h-to-*p* efficiently: a Nektar++ update on comparisons of CG and HDG

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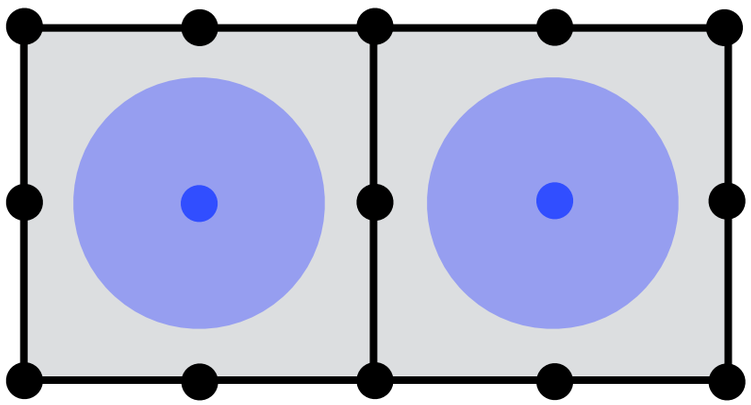
Outline

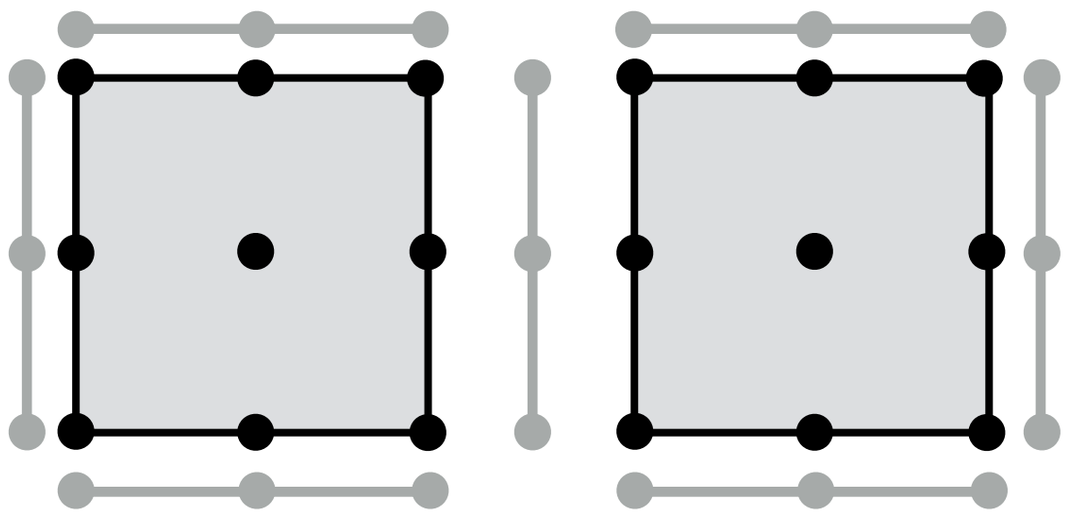
- Overview of CG and HDG formulations
- Goals
- Serial performance
- Parallel performance
- Conclusions

