Discontinuous Galerkin Methods

Part 1: Discretisation and efficient implementation

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Outline

DGM/IP methods

Framework : governing equations

Consider a generic set of N convection-diffusion-reaction equations

$$\mathcal{L}_m(\tilde{u}) = \frac{\partial \tilde{u}_m}{\partial t} + \nabla \cdot \vec{f}_m(\tilde{u}) + \nabla \cdot \vec{d}_m(\tilde{u}, \nabla \tilde{u}) + S_m(\tilde{u}, \nabla \tilde{u}) = 0$$

where

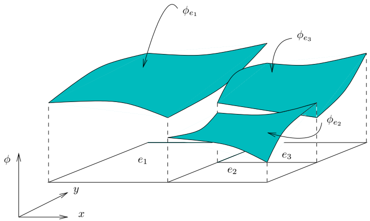
- $\tilde{u} \in (\mathbb{R}(\Omega))^N$ the state vector
- $\vec{f}$ the convective flux vector
- $\vec{d}$ the diffusive flux vector
- S the source term

with the first order expansion of $\vec{d}$

$$\vec{d}^k_m = \mathbf{D}^{kl}_{mn} \frac{\partial \tilde{u}_n}{\partial x^l} + \mathcal{O}((\nabla \tilde{u})^2)$$

DGM/IP methods

Framework : basic ingredients



Approximation $u \approx \tilde{u}$ on $\mathcal{E} = \cup e \approx \Omega$ is

- regular (polynomial, harmonic functions, waves, ...) on each element

$$u|_e \in (\mathcal{P}(e))^N$$

- not $\mathcal{C}_0$ continuous $\leftrightarrow$ standard FEM

$$u \in (\Phi(\mathcal{E}))^N = \cup (\mathcal{P}(e))^N$$

Galerkin formulation

$$a(u, v) \hat{=} \int_\Omega v_m \cdot \mathcal{L}_m(u) dV = 0 \ , \ \forall v \in \Phi$$

DGM/IP methods

Framework : Galerkin variational formulation

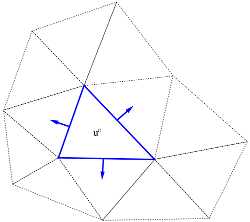
Take generic conservation equation

$$\frac{\partial \tilde{u}_m}{\partial t} + \nabla \cdot \vec{g}_m = 0$$

Naive Galerkin :

$$\int_\Omega v_m \frac{\partial u_m}{\partial t} dV + \int_\Omega v_m \nabla \cdot \vec{g}_m dV = 0 \ , \ \ \forall v \in \Phi$$

$$= \sum_e \int_e v_m \frac{\partial u_m}{\partial t} dV + \sum_e \left(- \int_e \nabla v_m \cdot \vec{g}_m dV + \oint_{\partial e} v_m \vec{g}_m \cdot \vec{n} dS \right)$$

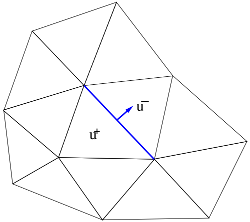


DGM/IP methods

Framework : Galerkin variational formulation

Take generic conservation equation

$$\frac{\partial \tilde{u}_m}{\partial t} + \nabla \cdot \vec{g}_m = 0$$



Naive Galerkin :

$$\int_\Omega v_m \frac{\partial u_m}{\partial t} dV + \int_\Omega v_m \nabla \cdot \vec{g}_m dV = 0 \ , \ \ \forall v \in \Phi$$

$$= \sum_e \int_e v_m \frac{\partial u_m}{\partial t} dV + \sum_e \left(- \int_e \nabla v_m \cdot \vec{g}_m dV + \oint_{\partial e} v_m \vec{g}_m \cdot \vec{n} dS \right)$$

Define operators on boundary (*trace*) wrt normal $\vec{n}^+ = \vec{n} = -\vec{n}^-$

$$[\![a]\!] = a^+ \vec{n}^+ + a^- \vec{n}^-$$

$$[\![\vec{g}]\!] = \vec{g}^+ \cdot \vec{n}^+ + \vec{g}^- \cdot \vec{n}^-$$

$$\{\!\{a\}\!\} = (a^+ + a^-)/2$$

Then we continue

$$\sum_e \int_e v_m \frac{\partial u_m}{\partial t} dV - \sum_e \int_e \nabla v_m \cdot \vec{g}_m dV + \sum_f \int_f [\![v_m]\!] \{\!\{\vec{g}_m\}\!\} + [\![\vec{g}_m]\!] \{\!\{v_m\}\!\} dS$$

DGM/IP methods

Framework : interface fluxes

The DGM discretisation is then defined as

$$\sum_e v_m \frac{\partial u_m}{\partial t} - \sum_e \int_e \nabla v_m \cdot \vec{g}_m dV + \sum_f \int_f \gamma_m(\tilde{u}^+, \tilde{u}^-, v^+, v^-, \vec{n}) dS = 0 \ , \ \ \forall v \in \Phi$$

Requirements for γ

- stability
- consistent as $u^+ = u^- = \tilde{u}$

$$\begin{aligned}\lim_{h \to 0} \int_f \vec{g}_m^* dS &= \int_f [[v_m \vec{g}_m(\tilde{u})]].\, dS \\ &= \int_f [[v_m]] \{\{\vec{g}_m(\tilde{u})\}\} + \{\{v_m\}\} [[\vec{g}_m(\tilde{u})]] \, dS \\ &= \int_f [[v_m]] \, \vec{g}_m(\tilde{u}) dS\end{aligned}$$

- conservative : let $W_m = 1 \ \ \forall x \in e \ , \ \ W_m = 0 \ \ \forall x \notin e$

$$a(W_m, u_m) = -\oint_e \gamma_m(u^+, u^-, 1, 0, \vec{n}) dS \Rightarrow \gamma_m(u^+, u^-, 1, 0, \vec{n}) = -\gamma_m(u^-, u^+, 1, 0, -\vec{n})$$

DGM/IP methods

Framework : local reinterpretation

Global formulation

$$\sum_e \int_e v_m \frac{\partial u_m}{\partial t} dV - \sum_e \int_e \nabla v_m \cdot \vec{g}_m dV + \sum_f \int_f \gamma_m(\tilde{u}^+, \tilde{u}^-, v^+, v^-, \vec{n}) dS = 0 \ , \ \ \forall v \in \Phi$$

Choose basis for Φ composed of locally supported v^e and expand

$$u = \sum_e u^e$$

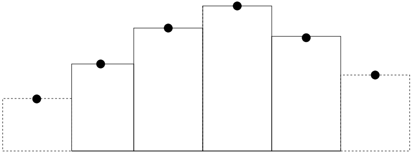
then the formulation reduces to elementwise FEM problems coupled by internal bc

$$\int_e v_m^e \frac{\partial u_m^e}{\partial t} dV - \int_e \nabla v_m^e \cdot \vec{g}_m dV + \int_{\partial e} \gamma_m(\tilde{u}^e, \tilde{u}^*, v^+, 0, \vec{n}) dS = 0 \ , \ \ \forall v^e \in (\Phi)_e$$

- internal bc provide guiding principle for choosing γ
- locally structured problem
- no global operations needed (in particular inversion of mass matrix)
- highly dense blocked matrix structure

DGM/IP methods

Convective terms : finite volume methods



Godunov scheme

- solution constant per element
- elementwise flux balance

$$V^e \frac{\partial u^e}{\partial t} + \oint_{\partial e} \mathcal{H}(u^e, u^*, \vec{n}) dS$$

- interface flux ~ local Riemann problem
  - consistency : $\mathcal{H}(u, u, n) = \vec{f}(u) \cdot \vec{n}$
  - conservation : $\mathcal{H}(u^-, u^+, -\vec{n}) = -\mathcal{H}(u^+, u^-, \vec{n})$
  - stability
  - entropy satisfying solutions

DGM/IP methods

Convective terms :

Unstructured maximum principle : *Local Extrema Diminishing* / positivity

Scalar problem

- E-flux

$$\frac{\mathcal{H}(u^+, u^-, \vec{n}) - \vec{f}(u) \cdot \vec{n}}{u^- - u^+} \leq 0 \ , \ \ \forall u \in [u^+, u^-]$$

- monotone fluxes

$$\frac{\partial \mathcal{H}}{\partial u^+} \geq 0 \qquad \frac{\partial \mathcal{H}}{\partial u^-} \leq 0 \forall u \in [u^+, u^-]$$

- upwind fluxes

$$\mathcal{H}(u^+, u^-, \vec{n}) = \mathtt{max}(0, (\vec{f} \cdot \vec{n})_u) u^+ + \mathtt{min}(0, (\vec{f} \cdot \vec{n})_u) u^- +$$

System of equations

- (approximate) Riemann solvers
- monotone fluxes

DGM/IP methods

Convective terms : Local Extrema Diminishing (LED)

If we can rewrite the FVM scheme as

$$\frac{du^e}{dt} = \sum_{ef} C_e (u_f - u_e)$$

with all $C_{ef} \geq 0$ then we can choose Δt such that the following is a convex combination

$$\begin{aligned}
\frac{du^e}{dt} &= \frac{1}{V^e} \sum_f \mathcal{H}(u^e, u^f, \vec{n}) \\
&= \frac{1}{V^e} \sum_f H(u^e, u^f, \vec{n}) - \vec{f}(u) \cdot \vec{n} \\
&= \frac{1}{V^e} \sum_f \frac{H(u^e, u^f, \vec{n}) - \vec{f}(u) \cdot \vec{n}}{u^f - u^e} (u^f - u^e) \\
&= \frac{1}{V^e} \sum_f \frac{\partial \mathcal{H}}{\partial u^-} (u^f - u^e)
\end{aligned}$$

and hence the scheme is *local extrema diminishing (LED)*

DGM/IP methods

Convective terms : finite volume reinterpreted as DGM

DGM formulation

$$\sum_e \int_e v_m \frac{\partial u_m}{\partial t} dV - \sum_e \int_e \nabla v_m \cdot \vec{g}_m dV + \sum_f \int_f \gamma_m(\tilde{u}^+, \tilde{u}^-, v^+, v^-, \vec{n}) dS = 0$$

Choose piecewise constant function space

$$\begin{aligned} v^e &= 1 \quad \forall x \in e \\ v^e &= 0 \quad \forall x \notin e \end{aligned}$$

Then

$$\begin{aligned} V^e \frac{du^e}{dt} + \oint_{\partial e} \gamma(u^e, u^*, 1, 0, \vec{n}) dS &= 0 \ , \ \forall e \\ V^e \frac{du^e}{dt} + \oint_{\partial e} \mathcal{H}(u^e, u^*, \vec{n}) dS &= 0 \end{aligned}$$

Generalisation

$$\sum_e \int_e v_m \cdot \frac{\partial u_m}{\partial t} dV - \sum_e \int_e \nabla v_m \cdot \vec{f}_m dV + \sum_f \int_f [[v_m]] \, \vec{n} \mathcal{H}_m(u^+, u^-, \vec{n}) dS = 0 \ , \ \forall v \in \Phi$$

DGM/IP methods

Convective terms : energy stability of HO version

LED in FVM is weakened to energy stability for DGM

Plug in $v = u$

$$\sum_e \int_e u \frac{\partial u}{\partial t} dV = \sum_e \int_e \nabla u \cdot \vec{f}(u) dV - \sum_f \int_f [\![u]\!] \cdot \vec{n} \mathcal{H}(u^+, u^-, \vec{n}) dS$$

$$\Downarrow \vec{g}(u) = \int^u \vec{f}(u) du$$

$$\frac{\partial}{\partial t} \sum_e \int_e \frac{u^2}{2} dV = \sum_e \int_e \nabla \cdot \vec{g}(u) dV - \sum_f \int_f [\![u]\!] \cdot \vec{n} \mathcal{H}(u^+, u^-, \vec{n}) dS$$

$$= - \sum_f \int_f \left([\![u]\!] \cdot \vec{n} \mathcal{H}(u^+, u^-, \vec{n}) - [\![\vec{g}(u)]\!] \right) dS$$

$$\Downarrow \text{midpoint rule}$$

$$= - \sum_f \int_f \left(u^+ - u^- \right) \left(\mathcal{H}(u^+, u^-, \vec{n}) - \vec{f}(u^*) \cdot \vec{n} \right) dS \ , \ \ u^* \in [u^+, u^-]$$

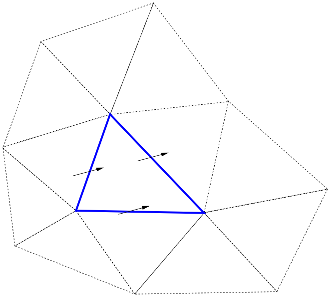
$$\Downarrow \text{E-flux} (\mathcal{H}(u^+, u^-, \vec{n}) - \vec{f}(u) \cdot \vec{n})(u^- - u^+) \leq 0$$

$$\leq 0$$

and a local elementwise entropy inequality (*Jiang* [JS94])

DGM/IP methods

Convective terms : local FEM reinterpretation



For each element e find $u^e \in \Phi(e)$

$$\int_e v^e_m \frac{\partial u^e_m}{\partial t} dV - \int_e \nabla v^e_m \cdot f_m(u^e) dV + \sum_{f \in e} \int_f v^e_m \mathcal{H}_m(u, u^*, \vec{n}) dS = 0 \ , \ \forall v^e_m \in \Phi(e)$$

then we find

- Galerkin FEM problem for each element e
- flux boundary conditions ensure "Dirichlet"-like coupling to the neighbours
- choice of $\mathcal{H}$ ensures stability of the bc
- if $\mathcal{H}$ is upwind flux imposes correct characteristics to/from external state $u^* = u^-$.

