Multigrid - raiders of the lost algorithm at exascale

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Research Questions & Project Goals

- How can exascale systems exploit the high arithmetic intensity of high-order DG while minimising time-to-solution?
- Can mathematically optimal MG deliver optimal performance at exascale?
- Can expensive assembly be overcome?
- Can we deliver MG as toolbox from which developers can pick and assemble their MG within their code base?
  (mature, holistic MG solvers do exist already)
- Can we integrate MG into our demonstrators such that we can do larger time steps (IMEX) or solve constraints more accurately?

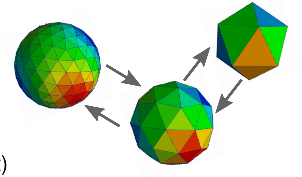
PROJECT GOALS

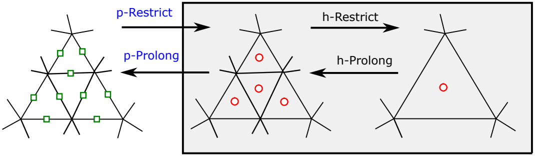
1. Combine ExaHyPE's higher-order discretisation with MG
2. Pair MG with spatial and temporal adaptive discretisations
3. Balance pros and cons of algebraic vs. geometric and matrix-free vs. matrix-based MG
4. Simulation of binary black holes

Multigrid

Why multigrid?

- **Optimal scaling**: Cost $\propto$ number of unknowns crucial for exascale
- **Parallelisation** well studied
- Compatible with **local mesh refinement**
- Supports **high-order finite elements** (p-refinement)
- Adapted to (Interior Penalty) **DG** [Bastian, Blatt, Scheichl (2012)] and **Hybridisable DG** [Cockburn, Dubois, Gopalakrishnan, Tan (2014)]



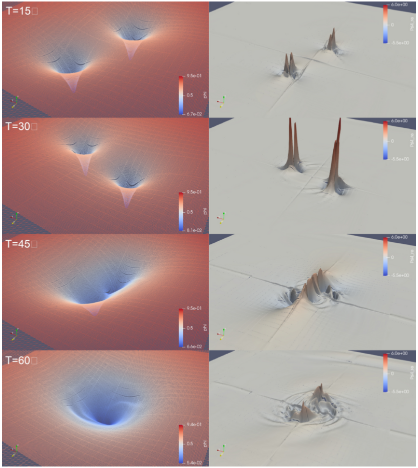


Challenges

- Coupling with **space-time** discretisation in ADER-DG, local timestepping
- Fast, **matrix-free** implementation [Bastian, Müller, Müthing, Piatkowski (2019)]
- Reputation of being difficult to implement (but is it?)

Challenges

- Methodological Challenges
  - Assembly expensive
  - Interplay MG-DG (hybridisation)
  - Higher order in time (ADER-DG)
  - Increase concurrency (additive/asynchronous) → new MG ingredients
- Science Challenges
  - Simulate binary black holes (CCZ4)
  - Switch to implicit/explicit time stepping
  - → larger time steps
  - → accurate constraints
  - → alternative models of gravity
- Software Challenges
  - Integrate into existing code bases
  - Pick n select rather than adopt to 3rd party code → open source toolbox



Current Progress

Durham University
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ExCALIBUR 10

- Developed **flexible Python - Peano interface** for DG matrix assembly from weak forms:

$$\underbrace{\int_\Omega \nabla u \cdot \nabla v \, dx}_{\text{weak form}} \xrightarrow{\text{Python}} \underbrace{a_{ij}^{F \mapsfrom C}, a_{ij}^{C \mapsfrom C}}_{\text{cell-local matrices}} \xrightarrow{\text{Peano}} \underbrace{\begin{pmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \\ \vdots & & \ddots \end{pmatrix}}_{\text{global matrix}}$$

  $\Rightarrow$ Interior Penalty DG, Hybridisable DG, ...
- Recreate Poisson equation solver with conforming FE* and DG discretisations
  - Aim to tackle Mixed/Hybrid DG next, as these are known to be compatible with Multigrid
- Instrumented Peano with PETSc backend
  - Allows us to use out-of-the-box solvers for validation
- Implemented matrix-free conforming FE Poisson solvers, with aim to develop this further

*lowest order, piecewise linear continuous finite elements

Next Steps

- Develop HDG with out-of-the-box solver to establish baseline
- Develop matrix-free formulations alongside
- Once hybridised DG methods are working with PETSc solver and with own matrix-free methods, begin to introduce multigrid, using previous results as a baseline
- Introduce ADER-DG for space-time discretisation

References

- Betteridge, J., Gibson, T.H., Graham, I.G. and Müller, E.H., 2021. Multigrid preconditioners for the hybridised discontinuous Galerkin discretisation of the shallow water equations. Journal of Computational Physics
- Cockburn, B., Dubois, O., Gopalakrishnan, J. and Tan, S., 2014. Multigrid for an HDG method. IMA Journal of Numerical Analysis
- Bastian, P., Müller, E.H., Müthing, S. and Piatkowski, M., 2019. Matrix-free multigrid block-preconditioners for higher order discontinuous Galerkin discretisations. Journal of Computational Physics, 394, pp.417-439.
- Bastian, P., Blatt, M. and Scheichl, R., 2012. Algebraic multigrid for discontinuous Galerkin discretizations of heterogeneous elliptic problems. Numerical Linear Algebra with Applications, 19(2), pp.367-388.