Formulations

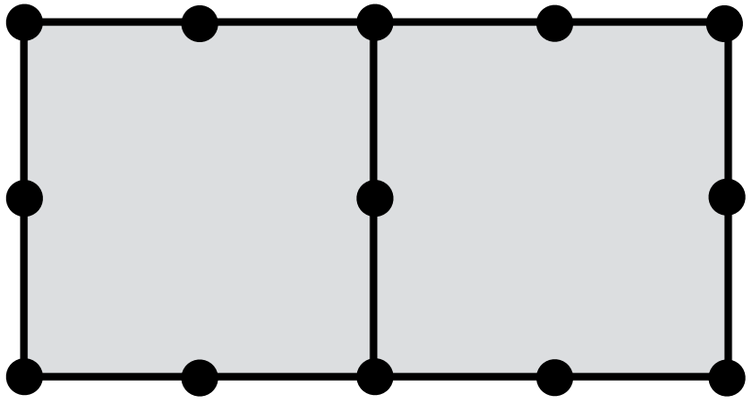
CG



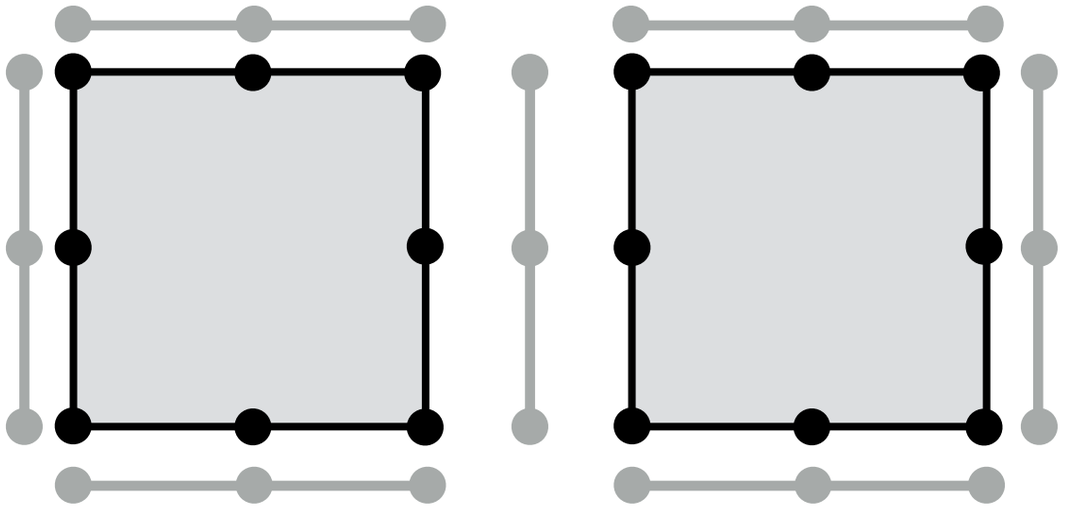
DG



static condensation



(statically condensed) CG



HDG

Formulations

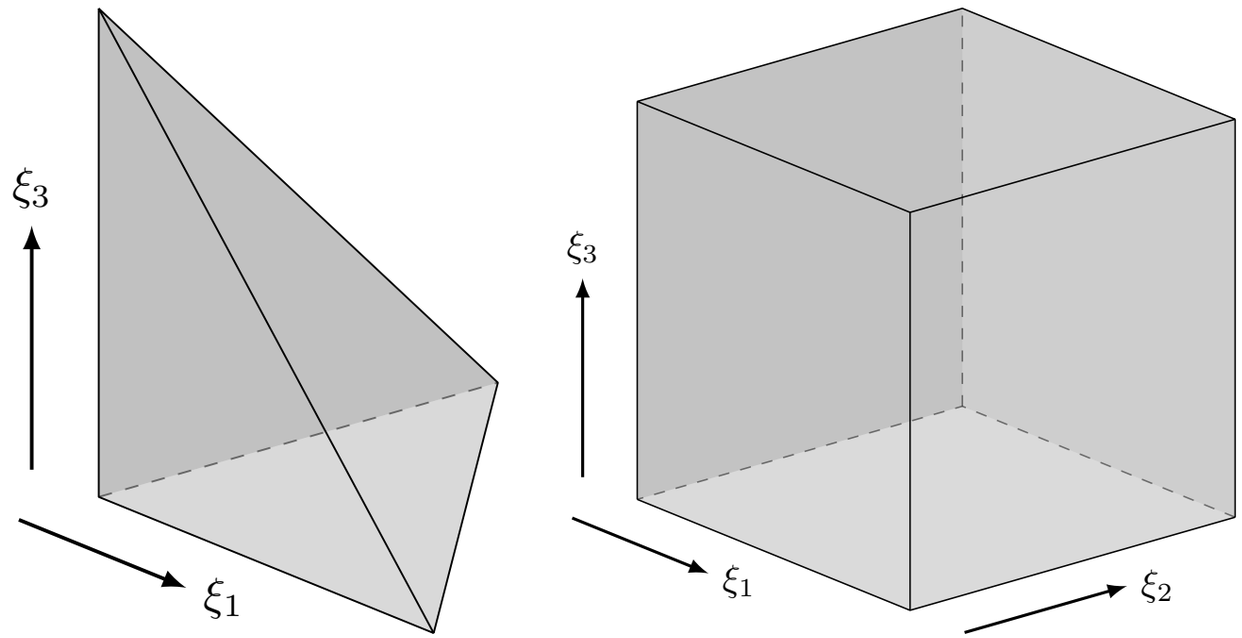
Continuous Galerkin (CG)

- Great for elliptic problems due to low degree of freedom (dof) count
- Established method: large body of knowledge

Discontinuous Galerkin (DG)