DGM/IP methods

Functional analysis : Lax-Milgram theorem

V is a Hilbert space

- Complete vector space
  - $x, y \in V \Rightarrow x + y \in V$
  - $x \in V \Rightarrow \alpha x \in V$
  - any Cauchy sequence converges in V
- Inner product $(.,.)$
  - $(u, v) = (v, u)$
  - $(u + w, v) = (u, v) + (w, v)$
  - $(u, u) \geq 0$

$a(.,.)$ is a *continuous* and *coercive bilinear* form $V \times V \to \mathbb{R}$

- $\exists c_1 > 0 : |a(u, v)| \leq c_1 ||u|| \cdot ||v|| \quad \forall u, v \in V$
- $\exists c_2 > 0 : a(u, u) \geq c_2 ||u||^2 \quad \forall u \in V$
- $a(u + v, w) = a(u, w) + a(v, w)$, $a(u, v + w) = a(u, v) + a(u, w)$

$< f, . >$ is a continuous linear form $V \to \mathbb{R}$

$$\exists c > 0 \ : \ |< f, u >| \ \leq \ c||u||$$

Then the problem

$$a(u, v) =< f, v > , \ \forall v \in V$$

has a unique solution $u \in V$

DGM/IP methods

Functional analysis : Lax-Milgram - illlustration for $\mathbb{R}^n$

Lax-Milgram is sufficient but not necessary condition for solvability (not applicable to convective DGM)

Eg. apply Lax-Milgram to solve for $\mathbf{A}\mathbf{x} = b$, $\mathbf{A} \in \mathbb{R}^{n\times n}, \mathbf{x}, \mathbf{b} \in \mathbb{R}^n$

- define inner product $(\mathbf{x}, \mathbf{y}) = \mathbf{y}^T \mathbf{x}$
- define bilinear form $a(\mathbf{x}, \mathbf{y}) = \mathbf{y}^T \mathbf{A}\mathbf{x}$
  - continuity implies $\mathbf{A}$ is *bounded*

$$|\mathbf{y}^T \mathbf{A}\mathbf{x}| = |\sum_i y_i^l \lambda_i \mathbf{l}_i^T \cdot \mathbf{x}| \leq \sum_i |\lambda_i y_i^l x_i^r| \leq |\lambda|_{max} ||x|| ||y||$$

  - coercivity implies $\mathbf{A}$ is *positive definite*

$$\mathbf{x}^T \mathbf{A}\mathbf{x} = \sum_i x_i^l \lambda_i \mathbf{r}_i \cdot \mathbf{x} = \sum_i \lambda_i x_i^l x_i^r \geq \lambda_{min} ||x||^2$$

- define a linear form $f(\mathbf{x}) = \mathbf{x}^T \cdot \mathbf{a}$, continuity implies $\mathbf{a}$ is *finite* : $|f(\mathbf{x})| \leq ||\mathbf{a}|| ||\mathbf{x}||$
- hence $\mathbf{y}^T \mathbf{A}\mathbf{x} = \mathbf{y}^T \cdot \mathbf{a}\ \forall \mathbf{y} \in \mathbb{R}^n$ has a unique solution

DGM/IP methods
Functional analysis : Broken Sobolev spaces

The broken Sobolev space $H^s(\mathcal{E})$ defined by its

- elements

$$H^s(\mathcal{E}) = \{v \in L^2(\Omega) \ : \ v|_e \in H^s(E) \ , \ \forall E \in \mathcal{E}\}$$

- broken norm

$$||u||_{H^s(\mathcal{E})} = \sum_{E \in \mathcal{E}} ||u||_{H^s(E)}$$

- broken inner product

$$(u,v)_{H^s(\mathcal{E})} = \sum_{E \in \mathcal{E}} (u,v)_{H^s(E)}$$

2nd order PDE : use $H^1(\mathcal{E})$

- natural norm :

$$||u||_{H^1()} = \sum_e ||u||_{H^1(e)} = \sum_e (|u|^2_{0,e} + |u|^2_{1,e})$$

- DG energy norm :

$$||u||_{DG} = \sum_e |\nabla u|^2_e + \sum_f |\,[\![u]\!]\,|^2_{0,f}$$

DGM/IP methods

Interior penalty methods : Naive Galerkin for elliptic/parabolic equations

Elliptic problem

$$
\begin{aligned}
\nabla \cdot \mu \nabla \tilde{u} &= f \\
u &= u^* \quad \forall x \in \Gamma_D \\
\partial_n u &= g \quad \forall x \in \Gamma_N
\end{aligned}
$$

Naive DG approach $\forall v \in \Phi$

$$
\begin{aligned}
a(u,v) &= \sum_e \int_e \nabla v \cdot \mu \nabla u \, dV - \sum_f \int_f [[v \mu \nabla u]] \, dS \\
&= \sum_e \int_e \nabla v \cdot \mu \nabla u \, dV - \sum_f \int_f [[v]] \cdot \{\{\nabla u\}\} + \cancel{[[\mu \nabla u]] \cdot \{\{v\}\}} \, dS \\
&= \sum_e \int_e \nabla v \cdot \mu \nabla u \, dV - \sum_f \int_f [[v]] \cdot \{\{\nabla u\}\} \, dS \forall v \in \Phi
\end{aligned}
$$

$$
\Rightarrow \exists v \in \Phi : a(v,v) \not> 0
$$

Conclusions :

- – is not coercive and hence unique solution is not guaranteed
- \+ however DG allows consistent stabilisation using solution jumps

DGM/IP methods

Interior penalty methods : Baumann-Oden (BO)

Bilinear form compensates consistent interface term

$$a(u,v) = \sum_e \int_e \nabla v \cdot \nabla u \, dV - \sum_f \int_f \left([\![v]\!] \cdot \{\!\{\nabla u\}\!\} - [\![u]\!] \cdot \{\!\{\nabla v\}\!\} \right) dS \ , \ \ u, v \in V_h$$

Coercivity ?

$$a(v,v) = \sum_e \int_e |\nabla v|^2 \, dV - \sum_f \int_f \left([\![v]\!] \cdot \{\!\{\nabla v\}\!\} - [\![v]\!] \cdot \{\!\{\nabla v\}\!\} \right) dS \quad = \sum_e \int_e |\nabla v|^2 \, dV \ , \ \ \forall u, v \in V_h$$

Conclusions

- \+ very natural way for stabilisation
- – not stable for pure diffusion (constant functions) since only larger than seminorm
- – formulation is not symmetric
  - non-symmetric Krylov iterator (`BiCG/GMRES`) instead of `CG`
  - convergence of stationary methods (`Jacobi/GS/SOR/...`)

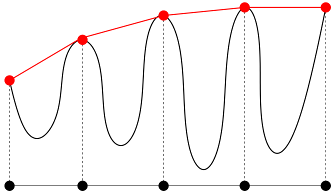
DGM/IP methods

Interior penalty methods : boundary penalty methods

Nitsche 71

Elliptic problem with rough Dirichlet bc

$$
\begin{aligned}
\nabla \cdot \mu \nabla u &= 0 \quad \forall x \in \Omega \\
u &= g \quad \forall x \in \partial\Omega
\end{aligned}
$$



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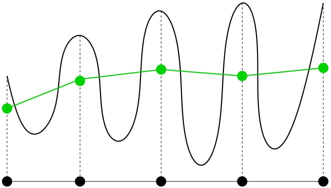

DGM/IP methods

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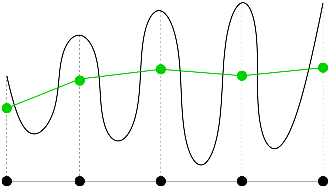

Elliptic problem with rough Dirichlet bc

$$\begin{aligned} \nabla \cdot \mu \nabla u = 0 \quad \forall x \in \Omega \\ u = g \quad \forall x \in \partial\Omega \end{aligned}$$

Penalty bc
+ consistency term - conditional stability ifo $\sigma \sim \mu C/h$

$$\int_\Omega \nabla u \cdot \mu \nabla v dV + \int_{\partial\Omega} \sigma (u-g) v dS - \int_{\partial\Omega} v \mu \nabla u \cdot \vec{n} dS = 0$$

DGM/IP methods

Interior penalty methods : boundary penalty methods

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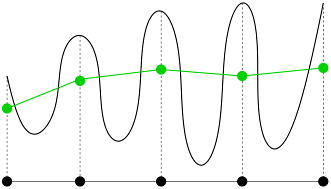


Penalty bc
+ consistency term - conditional stability ifo $\sigma \sim \mu C/h$

$$\int_\Omega \nabla u \cdot \mu \nabla v dV + \int_{\partial\Omega} \sigma (u-g) v dS - \int_{\partial\Omega} v \mu \nabla u \cdot \vec{n} dS = 0$$

Symmetrizing variant - conditional stability ifo $\sigma \sim C/h$

$$\int_\Omega \nabla u \cdot \mu \nabla v dV + \int_{\partial\Omega} \sigma (u-g) v dS - \int_{\partial\Omega} (v \mu \nabla u + (u-g) \mu \nabla v) \cdot \vec{n} dS = 0$$

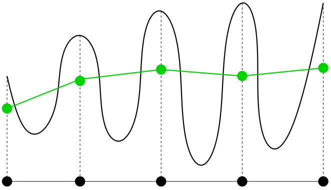
DGM/IP methods

Interior penalty methods : boundary penalty methods

Nitsche 71

Elliptic problem with rough Dirichlet bc

$$\nabla \cdot \mu \nabla u = 0 \quad \forall x \in \Omega$$
$$u = g \quad \forall x \in \partial\Omega$$



Penalty bc
+ consistency term - conditional stability ifo $\sigma \sim \mu C/h$

$$\int_\Omega \nabla u \cdot \mu \nabla v dV + \int_{\partial\Omega} \sigma (u-g) v dS - \int_{\partial\Omega} v \mu \nabla u \cdot \vec{n} dS = 0$$

Symmetrizing variant - conditional stability ifo $\sigma \sim C/h$

$$\int_\Omega \nabla u \cdot \mu \nabla v dV + \int_{\partial\Omega} \sigma (u-g) v dS - \int_{\partial\Omega} (v \mu \nabla u + (u-g) \mu \nabla v) \cdot \vec{n} dS = 0$$

Antisymmetric variant - stability for all $\sigma > 0$

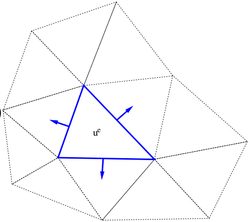
$$\int_\Omega \nabla u \mu \cdot \nabla v dV + \int_{\partial\Omega} \sigma (u-g) v dS - \int_{\partial\Omega} (v \mu \nabla u - \mu (u-g) \nabla v) \cdot n dS = 0$$

DGM/IP methods

Interior penalty methods : Interior Penalty Method - local view point

Local problem : for each element e find $u^e \in \Phi(e)$

$$\int_e \nabla v^e \cdot \nabla u^e dV + \int_{\partial e} \sigma v^e (u^e - u^o) dS$$
$$- \int_{\partial e} v^e \nabla u^e + \theta (u^e - u^*) \nabla v^e \vec{n} dS = 0 \ , \ \forall v^e \in \Phi(e)$$



with Nitsche penalties for coupling boundary conditions
Global problem : find $u \in \Phi$

$$\sum_e \int_e \nabla v \cdot \mu \nabla u dV + \sum_f \sigma \int_f [[u]] \, [[v]] \, dS$$
$$- \sum_f \int_f [[v]] \, \{\{\mu \nabla u\}\} + \cancel{[[\mu \nabla u]] \, \{\{v\}\}} dS$$
$$- \theta \sum_f \int_f [[u]] \, \{\{\mu \nabla v\}\} \, dS$$

DGM/IP methods

Interior penalty methods : properties

$$\sum_e \int_e \nabla v \cdot \mu \nabla u dV + \sum_f \sigma \int_f [[u]] \, [[v]] \, dS$$
$$- \sum_f \int_f [[v]] \, \{\{\mu \nabla u\}\} + \cancel{[[\mu \nabla u]] \, \{\{v\}\}} dS$$
$$- \theta \sum_f \int_f [[u]] \, \{\{\mu \nabla v\}\} \, dS$$

- *theta* = 1 *Non-Symmetric Interior Penalty (SIP)* - symmetric, conditionnally stable ($\sigma > \sigma_c$)
- *theta* = −1 *Incomplete Interior Penalty (NIP)* - antisymmetric, marginally stable ($\sigma > 0$)

Description Rivière [Riv08]
Relation to lifting based methods *Arnold et al. [ABCM02]*
Question : how do we choose σ for SIP

