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YOF

Spencer Sherwin Imperial College London David Moxey University of Exeter



Spectral/hp element Modelling

Outline

- Overview of Nektar++
- Challenges for modelling
 - Stabilisation and robustness
 - Performance
 - Mesh generation
- Applications
 - Hasegawa-Wakatani equations
 - Incompressible Flow Modelling









Computational cost ~ P⁴ Computational error ~ h^P







P accuracy



'Exact' solution



Bolis, Cantwell, Kirby, Sherwin Int J Num Meth. fluid, 2014

Nektar++: Spectral/hp element modelling

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Open Source & Continual Integration

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ctest: 450 small tests which can also act as demos



buildbot. nektar.info

Linux: CentOS, Debian, Fedora, Open SUSE Mac: Mavericks, Snow Leopard Windows: XP, 7

Quasi-3D

 A. Bolis, C. Cantwell, D. Moxey, D. Serson, and S. Sherwin, "An adaptable parallel algorithm for the direct numerical simulation of incompressible turbulent flows using a fourier spectral/hp element method and mpi virtual topologies," Computer physics communications, 2016.



Generalised Mapping

 D. Serson, J. Meneghini, and S. Sherwin, "Velocity-correction schemes for the incompressible Navier-Stokes equations in general coordinate systems," Journal of computational physics, 316, 243-254, 2016.









Adaptive Polynomial Order

• Example: Naca0012 with Re=50,000 and alpha=15 ($P_{min} = 2$, $P_{max} = 9$)







Variable P also available in 3D





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iLES/uDNS





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Wave interaction & Wave trapping











Spectral vanishing viscosity

Tadmor, (89) Maday, Kaber & Tadmor (93) :



Eigenanalysis informed SVV

R. Moura, J. Peiro, S. Sherwin

- Mengaldo G, De Grazia D, Moura RC, Sherwin SJ, 2018, Spatial eigensolution analysis of energy-stable flux reconstruction schemes and influence of the numerical flux on accuracy and robustness, Journal of Computational Physics, 358, 1-20
- Mengaldo G, Moura RC, Giralda B, Peiró J, Sherwin SJ 2017, Spatial eigensolution analysis of discontinuous Galerkin schemes with practical insights for under-resolved computations and implicit LES, Computers and Fluids, 0045-7930
- Moura RC, Sherwin SJ, Peiro J, 2016, Eigensolution analysis of spectral/hp continuous Galerkin approximations to advection-diffusion problems: Insights into spectral vanishing viscosity, Journal of Computational Physics, 307, 401-422
- Moura RC, Sherwin SJ, Peiro J, 2015, Linear dispersion-diffusion analysis and its application to under-resolved turbulence simulations using discontinuous Galerkin spectral/hp methods, Journal of Computational Physics, 298, 695-710,



Temporal analysis: (k real find $\omega = \omega(k)$)





DG-like properties of CG+SVV



R. C. Moura, S. J. Sherwin, and J. Peiró, J. computational physics, 307. 401-422, 2016.



Temporal analysis: (k real find $\omega = \omega(k)$)





Spatial analysis: (ω real find $k = k(\omega)$)





Spatial analysis: (ω real find $k = k(\omega)$)





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Example of CG or DG (Hyper upwinding) problem



DG-like properties of CG+SVV



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- Match log-log slope near origin
- Match CG+SVV at P with DG at P-2 to remove bubbles
- Have higher diffusion at higher frequencies
- SVV coefficient scaled to maintain mesh Peclet no.

0.6 2.5 0.5 0.4 0.3 Real (k* h) / P .t. Imag (k* h)/P $\mathbf{P}=\mathbf{3}$ $\mathbf{P}=\mathbf{3}$ $\mathbf{P} = \mathbf{8}$ $\mathbf{P} = \mathbf{8}$ 0.5 -0.1 -0.2 $\mathbf{P} = \mathbf{8}$ $\mathbf{P}=\mathbf{3}$ $\mathbf{P} = \mathbf{3}$ -0.3 1.5 3.5 0.5 1.5 3.5 0.5 2 2.5 3 0 1 2 2.5 3 1 ϖ h / P ϖ h / P

Reflected waves have strong diffusion enforced as part of optimisation





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Challenges in modern HPC

- Ideally: we want really fast single-core nodes with lots of memory bandwidth
- Instead, we get lots of FLOPS using many cores per node, lower clock speed
- Complicated memory hierarchies
- Very limited memory bandwidth

Need algorithms with high arithmetic intensities that can use available FLOPS: high-order methods

Performance



Imperial College Implementations





Moxey et al. CMAME, 2016



Exploiting vectorisation

- Key to achieving peak performance is exploiting vectorisation (SSE, FMA, AVX, AVX-512, ...)
- Recent work has focused on achieving this with tuned kernels for key operators
- Particular focus on 'matrix-free' approaches that avoid construction of a matrix perelement



Data layout

Natural to consider data laid out element by element





Data layout

Instead, could consider blocks that are equivalent to processor vector width (e.g. AVX = 4 doubles)





Exploiting vectorisation

- Perform multiple operations in a single cycle
- Combine with:
 - Hand-written loops for sum-factorisation
 - Explicit intrinsics for vector operations
 - C++ templating to allow for loop unrolling





Significant performance gains against benchmark solutions (libxsmm, Intel MKL) for backward transform

Still ongoing work!