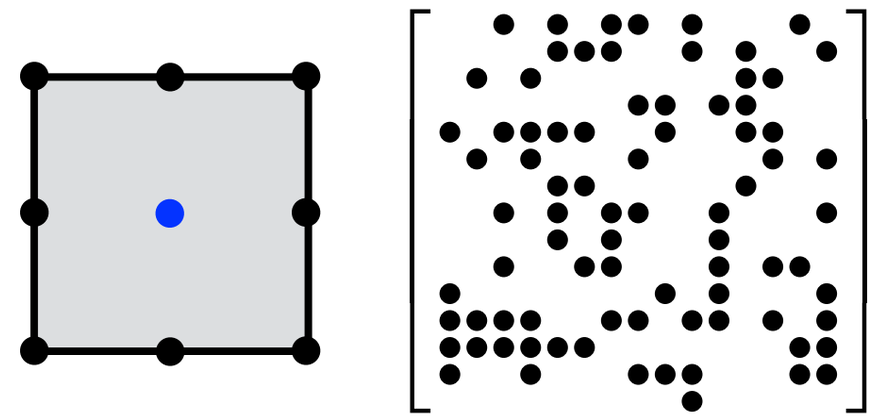
- Has attractive properties (local conservation)
- Great for hyperbolic problems
- Not as attractive for elliptic: higher DOF count

CG on an element



$\nabla^2 u$

Inner product with basis functions, integrate by parts



static cond.

$$\begin{bmatrix} L_{bb} & L_{ib} \\ L_{ib}^{\mathsf{T}} & L_{ii} \end{bmatrix}$$

Hex and tet standard elements

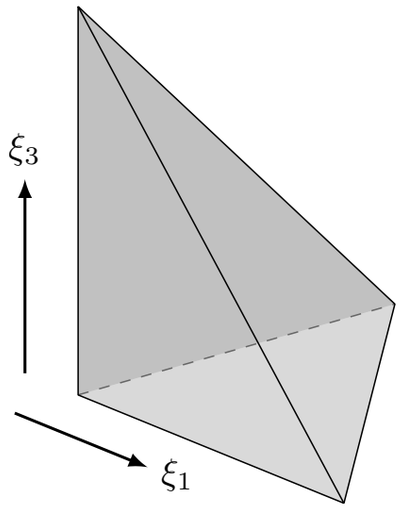
Modified orthogonal basis, order *P*

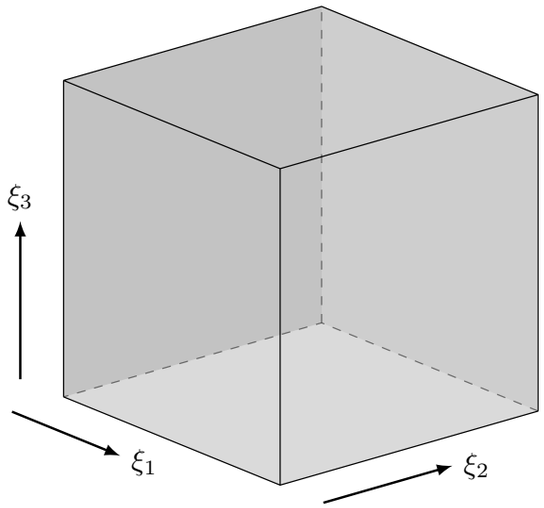
Isoparametric curvilinear elements

b = boundary

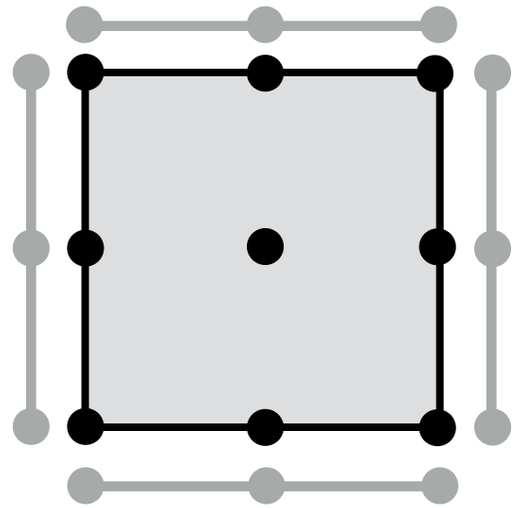
i = interior

HDG on an element

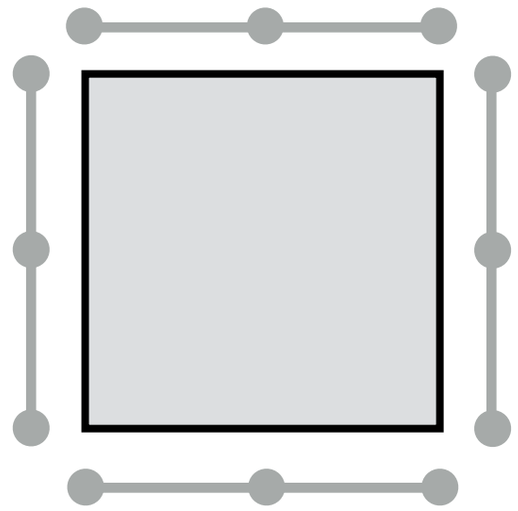




$$\boldsymbol{q} = \nabla u$$
$$u = \mathrm{div}(\boldsymbol{q}) \quad \text{on } \Omega$$