DGM/IP methods

Interior penalty methods : Coercivity of SIP [Sha05]

$$
\begin{aligned}
a(v,v) &= \sum_e \int_e |\nabla v|^2 \, dV - 2\sum_f \int_f \{\!\{\nabla v\}\!\} [\![v]\!] \, dS + \sum_f \sigma_f \int_f [\![v]\!]^2 \, dS > C_1 ||v||^2 \quad ? \\
&\geq \sum_e \int_e |\nabla v|^2 \, dV - \sum_f \frac{1}{\epsilon_F} \int_f \{\!\{\nabla v\}\!\}^2 \, dS + \sum_f (\sigma_f - \epsilon_f) \int_f [\![v]\!]^2 \, dS \\
&\geq \sum_e \int_e |\nabla v|^2 \, dV - \sum_f \frac{1}{4\epsilon_F} \int_f |\nabla v^+|^2 + |\nabla v^-|^2 + 2\nabla v^- \cdot \nabla v^+ \, dS + \dots \\
&\geq \sum_e \int_e |\nabla v|^2 \, dV - \sum_f \frac{1}{2\epsilon_F} \int_f |\nabla v^+|^2 + |\nabla v^-|^2 \, dS - \sum_{f \in \Gamma} \frac{1}{\epsilon_F} \int_f |\nabla v^-|^2 \, dS + \dots \\
&\geq \sum_e \left(1 - \sum_{f \in e} \frac{c^*_{f,e}}{\epsilon_f} \right) \int_e |\nabla v|^2 \, dV + \sum_f \int_f (\sigma_f - \epsilon_f) [v]^2 \, dS
\end{aligned}
$$

$$
\begin{aligned}
c^*_{f,e} &= c_{\mathfrak{f},\mathfrak{e}} \frac{\mathcal{A}(f)}{\mathcal{V}(e)} \quad , \quad \forall f \in \Gamma \\
&= \frac{c_{\mathfrak{f},\mathfrak{e}}}{2} \frac{\mathcal{A}(f)}{\mathcal{V}(e)} \quad , \quad \forall f \notin \Gamma
\end{aligned}
$$

DGM/IP methods

Interior penalty methods : Trace inequality constants

$e/\ f$	edge	triangle	quadrilateral
triangle*	$(p+1)(p+2)/2$	-	-
tetrahedron*	-	$(p+1)(p+3)/3$	-
quadrilateral†	$(p+1)^2$	-	-
hexahedron†	-	-	$(p+1)^2$
wedge†	-	$(p+1)^2$	$(p+1)(p+2)/2$
pyramid†	-	$1.05(p+1)(2p+3)/3$	$(p+1)(p+3)/3$

$$\int_f u^2 dS \leq c_{\mathfrak{e},\mathfrak{f}}(p) \cdot \frac{\mathcal{A}(f)}{\mathcal{V}(e)} \int_e u^2 dV \ , \ \forall u \in \Phi_p$$

Hillewaert & Remacle, submitted to Sinum

DGM/IP methods

Interior penalty methods : Coercivity of SIP - alternatives for σ

Choose ϵ_f and σ_f such that

$$a(v,v) \geq \sum_e \left(1 - \sum_{f \in e} \frac{c^*_{f,e}}{\epsilon_f}\right) \int_e |\nabla v|^2 dV + \sum_f \int_f (\sigma_f - \epsilon_f)[v]^2 dS$$

DGM/IP methods

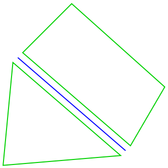
Interior penalty methods : Coercivity of SIP - alternatives for σ

Choose ϵ_f and σ_f such that

$$a(v,v) \geq \sum_e \left(1 - \sum_{f \in e} \frac{c^*_{f,e}}{\epsilon_f} \right) \int_e |\nabla v|^2 dV + \sum_f \int_f (\sigma_f - \epsilon_f) [v]^2 dS$$

Generalisation of Shahbazi (05)

$$\begin{aligned}
\sigma_f &> \epsilon_f \\
\epsilon_f &> \max_{e \ni f} \left(\sum_{f' \in e} c^*_{f',e} \right) = \max_{e \ni f} \left(\frac{1}{\mathcal{V}(e)} \sum_{f \in e} c_{f',e} \mathcal{A}(f') \right)
\end{aligned}$$



DGM/IP methods

Interior penalty methods : Coercivity of SIP - alternatives for σ

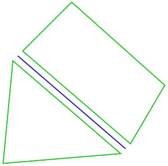
Choose ϵ_f and σ_f such that

$$a(v,v) \geq \sum_e \left(1 - \sum_{f\in e} \frac{c^*_{f,e}}{\epsilon_f}\right) \int_e |\nabla v|^2 dV + \sum_f \int_f (\sigma_f - \epsilon_f)[v]^2 dS$$

Generalisation of Shahbazi (05)

$$\sigma_f > \epsilon_f$$

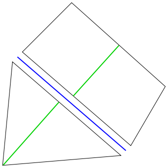
$$\epsilon_f > \max_{e\ni f}\left(\sum_{f'\in e} c^*_{f',e}\right) = \max_{e\ni f}\left(\frac{1}{\mathcal{V}(e)} \sum_{f\in e} c_{\mathfrak{f}',\mathfrak{e}} \mathcal{A}(f')\right)$$



Anisotropic definition

$$\sigma_f > \epsilon_f$$

$$\epsilon_f > \max_{e\ni f}\left(n c^*_{f,e}\right) = \max_{e\ni f}\left(n c_{\mathfrak{f},\mathfrak{e}} \frac{\mathcal{A}(f)}{\mathcal{V}(e)}\right)$$



DGM/IP methods

Interior penalty methods : verification

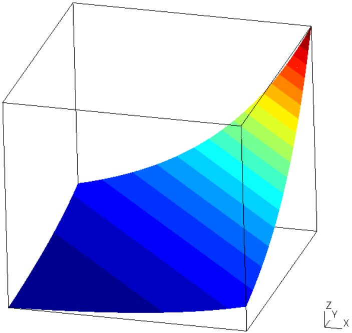
- manufactured solution

$$\Delta u = -\Delta f \ , \ \forall x \in \Omega$$
$$u = f \ , \ \forall x \in \Gamma$$
$$f = \prod_{i=1}^{d} e^{x_i}$$

- define

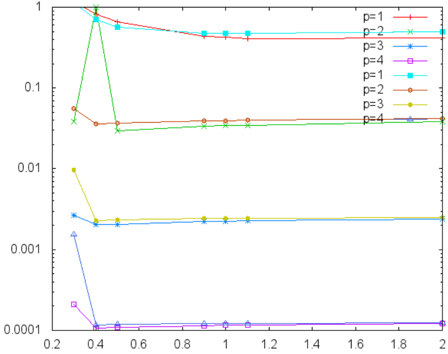
$$\sigma_f = \alpha \sigma_f^*$$

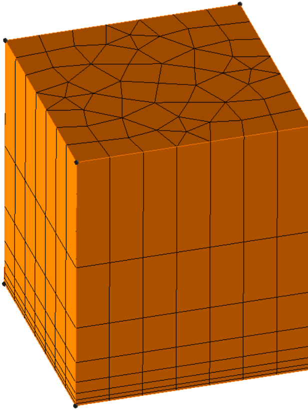
- plot
  L_2-norm of the error as a function of α
- single-precision
  direct solver ← conditioning



DGM/IP methods

Interior penalty methods : verification





DGM/IP methods

Interior penalty methods : extension to systems

Scalar penalty

$$\sum_e \int_e \frac{\partial v_m}{\partial x_k} \cdot \mathbf{D}^{kl}_{mn} \frac{\partial u_n}{\partial x_l}\, dV - \sum_f \int_f [[v_m]]^k \left\{\!\!\left\{ \mathbf{D}^{kl}_{mn} \cdot \frac{\partial u_n}{\partial x^l} \right\}\!\!\right\} dS$$
$$- \theta \sum_f \int_f [[u_n]]^k \left\{\!\!\left\{ \mathbf{D}^{kl}_{nm} \cdot \frac{\partial v_m}{\partial x^l} \right\}\!\!\right\} dS$$
$$+ \sum_f \sigma \int_f [[u_m]] \cdot [[v_m]]\, dS = 0$$

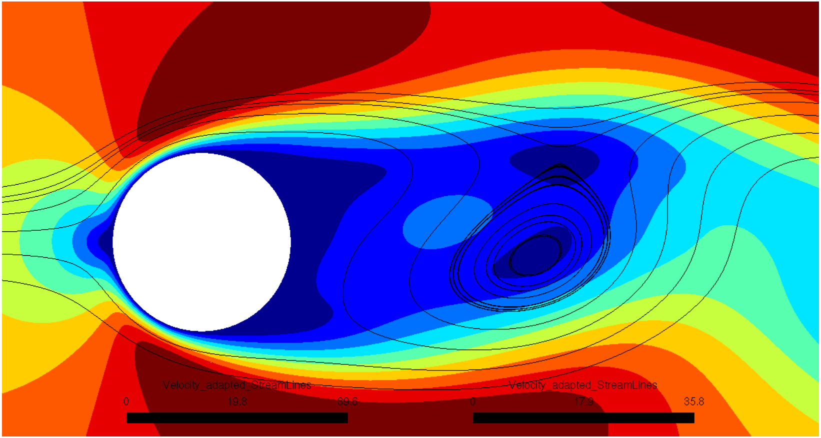
Matrix penalty

$$\sum_e \int_e \frac{\partial v_m}{\partial x_k} \cdot \mathbf{D}^{kl}_{mn} \frac{\partial u_n}{\partial x_l}\, dV - \sum_f \int_f [[v_m]]^k \left\{\!\!\left\{ \mathbf{D}^{kl}_{mn} \cdot \frac{\partial u_n}{\partial x^l} \right\}\!\!\right\} dS$$
$$- \theta \sum_f \int_f [[u_n]]^k \left\{\!\!\left\{ \mathbf{D}^{kl}_{nm} \cdot \frac{\partial v_m}{\partial x^l} \right\}\!\!\right\} dS$$
$$+ \sum_f \frac{\sigma^*}{2} \int_f \left([[v_m]]^l \left(\mathbf{D}^{kl}_{mn} + \mathbf{D}^{kl}_{nm} \right) [[u_n]]^k \right) dS = 0$$

DGM/IP methods

Interpolation and quadrature : need for curved meshes and mappings

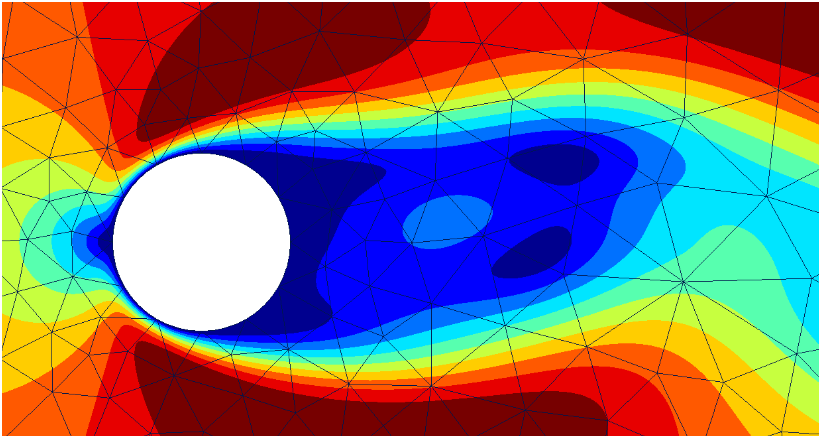
Example : von Karman street from cylinder Re=100, DGM(4)



DGM/IP methods

Interpolation and quadrature : need for curved meshes and mappings

Example : von Karman street from cylinder Re=100, DGM(4)



DGM/IP methods

Interpolation and quadrature : need for curved meshes and mappings

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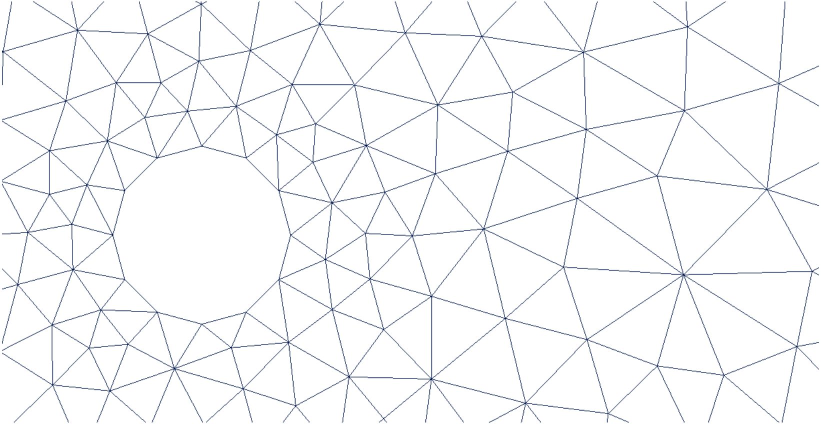
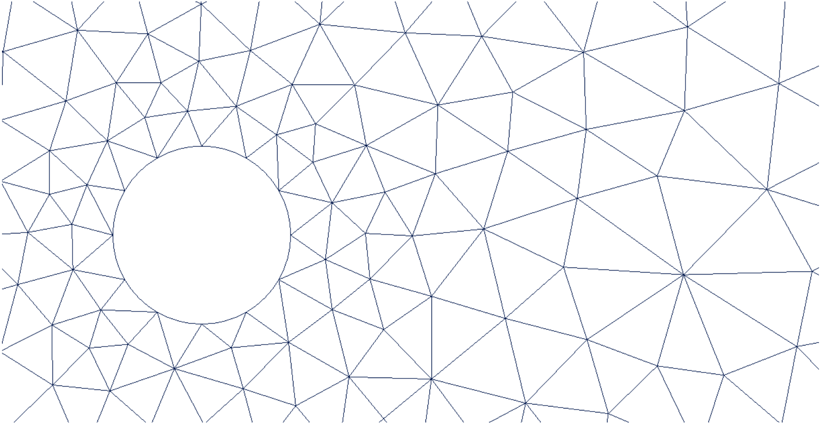