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High-order mesh



B-Rep

High-order mesh generation

Curving coarse meshes leads to invalid elements Most existing MG packages cannot deal with this









Surface mesh sliding

Often surface mesh will never yield valid volume to be generated: solve by sliding elements on the CAD surface





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Imperial College DLR F6 engine













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Hasegawa-Wakatani

- Model for drift wave instability in fusion edge turbulence simulations
- State variables: φ is the electrostatic potential, ζ is vorticity, n is the perturbed number density
- Parameters: α is the adiabaticity operator, κ is a constant density gradient scale-length
- Determine how to implement these equations



Hasegawa-Wakatani equations

$$\frac{\partial \zeta}{\partial t} + \{\phi, \zeta\} = \alpha(\phi - n) - \mu \nabla^4 \zeta$$
$$\frac{\partial n}{\partial t} + \{\phi, n\} = \alpha(\phi - n) - \kappa \frac{\partial \phi}{\partial y} - \mu \nabla^4 n$$
$$\nabla^2 \phi = \zeta$$

{a,b} is the canonical Poisson bracket operator

$$\{a,b\} = \frac{\partial a}{\partial x} \frac{\partial b}{\partial y} - \frac{\partial a}{\partial y} \frac{\partial b}{\partial x}$$



Hasegawa-Wakatani equations

- Mixture of convective term and elliptic solve for ζ from ϕ
- Therefore can leverage **mixed** formulation: CG for elliptic solve, DG for convection
- Since we're using DG, omit the hyper diffusion term for stability
- Rewrite in conservative form
- Leverage Nektar++ framework for rapid development

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Hasegawa-Wakatani equations

$$\mathbf{u}_E = \left(-\frac{\partial \phi}{\partial y'}, \frac{\partial \phi}{\partial x}\right)$$

$$\{\phi, \zeta\} = \nabla \cdot (\mathbf{u}_E \zeta)$$
$$\{n, \zeta\} = \nabla \cdot (\mathbf{u}_E n)$$

Apply DG formulation with \mathbf{u}_E and upwinding

Sample output



 spectral/hp simulation of the Hasegawa-Wakatani equations

- Joint CG/DG implementation
- Simple model for drift-wave turbulence

Navier-Stokes Time-stepping Navier–Stokes: $\frac{\partial_t \mathbf{u} + \mathbf{N}(\mathbf{u})}{\nabla \cdot \mathbf{u}} = -\nabla p + \nu \nabla^2 \mathbf{u}$ $\mathbf{N}(\mathbf{u}) \models \mathbf{u} \cdot \nabla \mathbf{u} \\ \mathbf{u}^n$ $\mathbf{u} \cdot \nabla \mathbf{u}$ Velocity correction scheme (aka stiffly stable): Orszag, Israeli, Deville (90), Karnaidakis Israeli, Orszag (1991), Guermond & Shen (2003) \mathbf{u}^* Advection: $u^* = -\sum_{q} \alpha_q \mathbf{u}^{n-q} - \Delta t \sum_{q} \beta_q \mathbf{N}(\mathbf{u}^{n-q})$ $\nu \nabla^2 \mathbf{u} - \nabla p = \mathbf{f}$ $\nabla \cdot \mathbf{u} = 0$ $\nabla^2 p^{n+1} = \frac{1}{\Lambda t} \nabla \cdot \mathbf{u}^*$ n^{n+1} Pressure Poisson: n = n + 1 $\nabla^2 \mathbf{u}^{n+1} - \frac{\alpha_0}{\nu \Lambda t} \mathbf{u}^{n+1} = -\frac{\mathbf{u}^*}{\nu \Lambda t} + \frac{1}{\nu} \nabla p^{n+1}$ Helmholtz: Imperial College

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Meshing for F1 applications



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F1 Geometry

McLəren

Elemental ro P = 4







Moxey, Turner, Jassim, Taylor Sherwin Design 3: +270% Downforce

Imperial College Turbomachinery application



T106 using NekMesh

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Re=1.5M







Summary/Confessions

- Applying spectral/hp element techniques to challenging industrial flow problems.
- Compactness of methods attractive on current/ emerging HPC architecture
- Accurate, transient flow modelling is an enabling technology for high-end engineering/physics.
- But ...
 - Meshing for 3D geometries is a specialist skill
 - Robustness has required careful analysis and probably requires more!