$u = \lambda$ on $\partial\Omega$
(static condensation)



A_λ local boundary system

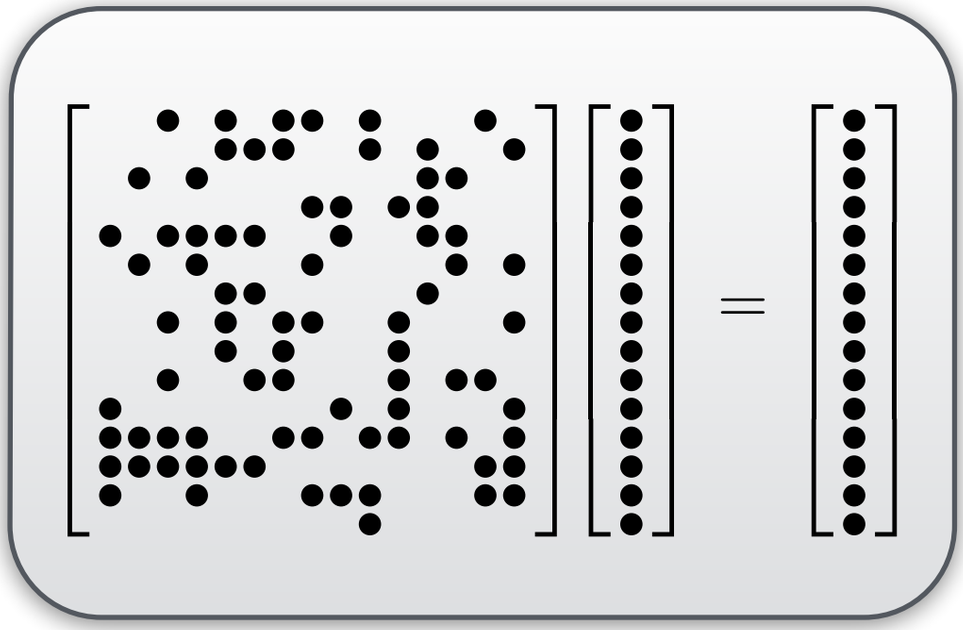
A_i interior solve

$A_{\lambda \to u}$ project λ onto u

Global matrices

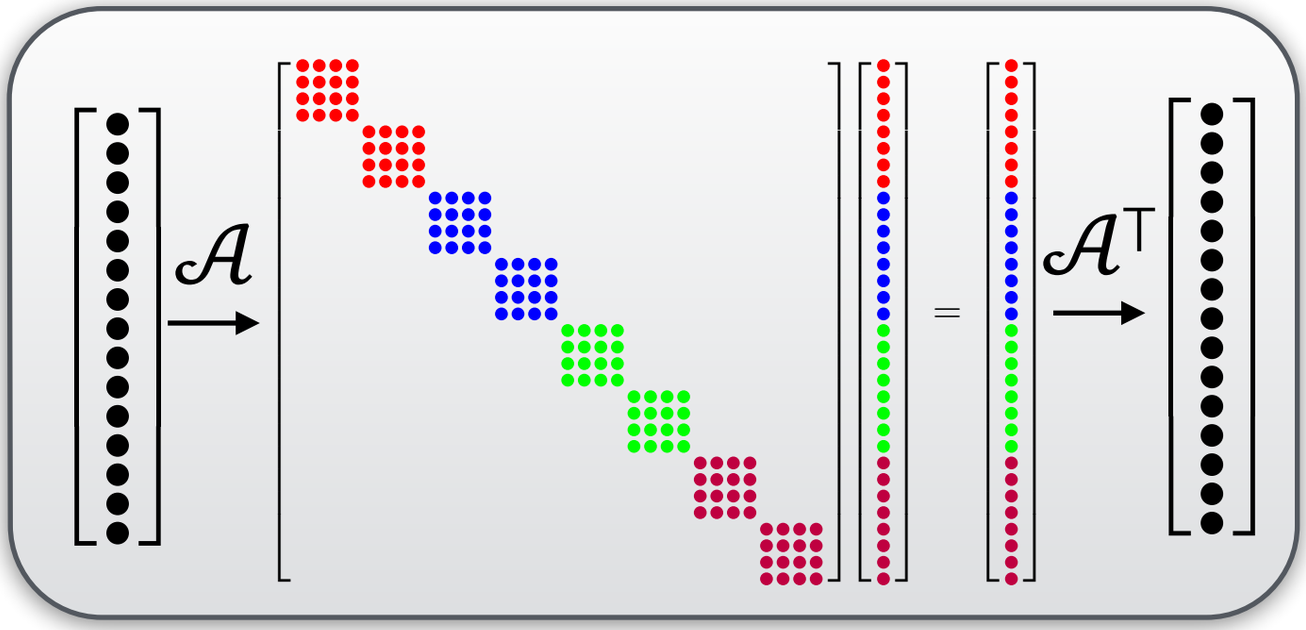
- Once we have *local* elemental matrices, need to form a *global* matrix for the entire system
- Create an *assembly map* $\mathcal{A}$ that establishes connections between elements based on mesh
- Can be seen as a global-to-local operator
- **Serial:** construct a global matrix and solve directly
- **Parallel:** form action of the global matrix using elemental matrices and assembly map