DGM/IP methods

Interpolation and quadrature : need for curved meshes and mappings

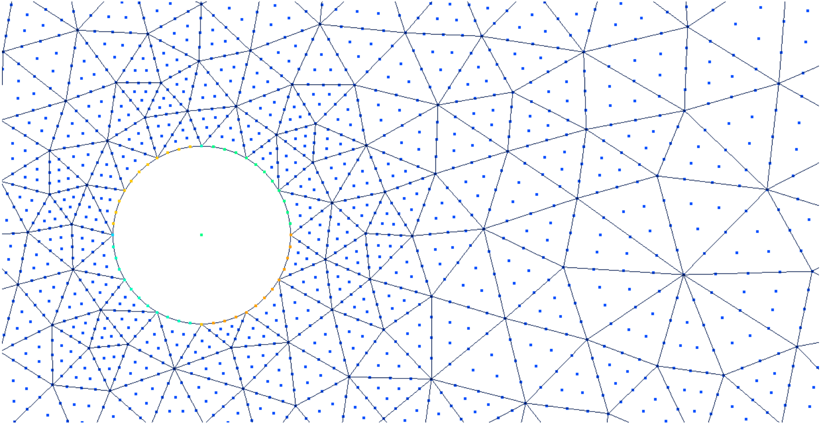
Example : von Karman street from cylinder Re=100, DGM(4)



DGM/IP methods

Interpolation and quadrature : need for curved meshes and mappings

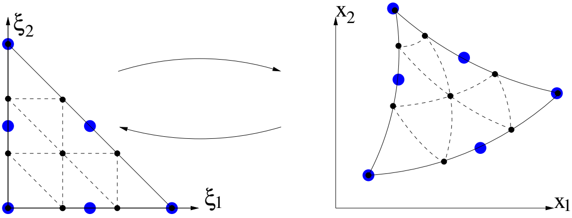
Example : von Karman street from cylinder Re=100, DGM(4)



Pre- and postprocessing tools are (not enough) subject of research
Gmsh (http ://www.geuz.org/gmsh)

DGM/IP methods

Interpolation and quadrature : Taxonomy of base functions



DGM : basis ϕ_i for Φ is supported on a single element $\rightarrow$ total freedom

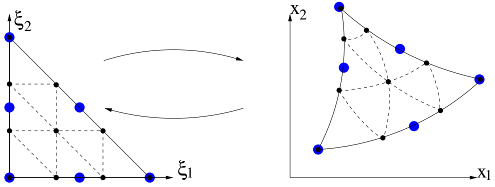
- *modal* : easy/well-conditioned base irrespective of geometry
  - monomials $1, \xi, \xi^2, \ldots$
  - orthogonal polynomials, eg. Legendre in 1D $\mathcal{P}^n(\xi)$
  - fundamental solutions : eg. plane waves
  - ...
- *nodal* : control points associated to the geometry
  - Lagrangian (equidistant, optimised, spectral elements)
  - Splines

Coordinate system

- Parametric
- Cartesian

DGM/IP methods

Interpolation and quadrature : Standard choice : parametric Lagrangian interpolation



Solutions and coordinates expanded in parametric coordinates $\boldsymbol{\xi}$

$$u_m = \sum_{i=1}^{N_\phi} \mathbf{u}_{im} \phi_i(\boldsymbol{\xi}) \qquad x^k = \sum_{i=1}^{N_\psi} \mathbf{x}_i^k \psi_i(\boldsymbol{\xi})$$

Jacobian $\mathbf{J}$ of $\mathbf{x}$ wrt $\boldsymbol{\xi}$

$$\mathbf{J}_{kl} = \frac{\partial x^k}{\partial \xi^l} = \sum_{i=1}^{N_c} \frac{\partial \psi_i}{\partial \xi^l} \qquad \left(\mathbf{J}^{-1}\right)_{kl} = \frac{\partial \xi^k}{\partial x^l}$$

Classical Gauss-Legendre quadrature $\mathcal{O}(2p+1)$

$$\int_V \nabla \phi_i (\mathbf{f}_c(u) + \mathbf{f}_d(u, \nabla u)) dV \approx \sum_{q=1}^{N_q} w_q \left(\frac{\partial \phi_i}{\partial \xi^k} \mathbf{J}_{kl}^{-1} \left(f_c^l(u) + f_d^l(u, \nabla u) \right) |\mathbf{J}| \right)_{\xi_q}$$

DGM/IP methods

Interpolation and quadrature : Lagrangian boundary closures

Suppose

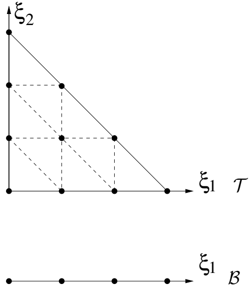
- $\Lambda(\psi_i, \xi_i) = \{\lambda_i\}$
- suppose $span\{\psi_k\}_f = span\{\psi_k^f\}$
- $\mathbf{V}^f$ is invertible, with $\mathbf{V}_{ij}^f = \psi_i^f(\xi_j^f)$

For any λ_i

$$\lambda_i\big|_f = \sum_j \beta_{ij}\psi_j^f = \sum_{j \in \Xi^f} \beta_{ij}\lambda_j^f$$

$$\lambda_i(\xi_k) = 0$$

$$= \sum_j \beta_{ij}\lambda_j^f(\xi_k) = \beta_{ik} \ , \ \ \forall \xi_k \in \Xi^f$$



and hence

$$\lambda_k\big|_f = 0 \ , \ \ \forall \xi_k \notin f$$

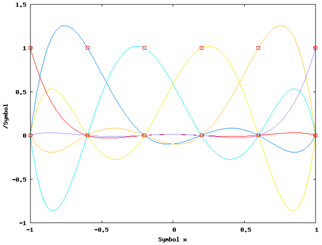
$\Rightarrow$ whatever the basis ψ_i, Lagrangian elements with complete boundary spaces will result interpolations on the boundary that only depend on the interpolation nodes on that same boundary

- $\mathcal{C}^0$ continuity (mesh generation)
- efficient assembly

DGM/IP methods

Interpolation and quadrature : computation

Lagrangian interpolants λ_i based on points ξ_i
and whatever set of basis functions $\psi_i : \Phi = \text{span}(\psi_i)$



$$\lambda_i \in \Phi : \lambda_i\left(\xi_j\right) = \delta_{ij}$$

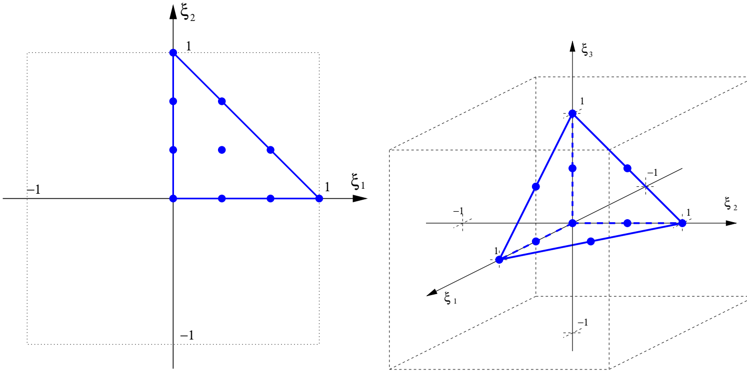
$$\lambda_i = \sum_j \mathbf{A}_{ij} \psi_j$$

$$\underbrace{\begin{bmatrix} \lambda_1(\xi_1) & \lambda_1(\xi_2) & \dots & \lambda_1(\xi_n) \\ \lambda_2(\xi_1) & \lambda_2(\xi_2) & \dots & \lambda_2(\xi_n) \\ \dots & & & \\ \lambda_n(\xi_1) & \lambda_n(\xi_2) & \dots & \lambda_n(\xi_n) \end{bmatrix}}_{I} = \mathbf{A} \cdot \underbrace{\begin{bmatrix} \psi_1(\xi_1) & \psi_1(\xi_2) & \dots & \psi_1(\xi_n) \\ \psi_2(\xi_1) & \psi_2(\xi_2) & \dots & \psi_2(\xi_n) \\ \dots & & & \\ \psi_n(\xi_1) & \psi_n(\xi_2) & \dots & \psi_n(\xi_n) \end{bmatrix}}_{\mathbf{V}}$$

$$\Rightarrow \mathbf{A} = \mathbf{V}^{-1}$$

DGM/IP methods

Interpolation and quadrature : simplex templates

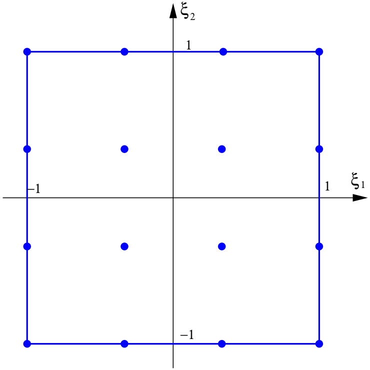


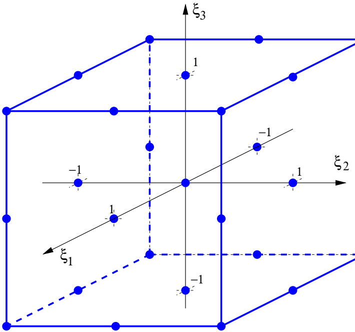
Functional space $\mathbb{P}^d_p = \mathrm{span}\{\prod_{i=1}^d \xi_i^{p_i} : 0 \leq \sum_{i=1}^p p_i \leq p\}$

Compendium of quadrature rules in *Solin 2004* [SSD04]

DGM/IP methods

Interpolation and quadrature :tensor product element templates





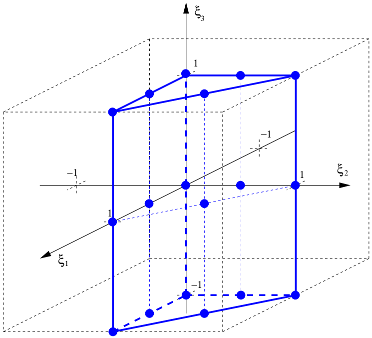
Functional space $\mathbb{Q}_p^d = \mathrm{span}\{\prod_{i=1}^d \xi_i^{p_i} : 0 \leq p_i \leq p\}$

Quadrature rules : tensor product of 1D Gauss-Legendre

Caveat : optimised quadrature rules (Solin) often apply to Pascal space

DGM/IP methods

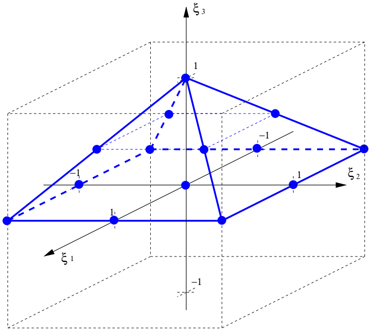
Interpolation and quadrature : prisms



Functional space and quadrature : Tensor product of triangle and lines

DGM/IP methods

Interpolation and quadrature :transition element templates



Bergot et al. [BCD10] boundary compliant functional space

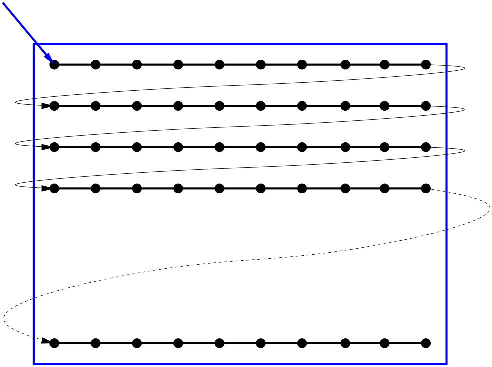
$$
\begin{aligned}
\Phi^e &= \operatorname{span}\left\{\psi_{ijk}, 0 \leq i,j \leq p \ , \ 0 \leq k \leq p - \mu_{ij}\right\} \\
\psi_{ijk} &= \mathcal{P}_i\left(\frac{\xi_1}{1-\xi_3}\right)\ \mathcal{P}_j\left(\frac{\xi_2}{1-\xi_3}\right)\ (1-\xi_3)^{\mu_{ij}}\ \mathcal{P}_k^{2\mu_{ij}+2,0}\left(2\xi_3 - 1\right) \\
\mu_{ij} &= \max\left(i,j\right)
\end{aligned}
$$

