR grid: 1953 cells. Less than **30%** of full grid!
Relative L_2-error between AMR and fully refined: 2.6×10^{-6}.

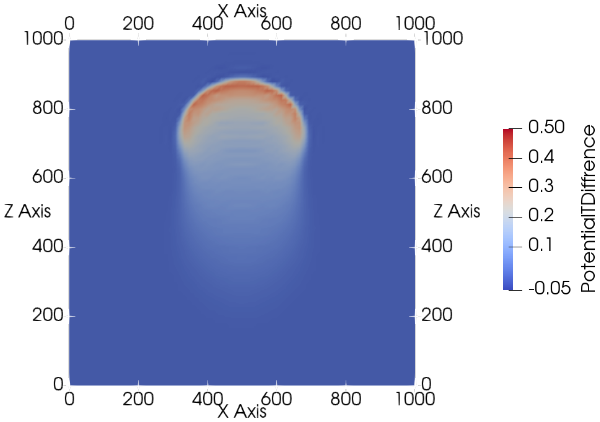
AMR vs. Fully Refined Grid: Grid

AMR vs. Fully Refined Grid: Error



Potential temperature of fully refined solution minus AMR solution.

3D Cosine Bubble[6]



- Polynomial Order 3
- 25^3 cells
- Time: 400 s
- Viscosity: $\mu = 0.05$

[6] J. F. Kelly and F. X. Giraldo. 'Continuous and discontinuous Galerkin methods for a scalable three-dimensional nonhydrostatic atmospheric model: Limited-area mode'. In: *Journal of Computational Physics* 231.24 (Oct. 2012).

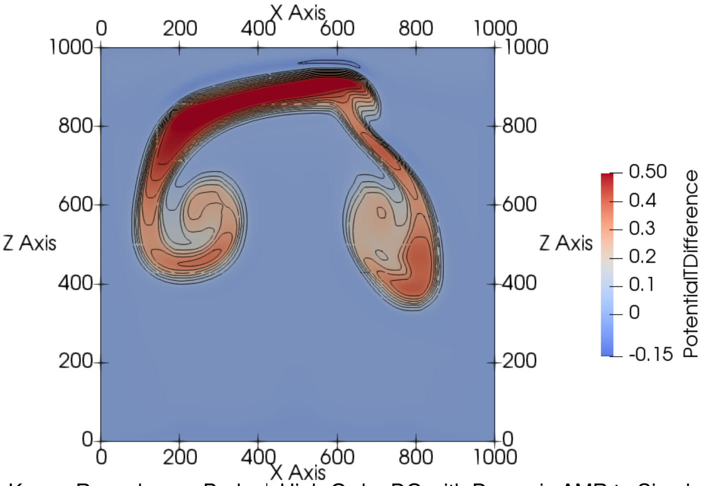
MUSCL-Hancock Scheme

Finite Volume scheme: store only **cell averages**
Reconstruction of linear function
Second order in time and space[7]
Stabilized with (Van Albada[8]) slope limiter
Very stable, larger **numerical viscosity**

[7] B. van Leer. ‘Towards the ultimate conservative difference scheme. V. A second-order sequel to Godunov’s method’. In: *Journal of Computational Physics* 32.1 (July 1979).

[8] G. Van Albada, B. Van Leer and W. Roberts. ‘A comparative study of computational methods in cosmic gas dynamics’. In: *Upwind and High-Resolution Schemes*. 1997.

Two Bubbles: Finite Volume



- 7^2 patches with 90^2 cells each
- Euler equations ($\mu = 0$)
- Numerical viscosity smooths solution

Summary

- **ADER-DG** can be used to simulate Navier-Stokes equations.
- Total variation **measures edges** of numerical solution.
- Chebyshev's criterion finds **interesting cells**.
- Combination of both **accurately tracks** cloud.
- AMR solution is close to fully refined solution but needs **fewer** cells.
- **Artificial viscosity** of Finite Volume has a similar effect as **physical viscosity** of Navier-Stokes.

Acknowledgments

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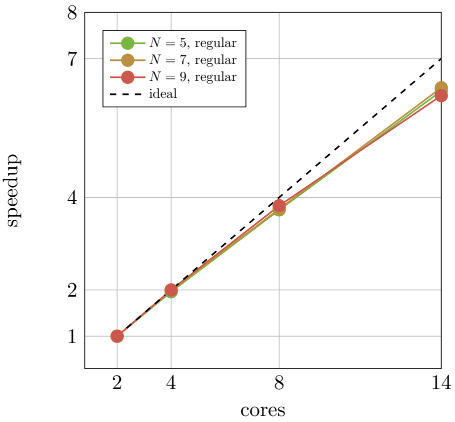
Shared-Memory Scaling (from[9])



[9] A. Reinarz et al. 'ExaHyPE: An Engine for Parallel Dynamically Adaptive Simulations of Wave Problems'. In: *arXiv e-prints* (May 2019).