Global matrices



Global approach

serial + direct solve



Local approach
(gather-scatter)

parallel + PCG solve

Goals

- Follow on from previous study in 2D: **3D mixed elements**
- How does HDG fare against CG for:
  - Smaller problems (direct solve, **serial**)
  - Large problems (iterative solve, **parallel**)
- Performance for **elliptic** vs. **parabolic** solve
- Effect of **structured** vs. **unstructured** mesh
- In parallel, how does each method **scale**?
- How might these performance characteristics reflect in terms of complex systems?
- **Be fair** to both methods: same codebase, Nektar++

Models

$$\nabla^2 u + \lambda u = f$$

Helmholtz equation
(elliptic)

$$\frac{\partial u}{\partial t} = \nabla^2 u$$

Diffusion equation
(parabolic)

- Fundamental elliptic and parabolic equations with known non-polynomial exact solutions
- The building blocks of more complex operators
- e.g. incompressible Navier-Stokes: 1 x Poisson solve (pressure) + 3 x Helmholtz solve (velocity)

A priori expectations

- In both cases, we expect there might be a crossover point

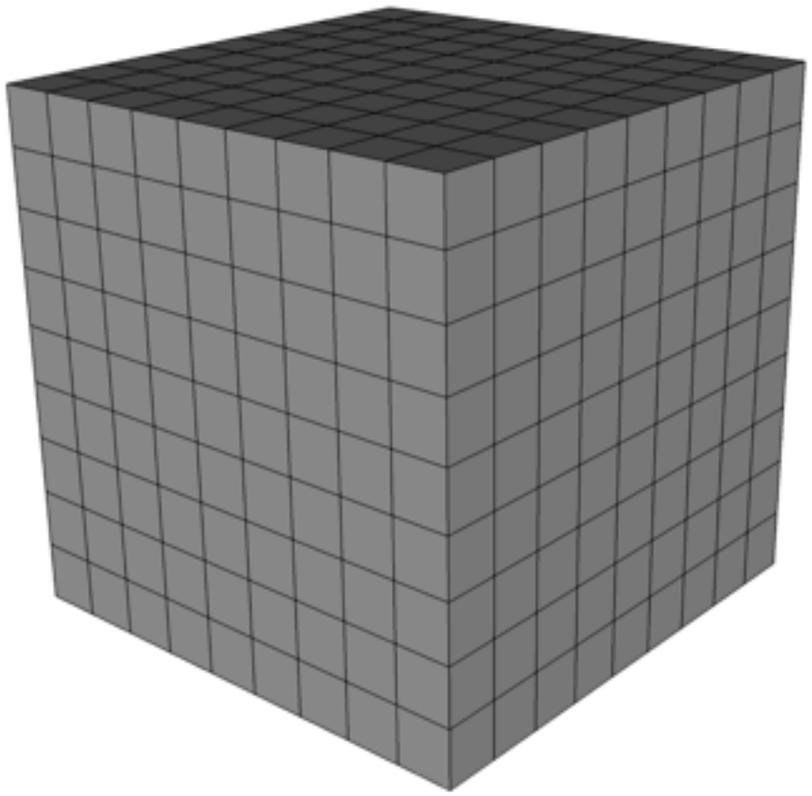
- **Serial:** factors include system bandwidth (as in 2D case), efficiency of direct solver

- **Parallel:** could depend on a number of factors: preconditioner/condition number, interconnect, mesh topology, communication patterns, ...