Quadrature rules based on degenerated hex

Outline

Practical implementation

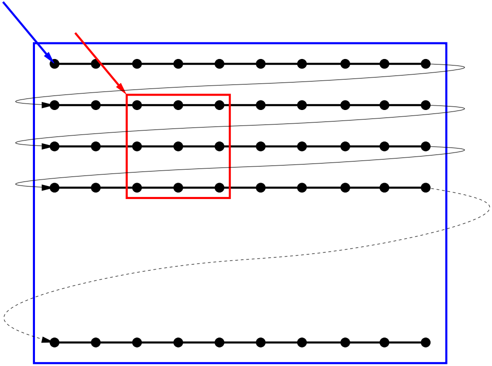
Computational kernels : matrix and vector proxies



$$\mathbf{A} \in \mathbb{R}^{m \times n} = (\mathbf{a}, n, m, lda)$$
$$\mathbf{A}_{ij} = *(\mathbf{a} + i * n + j)$$
$$\mathbf{A}_{ij} = *(\mathbf{a} + i * lda + j)$$

Practical implementation

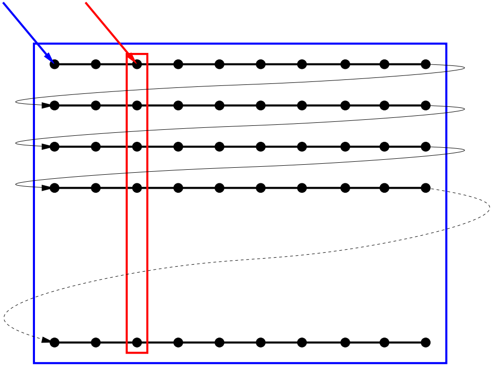
Computational kernels : matrix and vector proxies



$$\mathbf{B} \in \mathbb{R}^{p \times q} = (\mathbf{b}, p, q, lda)$$
$$\mathbf{b} = \mathbf{a} + i_b * lda + j_b$$
$$\mathbf{B}_{ij} = *(\mathbf{b} + i * lda + j) = *(\mathbf{a} + (i + i_b) * n + (j + j_b))$$

Practical implementation

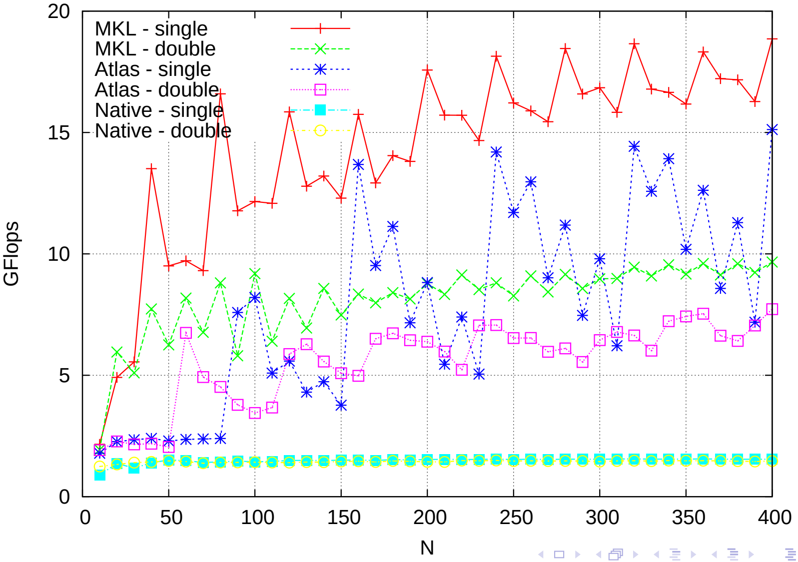
Computational kernels : matrix and vector proxies



$$\mathbf{b} \in \mathbb{R}^p = (\mathbf{b}, p, lda)$$
$$\mathbf{b} = \mathbf{a} + i_b * lda$$
$$\mathbf{b}_i = *(\mathbf{b} + i * lda) = *(\mathbf{a} + (i + i_b) * n$$

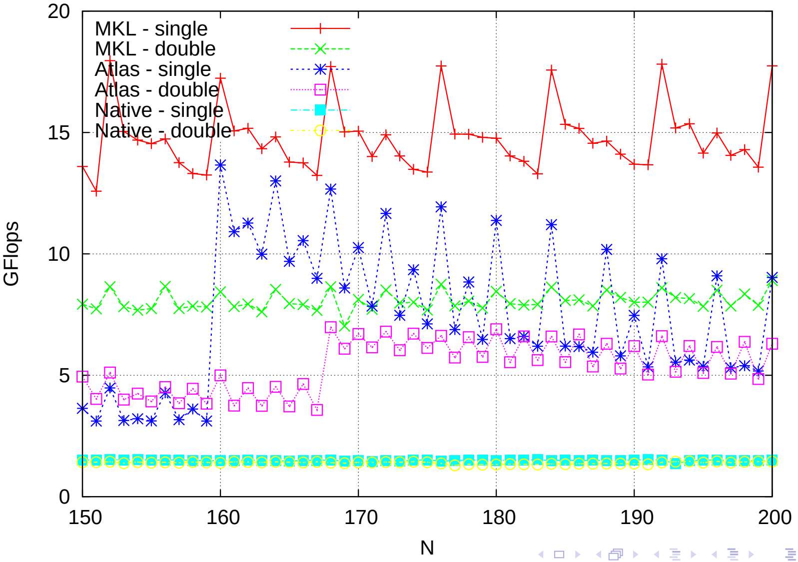
Practical implementation

Computational kernels : BLAS GEMM



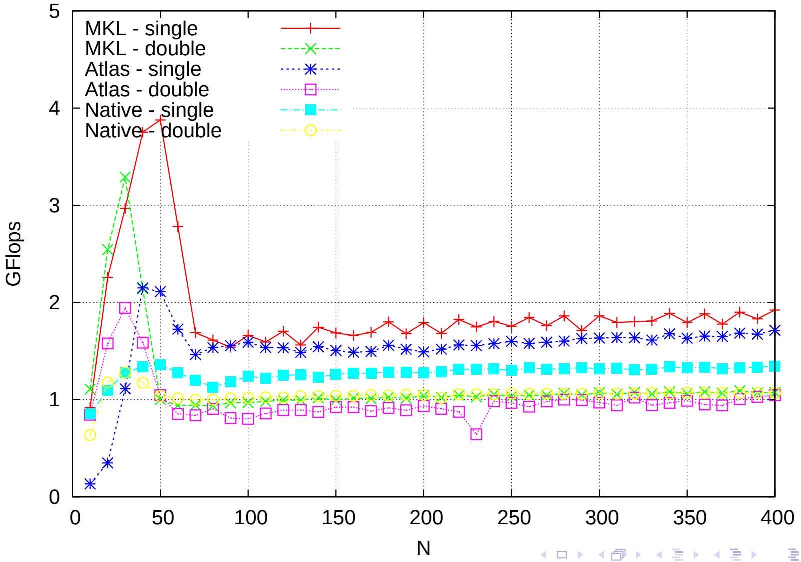
Practical implementation

Computational kernels : BLAS GEMM



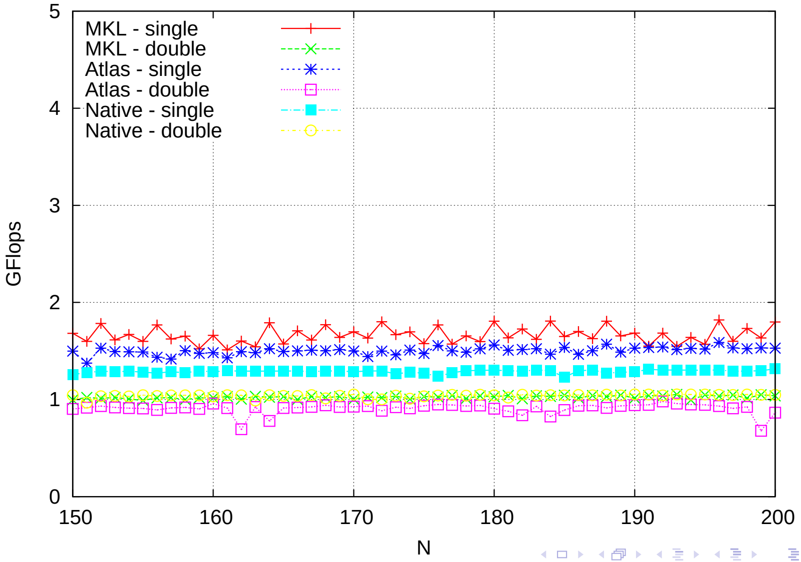
Practical implementation

Computational kernels : BLAS GEMV



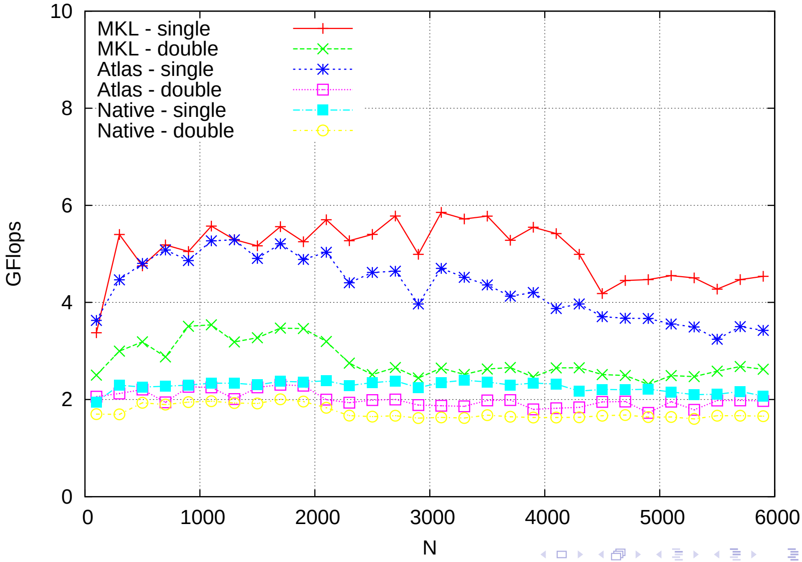
Practical implementation

Computational kernels : BLAS GEMV



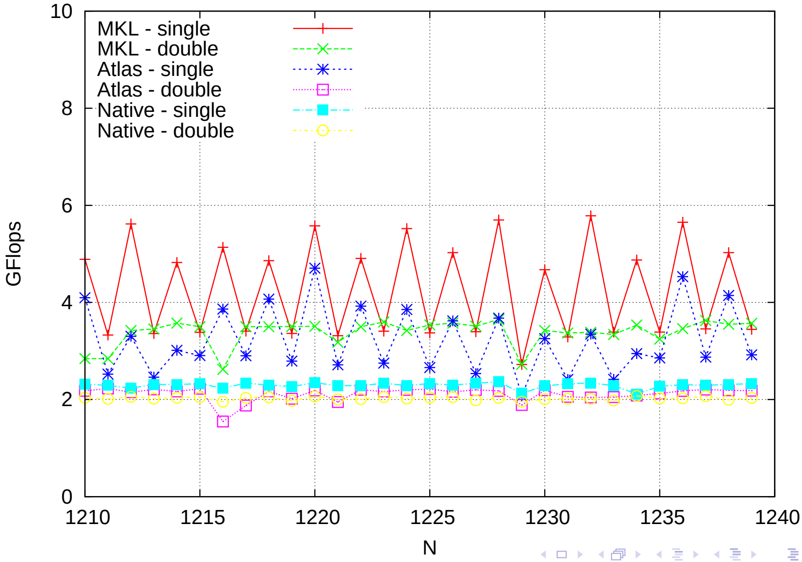
Practical implementation

Computational kernels : BLAS AXPY



Practical implementation

Computational kernels : BLAS AXPY



Practical implementation

Practical implementation : lessons

- peak flop rate : multiple of clock-speed due to inherent vectorisation (*SIMD*)
  - AMD, Intel $\leq$ Harpertown : SSE4 - 4 double, 8 single
  - Intel Sandy Bridge : AVC - 8 double, 16 single
  - BG/P 4 double (fma)
  - BG/Q 8 double (fma)

  requires efficient pipelining (data alignment and cache)
- efficiency increases with BLAS level ~ cache effects and pipelining effects - work to memory $\sim n^l/n$
- data packing effects clearly visible in efficiency → interest for padding
- efficiency depends very much on library

Practical quadrature

Full quadrature

eg. volume terms

Classical Gauss-Legendre quadrature $\mathcal{O}(2p+1)$

$$\mathbf{r}_{im} \leftarrow \mathbf{r}_{im} + \int_V \nabla\phi_{im}(\vec{f}_m(u) + \vec{d}_m(u,\nabla u))dV \approx \mathbf{r}_{im} + \sum_{q=1}^{N_q} w_q \left(\frac{\partial \phi_i}{\partial \xi^k} \mathbf{J}^{-1}_{kl} \left(f^l_c(u) + f^l_d(u,\nabla u) \right) |\mathbf{J}| \right)_{\xi_q}$$

efficient implementation : split up in *parametric* and *physical* steps :

1. Collocation

$$u_m(\xi_q) = \sum_{i=1}^{N_\phi} \phi_i(\xi_q)\mathbf{u}_{im}$$

$$\left(\frac{\partial u_m}{\partial \xi^l} \right)_{\xi_q} = \sum_{i=1}^{N_\phi} \mathbf{u}_{im} \left(\frac{\partial \phi_i}{\partial \xi^l} \right)_{\xi_q}$$

2. Evaluation of geometry and physics

$$\left(\frac{\partial u_m}{\partial x^k} \right)_{\xi_q} = \sum_{l=1}^{d} \left(\mathbf{J}^{-1}_{lk} \frac{\partial u_m}{\partial \xi^l} \right)_{\xi_q}$$

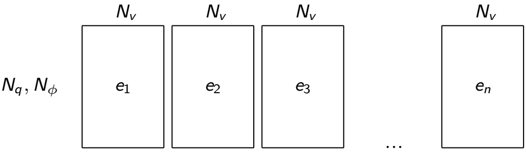
$$\mathfrak{f}^k_{qm} = |\mathbf{J}|\mathbf{J}^{-1}_{kl} \left(f^k_{c,m}(u) + f^k_{d,m}(u,\nabla u) \right)_{\xi_q}$$

3. Flux redistribution

$$\mathbf{r}_{im} \leftarrow \mathbf{r}_{im} + \sum_{q=1}^{N_q} w_q \left(\frac{\partial \phi_i}{\partial \xi^k} \right)_{\xi_q} \mathfrak{f}^k_{qm}$$

Practical implementation

Practical quadrature :Matrix operations in parametric



Solution collocation

$$u_m(\xi_q) = \sum_{i=1}^{N_\phi} \phi_i(\xi_q)\mathbf{u}_{im} \qquad \mathfrak{u}_{qm} = \sum_{i=1}^{N_\phi} \mathbf{C}_{qi}\mathbf{u}_{im}$$

Gradient collocation

$$\left(\frac{\partial u_m}{\partial \xi^l}\right)_{\xi_q} = \sum_{i=1}^{N_\phi} \mathbf{u}_{im}\left(\frac{\partial \phi_i}{\partial \xi^l}\right)_{\xi_q} \qquad \mathfrak{g}^l_{qm} = \sum_{i=1}^{N_\phi} \mathfrak{G}^l_{qi}\mathbf{u}_{im}$$

Flux redistribution

$$\mathbf{r}_{im} + = \sum_{q=1}^{N_q} w_q \left(\frac{\partial \phi_i}{\partial \xi^k}\right)_{\xi_q} \mathfrak{f}^k_{qm} \qquad \mathbf{r}_{im} + = \sum_k \sum_q \mathfrak{R}^k_{iq}\mathfrak{f}^k_{qm}$$

Premultiplication with the mass matrix

$$\mathbf{r}^*_{im} + = \mathfrak{M}_{ij}\mathbf{r}_{jm}$$

Practical implementation

Implicit solver : Damped inexact Newton

Backward-Euler with one Newton solve

$$\mathbf{r}^{\star}_{im} = \left(\phi_i, \frac{u^n_m - u^{n-1}_m}{\Delta\tau^n} + \mathcal{L}_m\left(u^n\right)\right) = 0 \ , \ \forall m, \ \forall \phi_i \in \Phi$$

$$\mathbf{A}^{\star} \cdot \Delta\mathbf{u}^n = -\mathbf{r}^{\star}$$

$$\mathbf{A}^{\star} = \frac{\partial \mathbf{r}^{\star}}{\partial \mathbf{u}} = \frac{\mathbf{M}}{\Delta\tau^n} + \mathbf{A}$$

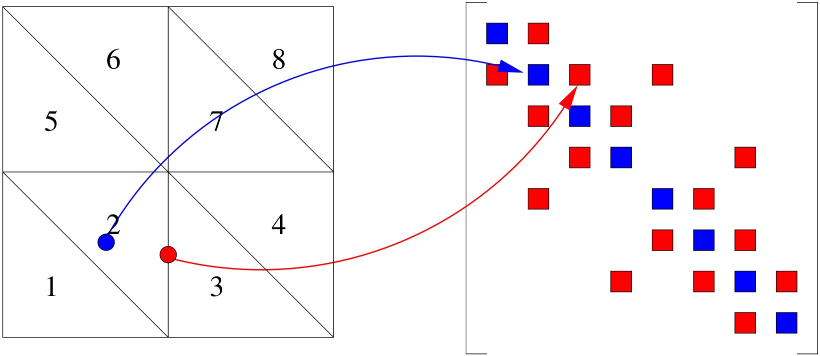
Strategy for global CFL

$$\Delta\tau^n = CFL^n \frac{\Delta x}{u \cdot (2p+1)}$$

$$CFL^n = CFL^0 \cdot \left(\frac{||\mathbf{r}^o||_2}{||\mathbf{r}^{n-1}||_2}\right)^{\alpha}$$

Options

- direct solvers (Gauss)
- Matrix iterative solvers - Krylov subspace



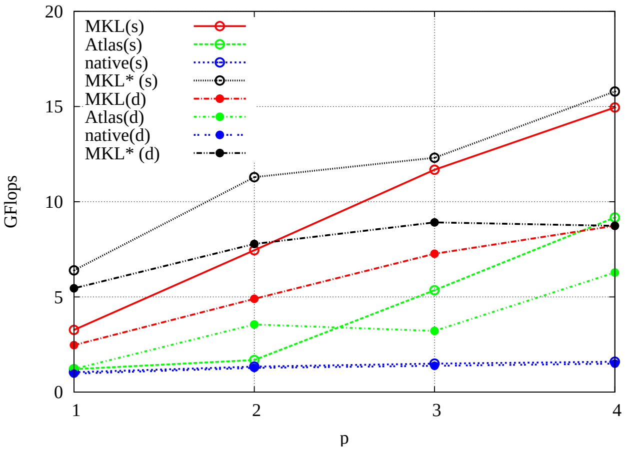
block CSR structure

+ very low indexing overhead allowing simple and flexible datastructure
+ computations recastable in dense gemm, inversion and gemv
    - datastructure can be deallocated/allocated on the fly
    - internal renumbering independent of the mesh
- large block size $N_\phi N_v \sim p^3 N_v$ (eg. DGM(4) hex, Navier-Stokes : 625) → memory bottle-neck

Implicit solver

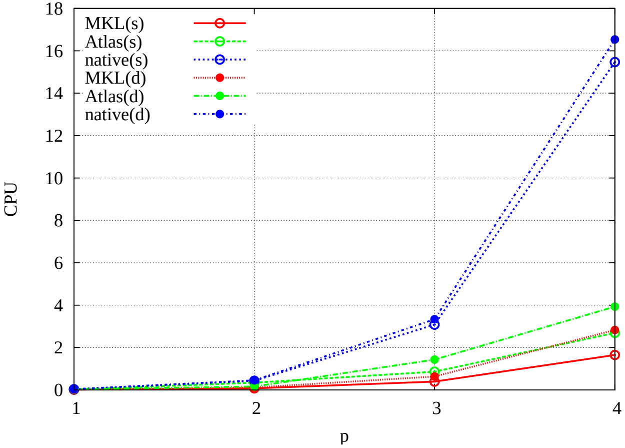
Matrix operations efficiency

inversion



Implicit solver
Matrix operations efficiency

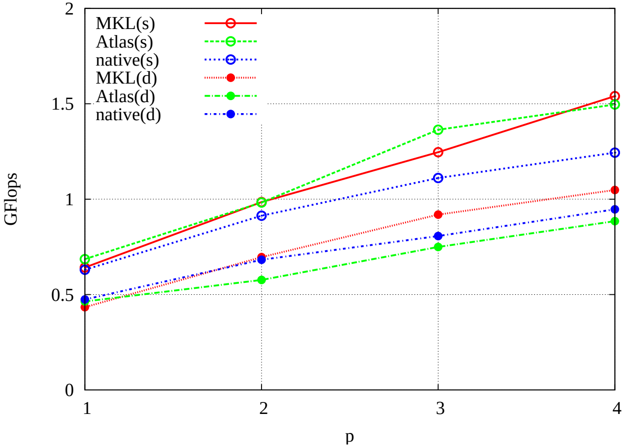
inversion



Implicit solver

Matrix operations efficiency

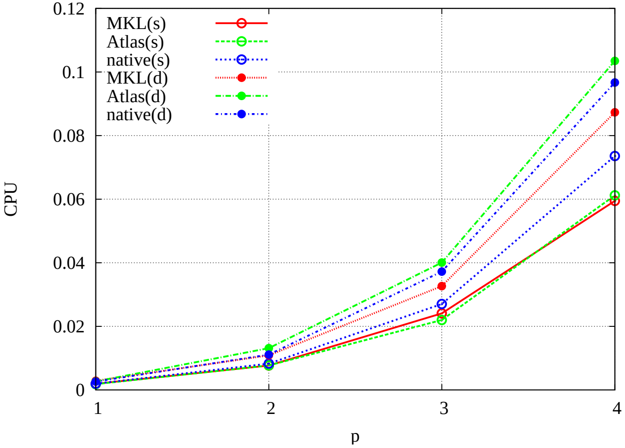
matrix-vector product



Implicit solver

Matrix operations efficiency

matrix-vector product



Practical implementation

Implicit solver : Krylov subspace methods (see Saad00 [Saa00])

Look for correction $\Delta u^n \in \mathcal{K}_n\left(\mathbf{A}^\star, \mathbf{r}^\star\right)$

$$\mathcal{K}_n\left(\mathbf{A}^\star, \mathbf{r}^\star\right) = \mathrm{span}\{\mathbf{r}^\star, \mathbf{A}^\star \cdot \mathbf{r}^\star, \ldots, \left(\mathbf{A}^\star\right)^n \cdot \mathbf{r}^\star\}$$

Needs

- operator to provide $\mathbf{A}^* \cdot p$ for generic p matrix-free Krylov

$$\mathbf{A}^\star \cdot \mathbf{p} \approx \frac{\mathbf{r}^\star\left(\mathbf{u}^n + \epsilon\ \mathbf{p}\right) - \mathbf{r}^\star\left(\mathbf{u}^n\right)}{\epsilon}$$
$$\epsilon = \sqrt{\mu}\frac{||u||}{||p||}$$

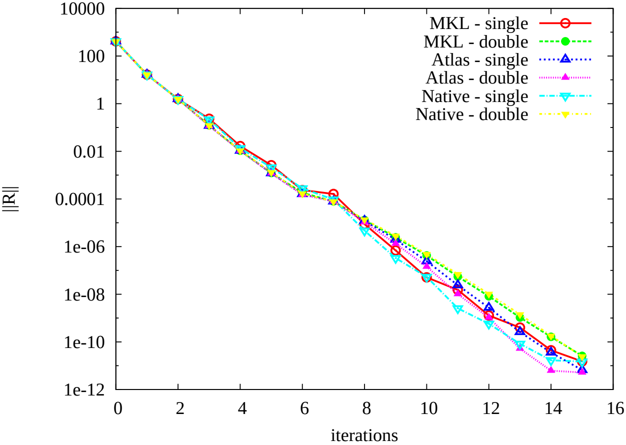
- vector internal product (parallellisation) (Gramm-Schmidt)
- preconditioning : pick iterative method $\mathbf{P} \sim A^-1$

$$\mathbf{A}^\star \cdot \mathbf{P} \cdot \mathbf{x} = -\mathbf{r}^\star$$
$$\Delta \mathbf{u}^n = \mathbf{P} \cdot \mathbf{x} \sim \left(\mathbf{A}^\star\right)^{-1} \cdot \mathbf{x}$$

  matrix preconditioners (BILU, BJacobi), hp-multigrid

Practical implementation

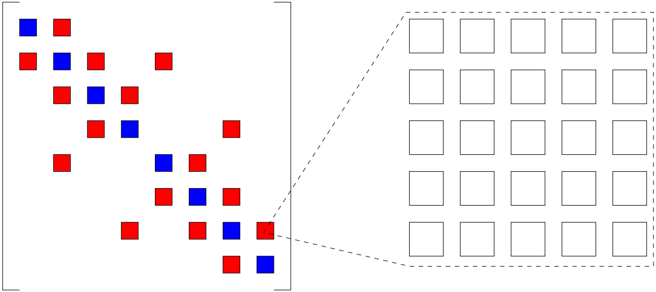
Implicit solver : single precision preconditioner



- still solve a double precision problem
- preconditioning only requires approximate solution
- halves the memory
- up to twice as efficient