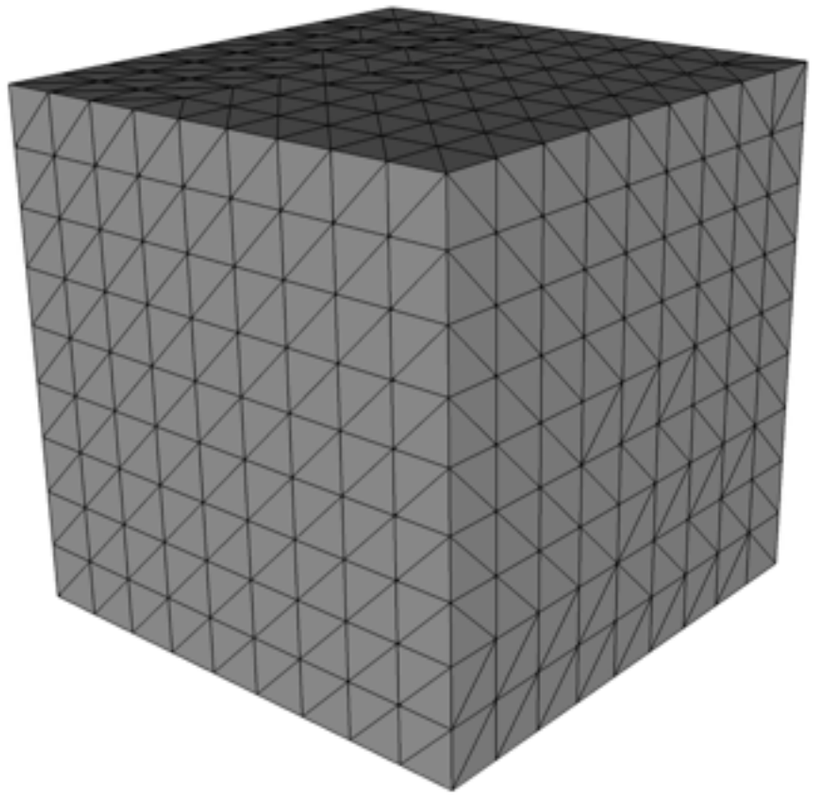
HDG postprocessing

- For some PDEs we can use an order *p* solution to construct a solution which is ***p* + 1** accurate
- Not clear whether this can hold for non-linear or time evolved systems
- However important to take into consideration when doing our timings

Serial performance



9^3 hex mesh



6 x 9^3 tet mesh

Helmholtz equation, Dirichlet boundary conditions

$\Omega = [-1,1]^3$, $u(\boldsymbol{x}) = \sin(5\pi x)\sin(5\pi y)\sin(5\pi z)$

Convergence validation

N_{CG}	Hexahedra		Tetrahedra		N_{HDG}
	L^2_{CG}	L^2_{HDG}	L^2_{CG}	L^2_{HDG}	
3	1.944e-02	8.301e-02	1.686e-01	1.323e-01	2
4	2.126e-03	6.046e-03	5.522e-02	4.367e-02	3
5	1.833e-04	3.449e-04	1.673e-02	1.373e-02	4
6	1.325e-05	2.504e-05	4.431e-03	3.981e-03	5
7	8.201e-07	1.460e-06	1.085e-03	9.973e-04	6
8	4.460e-08	7.863e-08	2.388e-04	2.283e-04	7
9	2.151e-09	3.828e-09	4.707e-05	4.562e-05	8

Serial performance

N_{CG}	DSC			DMSC			N_{HDG}
	CG	HDG	$\frac{\text{HDG}}{\text{CG}}$	CG	HDG	$\frac{\text{HDG}}{\text{CG}}$	
3	4.92	6.07	1.24	7.46	4.96	0.66	2
4	80.96	48.44	0.60	48.32	31.51	0.65	3
5	564.31	243.17	0.43	297.90	169.73	0.57	4
6	2661.04	947.12	0.36	1103.36	791.51	0.72	5
7	8765.75	2709.26	0.31	3397.99	2642.24	0.78	6
8	25450.47	6917.71	0.27	8789.20	7051.14	0.80	7
9	58228.23	16177.59	0.28	19580.75	17786.10	0.91	8

Hex cube mesh

DSC: direct static condensation

DMSC: direct **multi-level** static condensation

Serial performance

N_{CG}	DSC			DMSC			N_{HDG}
	CG	HDG	$\frac{\text{HDG}}{\text{CG}}$	CG	HDG	$\frac{\text{HDG}}{\text{CG}}$	
3	0.73	3.28	4.52	3.46	2.92	0.84	2
4	4.86	12.29	2.53	14.02	9.05	0.65	3
5	42.04	46.71	1.11	59.39	29.30	0.49	4
6	220.04	144.82	0.66	154.89	92.03	0.59	5
7	819.23	399.07	0.49	777.43	297.04	0.38	6
8	2282.90	885.17	0.39	2057.15	796.64	0.39	7
9	5747.78	1852.25	0.32	4081.03	1712.52	0.42	8