Practical implementation

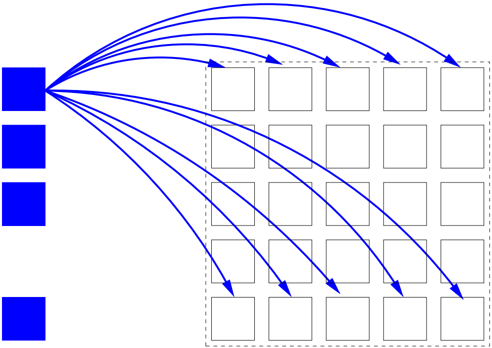
Efficient Jacobian assembly : volume Jacobian assembly (naive)



$$\mathbf{r}_{im} = \int_V \nabla\phi \vec{f}_c dV = \sum_q w_q \left(|\mathbf{J}| \frac{\partial \phi_i}{\partial \xi^k} \mathbf{J}^{-1}_{kl} f^l_m(u) \right)_{\xi_q} \Rightarrow \frac{\partial \mathbf{r}_{im}}{\partial \mathbf{u}_{jn}} = \sum_q \left(w_q \frac{\partial \phi_i}{\partial \xi^k} \phi_j \right)_{\xi_q} \left(|\mathbf{J}| \mathbf{J}^{-1}_{kl} \frac{\partial f^l_m}{\partial u_n}(u) \right)_{\xi_q}$$

Practical implementation

Efficient Jacobian assembly : volume Jacobian assembly (contiguous)

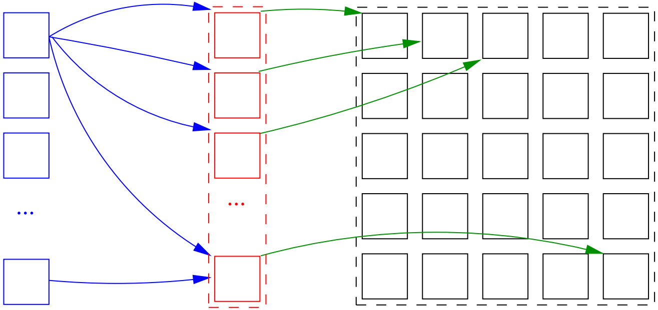


$$\mathbf{r}_{im} = \int_V \nabla \phi \vec{f}_c dV = \sum_q w_q \left(|\mathbf{J}| \frac{\partial \phi_i}{\partial \xi^k} \mathbf{J}^{-1}_{kl} f^l_m(u) \right)_{\xi_q} \Rightarrow \frac{\partial \mathbf{r}_{im}}{\partial \mathbf{u}_{jn}} = \sum_q \left(w_q \frac{\partial \phi_i}{\partial \xi^k} \phi_j \right)_{\xi_q} \left(|\mathbf{J}| \mathbf{J}^{-1}_{kl} \frac{\partial f^l_m}{\partial u_n}(u) \right)_{\xi_q}$$

- subblock (right) is proxy → not contiguous in memory → addition is done row per row

Practical implementation

Efficient Jacobian assembly : volume Jacobian assembly (optimized)

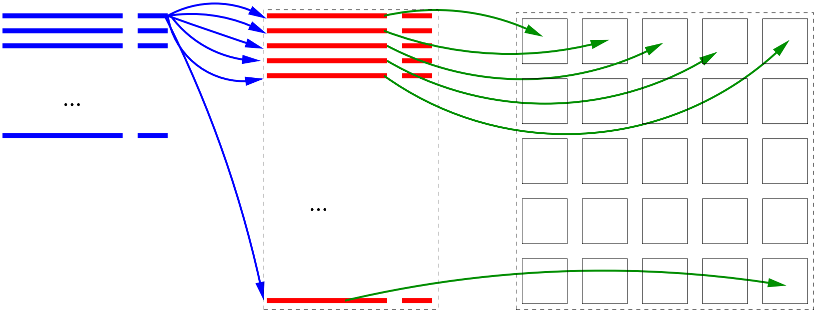


$$\mathbf{r}_{im} = \int_V \nabla \phi \vec{f}_c dV = \sum_q w_q \left(|\mathbf{J}| \frac{\partial \phi_i}{\partial \xi^k} \mathbf{J}^{-1}_{kl} f^l_m(u) \right)_{\xi_q} \Rightarrow \frac{\partial \mathbf{r}_{im}}{\partial \mathbf{u}_{jn}} = \sum_q \left(w_q \frac{\partial \phi_i}{\partial \xi^k} \phi_j \right)_{\xi_q} \left(|\mathbf{J}| \mathbf{J}^{-1}_{kl} \frac{\partial f^l_m}{\partial u_n}(u) \right)_{\xi_q}$$

- subblock (right) is proxy → not contiguous in memory
- intermediate blocks contiguous → single contiguous sum for N_q assembly steps (blue) + single copy (green)

Practical implementation

Efficient Jacobian assembly : volume Jacobian assembly



$$\mathbf{r}_{im} = \int_V \nabla\phi \vec{f}_c dV = \sum_q w_q \left(|\mathbf{J}| \frac{\partial \phi_i}{\partial \xi^k} \mathbf{J}^{-1}_{kl} f^l_m(u) \right)_{\xi_q} \Rightarrow \frac{\partial \mathbf{r}_{im}}{\partial \mathbf{u}_{jn}} = \sum_q \left(w_q \frac{\partial \phi_i}{\partial \xi^k} \phi_j \right)_{\xi_q} \left(|\mathbf{J}|\mathbf{J}^{-1}_{kl} \frac{\partial f^l_m}{\partial u_n}(u) \right)_{\xi_q}$$

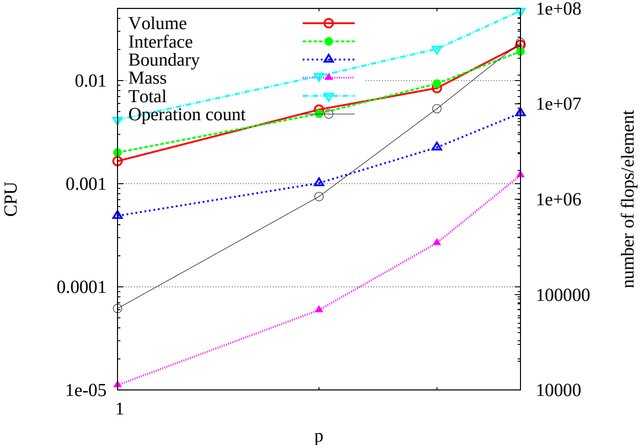
- subblock (right) is proxy → not contiguous in memory
- intermediate blocks contiguous → single contiguous sum for N_q assembly steps (blue) + single copy (green)
- padding increases flop efficiency in the assembly sums (blue)

Similar optimisations for interface terms etc. See [Hil10] for details.

Efficient Jacobian assembly

Evolution of assembly cost

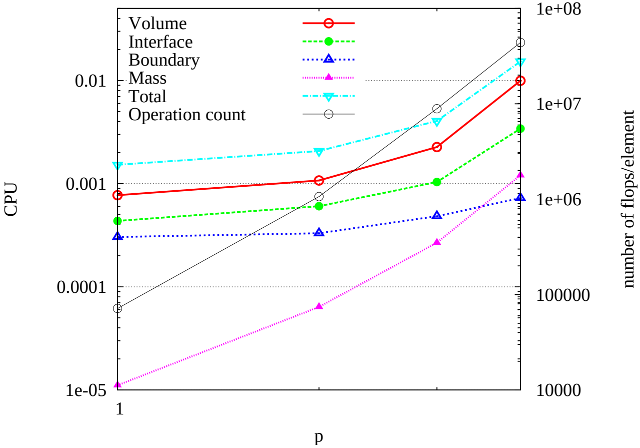
MKL - naive



Efficient Jacobian assembly

Evolution of assembly cost

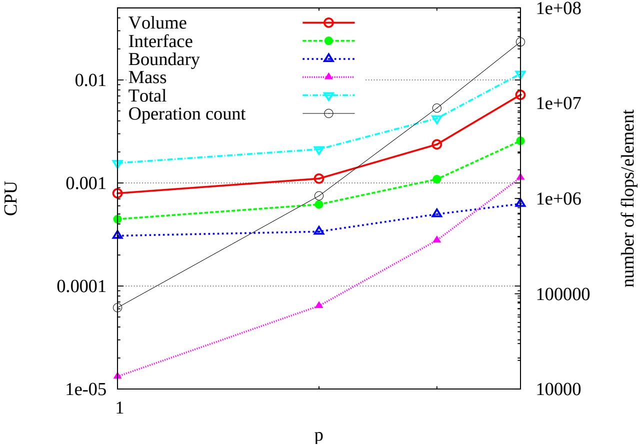
MKL - contiguous



Efficient Jacobian assembly

Evolution of assembly cost

MKL - optimized

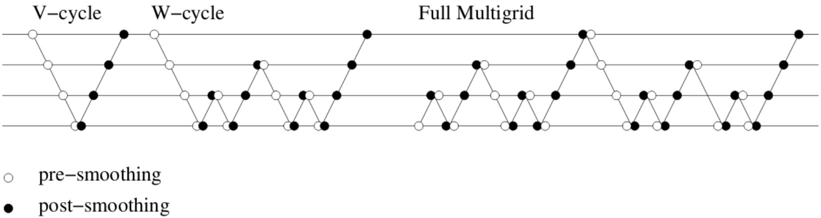


Computational complexity $\neq$ computational effort

Outline

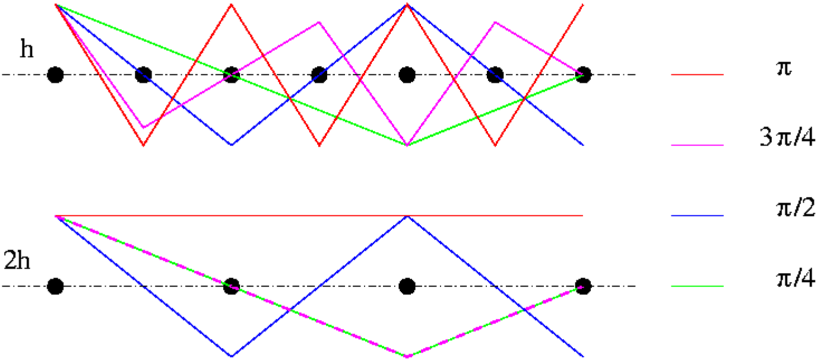
hp-multigrid

Basics : multilevel methods



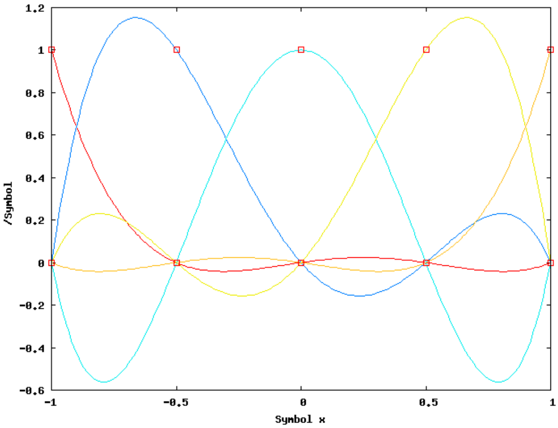
hp-multigrid

Basics : h-Multigrid → element size coarsening



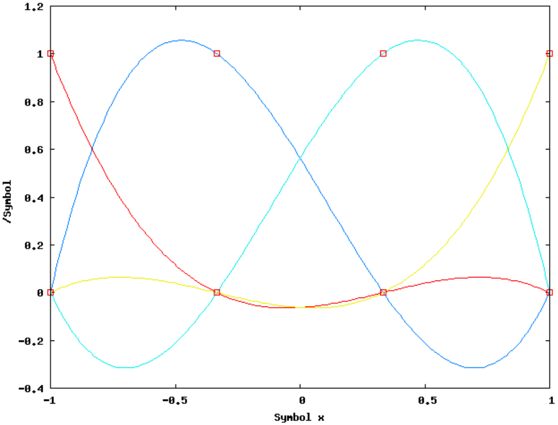
hp-multigrid

Basics : p-Multigrid → element order coarsening [FOLD05]



hp-multigrid

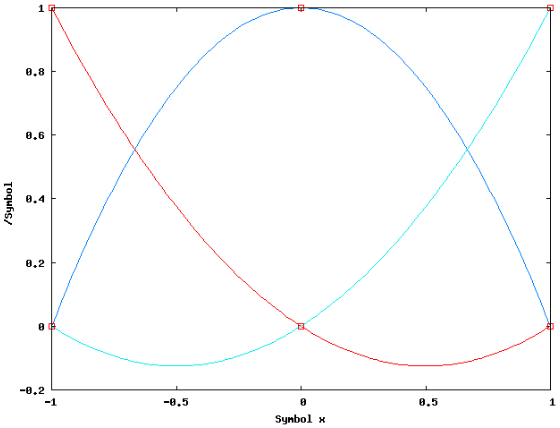
Basics : p-Multigrid → element order coarsening [FOLD05]



hp-multigrid

Basics : p-Multigrid → element order coarsening

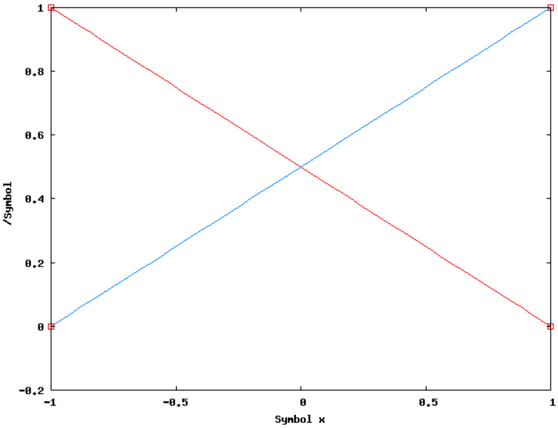
[FOLD05]



hp-multigrid

Basics : p-Multigrid → element order coarsening

[FOLD05]



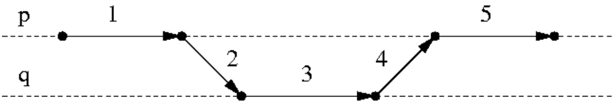
hp-multigrid

Basics : DGM - variational FAS

[HCGR06, HRC+06]

Define fine (p) and coarse level (q) by either grid- or order-coarsening

$$u^p \in \Phi^p$$
$$u^q \in \Phi^q$$



FAS cycle :

1. iterate on the fine level : $u^p \rightarrow u^{p'}$
2. restrict the fine level solution : $u^{q'} = \mathcal{T}^{qp}\left(u^{p'}\right)$
3. solve variational formulation of the defect correction equation

$$\left(\mathcal{L}\left(u^q\right) - \mathcal{L}\left(u^{q'}\right) + \mathcal{L}\left(u^{p'}\right), \phi_j^q\right) = 0 \quad \forall \phi_j^q \in \Phi^q$$

4. prolongate the correction $u^p := u^{p'} + \mathcal{T}^{pq}\left(u^q - u^{q'}\right)$
5. iterate on the finest level to smooth the error

hp-multigrid

Transfer operators : Solution transfer between levels a and b [HCGR06, HRC+06]

Both restriction and prolongation : use Galerkin projection

$u^a \in \Phi^a \rightarrow u^b \in \Phi^b$

$$
\begin{aligned}
u^a_m &= \mathbf{u}^a_{im}\phi^a_i \ , \ \phi^a_i \in \Phi^a \\
\mathcal{T}^{ba} u^a_m = u^b_m &= \mathbf{u}^b_{jm}\phi^b_j \ , \ \phi^b_j \in \Phi^b
\end{aligned}
$$

L_2 projection $\Phi^a \rightarrow \Phi^b$

$$
\left(\phi^b_k, \phi^b_j\right)\mathbf{u}^b_{jm} = \left(\phi^b_k, \phi^a_i\right)\mathbf{u}^a_{im}, \ \ \forall \phi^b_k \in \Phi^b
$$

Solution transfer matrix $\mathbf{T}^{ba}$

$$
\mathbf{u}^b = \mathbf{T}^{ba} \cdot \mathbf{u}^a = \left(\mathbf{M}^{bb}\right)^{-1} \cdot \mathbf{M}^{ba} \cdot \mathbf{u}^a
$$

hp-multigrid

Transfer operators : Residual transfer

[HCGR06, HRC+06]

Expand $\mathcal{L}(u^p)$ in Φ^p using L_2 projection

$$\mathcal{L}_m(u^p) \approx \sum_i \mathbf{l}^p_{im} \phi^p_i$$

$$\sum_i \mathbf{l}^p_{im} \left(\phi^p_i, \phi^p_j\right) \approx \left(\phi^p_j, \mathcal{L}(u^p)\right) = \mathbf{r}^p_{jm}$$

then weigh with ϕ^q_j

$$\mathbf{r}^{q\prime}_{im} = \left(\phi^q_i, \mathcal{L}_m(u^p)\right) \approx \left(\phi^q_i, \sum \mathbf{l}^p_{im} \phi^p_i\right)$$

residual transfer matrix $\tilde{\mathbf{T}}^{qp}$

$$\begin{aligned} \mathbf{r}^{q\prime} &= \mathbf{M}^{qp} \cdot \left(\mathbf{M}^{pp}\right)^{-1} \mathbf{r}^p \\ &= \tilde{\mathbf{T}}^{qp} \mathbf{r}^p = \left(\mathbf{T}^{pq}\right)^T \mathbf{r}^p \end{aligned}$$

hp-multigrid

Transfer operators : equivalence of DCGA and GCGA [HCGR06, HRC+06]

$\mathcal{L}$ is linear :

$$\mathbf{A}^p \cdot \mathbf{u}^p = \mathbf{s}^p$$
$$\mathbf{A}^p_{ij} = \left(\phi^p_i, \mathcal{L}\left(\phi^p_j\right)\right)$$

$\mathbf{\Phi}^q \in \mathbf{\Phi}^p$

$$\phi^q_i = \alpha^{qp}_{ij} \cdot \phi^p_j \ , \ \forall \phi^q_i \in \mathbf{\Phi}^q$$
$$\alpha^{qp} = \mathbf{M}^{qp} \cdot \left(\mathbf{M}^{pp}\right)^{-1} = \tilde{\mathbf{T}}^{qp} = \left(\mathbf{T}^{pq}\right)^T$$

then we can compute the *Coarse Grid Approximation (CGA)* of $\mathbf{A}^q$

$$\mathbf{A}^q_{ij} = \left(\phi^q_i, \mathcal{L}\left(\phi^q_j\right)\right) = \alpha^{qp}_{ik} \cdot \left(\phi^p_k, \mathcal{L}(\phi^p_l)\right) \cdot \alpha^{qp}_{jl}$$
$$\mathbf{A}^q = \alpha^{qp}\mathbf{A}p\left(\alpha^{qp}\right)^T = \tilde{\mathbf{T}}^{qp} \cdot \mathbf{A}^p \cdot \mathbf{T}^{pq}$$

Using Galerkin projection and variational FAS, we get *optimal* Galerkin CGA from *simple/standard* discretisation CGA

hp-multigrid

Transfer operators : Galerkin CGA and error propagation

- restriction of residual after correction is exactly 0

$$\tilde{\mathbf{T}}^{qp}\left(\mathbf{A}^p\cdot\left(\mathbf{u}^{p\prime}+\mathbf{T}^{pq}\cdot\left(\mathbf{u}^q-\mathbf{u}^{q\prime}\right)\right)-\mathbf{s}^p\right)=0$$

- the error after coarse grid correction depends only on the smooth part of the initial error

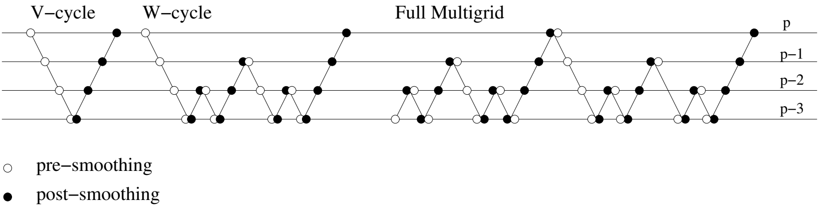
$$\begin{aligned}
\mathbf{A}^p\mathbf{e}^p &= \mathbf{A}^p\mathbf{u}^p-\mathbf{s}^p=\mathbf{r}^p\\
\mathbf{e}^{p\prime}_S &= \left(\mathbf{T}^{pq}\cdot\left(\tilde{\mathbf{T}}^{qp}\mathbf{T}^{pq}\right)^{-1}\cdot\tilde{\mathbf{T}}^{qp}\right)\cdot\mathbf{e}^{p\prime}\in\mathrm{ran}\left(\mathbf{T}^{qp}\right)\\
\mathbf{e}^{p\prime}_R &= \left(\mathbf{I}p-\mathbf{T}^{pq}\cdot\left(\tilde{\mathbf{T}}^{qp}\mathbf{T}^{pq}\right)^{-1}\cdot\tilde{\mathbf{T}}^{qp}\right)\cdot\mathbf{e}^{p\prime}\in\ker\left(\tilde{\mathbf{T}}^{pq}\right)
\end{aligned}$$

then

$$\mathbf{e}^p=\left(\mathbf{I}p-\mathbf{T}^{pq}\cdot\left(\mathbf{A}^q\right)^{-1}\cdot\tilde{\mathbf{T}}^{qp}\cdot\mathbf{A}^p\right)\cdot\mathbf{e}^{p\prime}_R$$

hp-multigrid

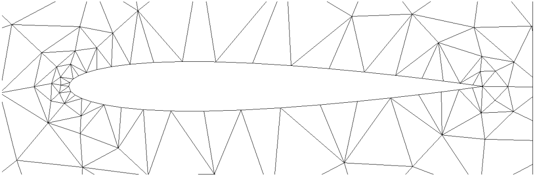
Performance for convective problems : Strategy

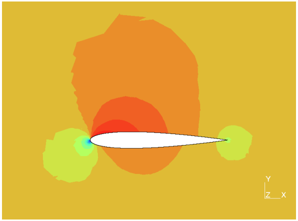


Schemes

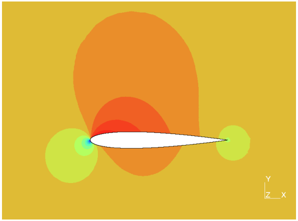
- 4step explicit Runge-Kutta on finest levels
- 10 pre- and postsmoothing steps
- hybrid cycles : Newton step at coarsest level

hp-multigrid : Performance for convective problems
NACA0012





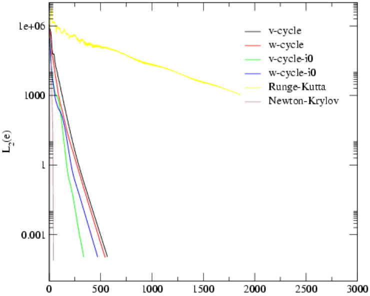
(f) p=2



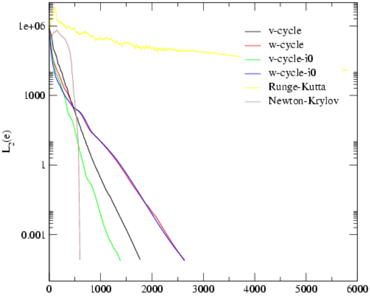
(g) p=4

hp-multigrid : Performance for convective problems

CPU comparison with Newton-Krylov - coarse mesh



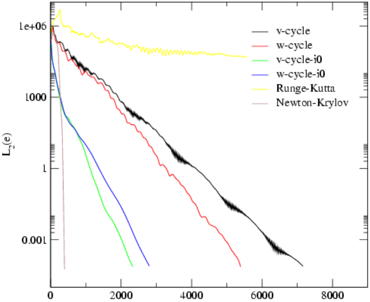
(h) p=2



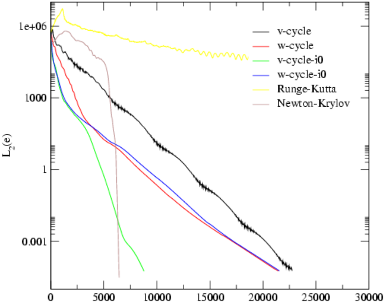
(i) p=4

hp-multigrid : Performance for convective problems

CPU comparison with Newton-Krylov - fine mesh



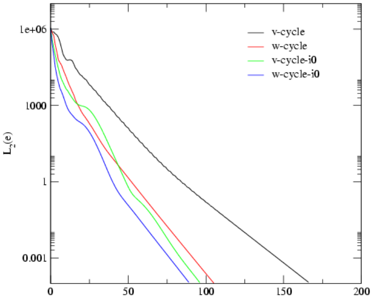
(j) p=2



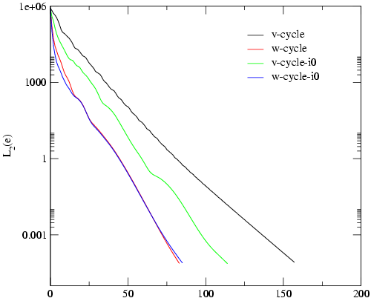
(k) p=4

hp-multigrid

Performance for convective problems : Cycling strategies - coarse mesh



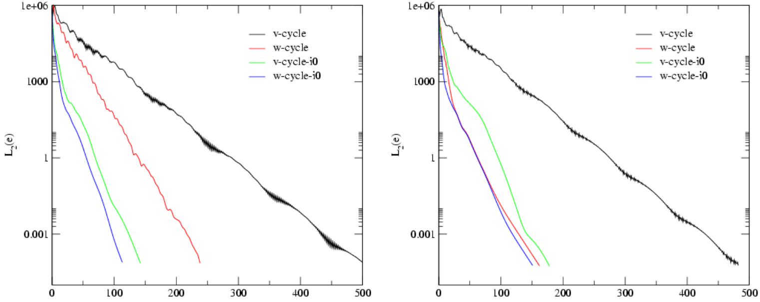
(l) p=2



(m) p=4

hp-multigrid

Performance for convective problems : Cycling strategies - fine mesh



(n) p=2 (o) p=4

hp-multigrid : Concluding remarks

Concluding remarks

Conclusions

- easy multigrid implementation for DG
- optimal transfer operators
- hybrid p-multigrid approach promising for inviscid flows (hybrid cycle)
- very easy to use for nested initial iterations

Further work

- h-Multigrid implementations on unstructured meshes
  - agglomeration multigrid *Tesini 2008* [Tes08]
  - nested meshes
  - independent meshes
  - directional coarsening
- design of smoothers for viscous flows *VdVegt, JCP [vdVR12a, vdVR12b]*, ?

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