Tet cube mesh

Parallel performance

- Most operations (e.g. matrix construction) are trivially parallelisable: hard part is matrix solve

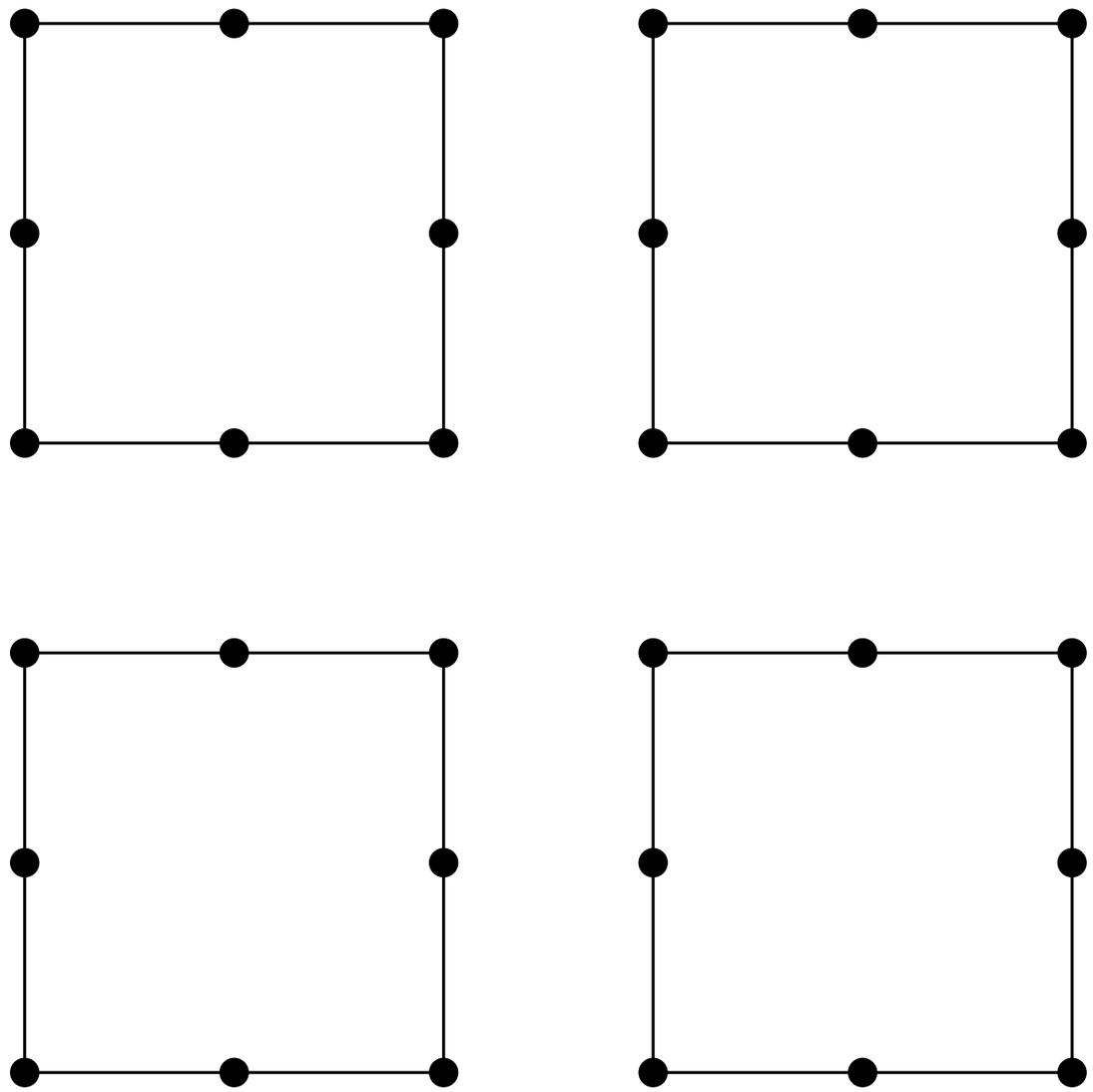
- Use preconditioned conjugate gradient (PCG)

- Most complex operation: gather-scatter required for matrix action: we use gslib (part of Nek5000)

- Measure both **weak** and **strong** scaling

- Tests on **HECToR**: 32 and 4,096 cores, **ARCHER**: 24 and 3,072 cores (1 to 128 nodes)

Communication patterns



HDG: elemental pairwise

CG: much more complex

Preconditioners and fair metrics

- CG and HDG systems will have different sizes and conditioning properties

- Therefore timings will depend (mostly) on:
  - # iterations / choice of preconditioner
  - cost of block matrix-vector multiply
  - interconnect and communication properties

- We can always build better preconditioners

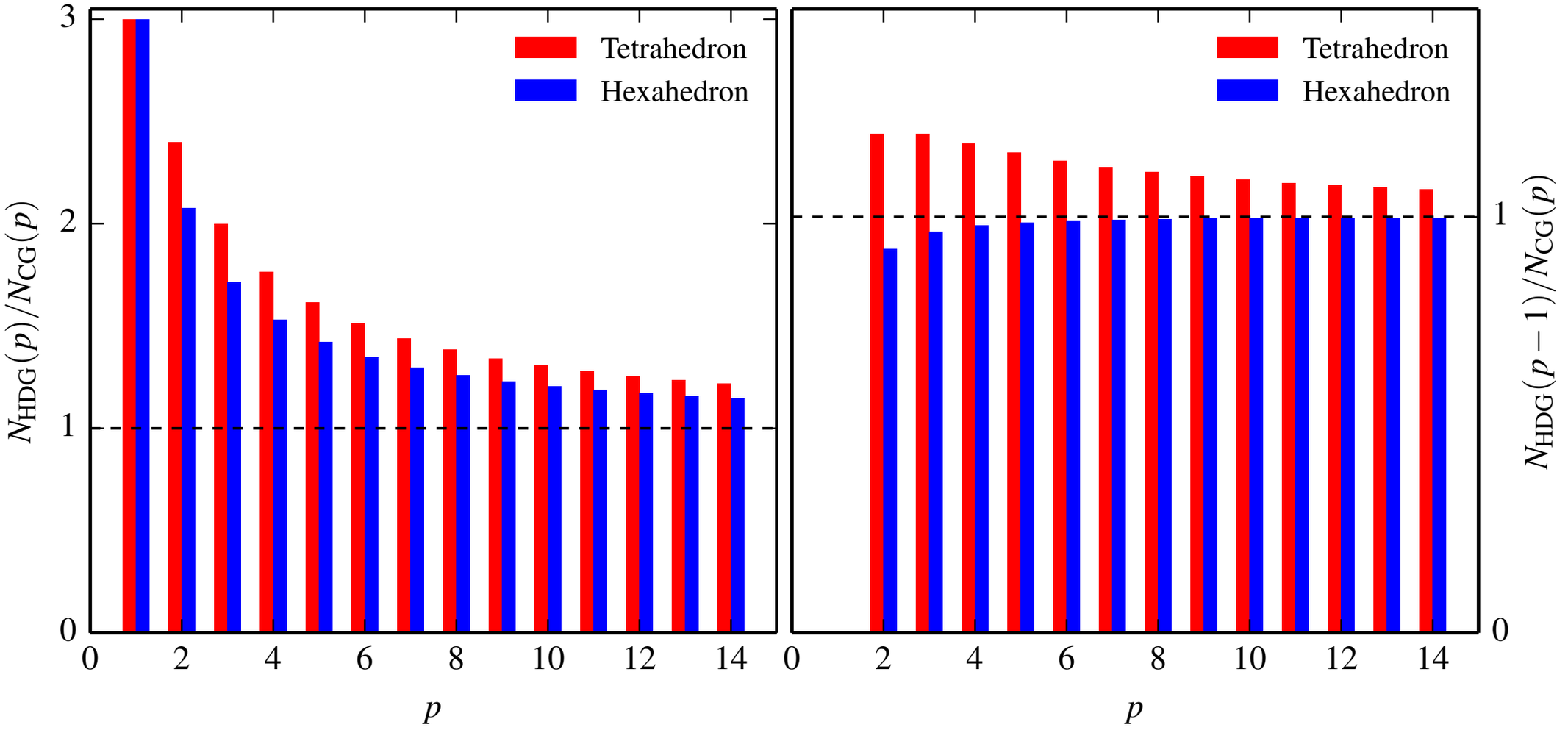
- **Fairness:** use Jacobi precon, measure time/iteration

Preconditioners: justification

N_{HDG}	HDG block	CG block	CG low energy	CG linear space	N_{CG}
2	130	51	37	29	3
3	157	98	53	35	4
4	203	150	62	38	5
5	223	204	69	40	6
6	245	252	74	41	7
7	258	295	78	42	8
8	279	345	82	44	9

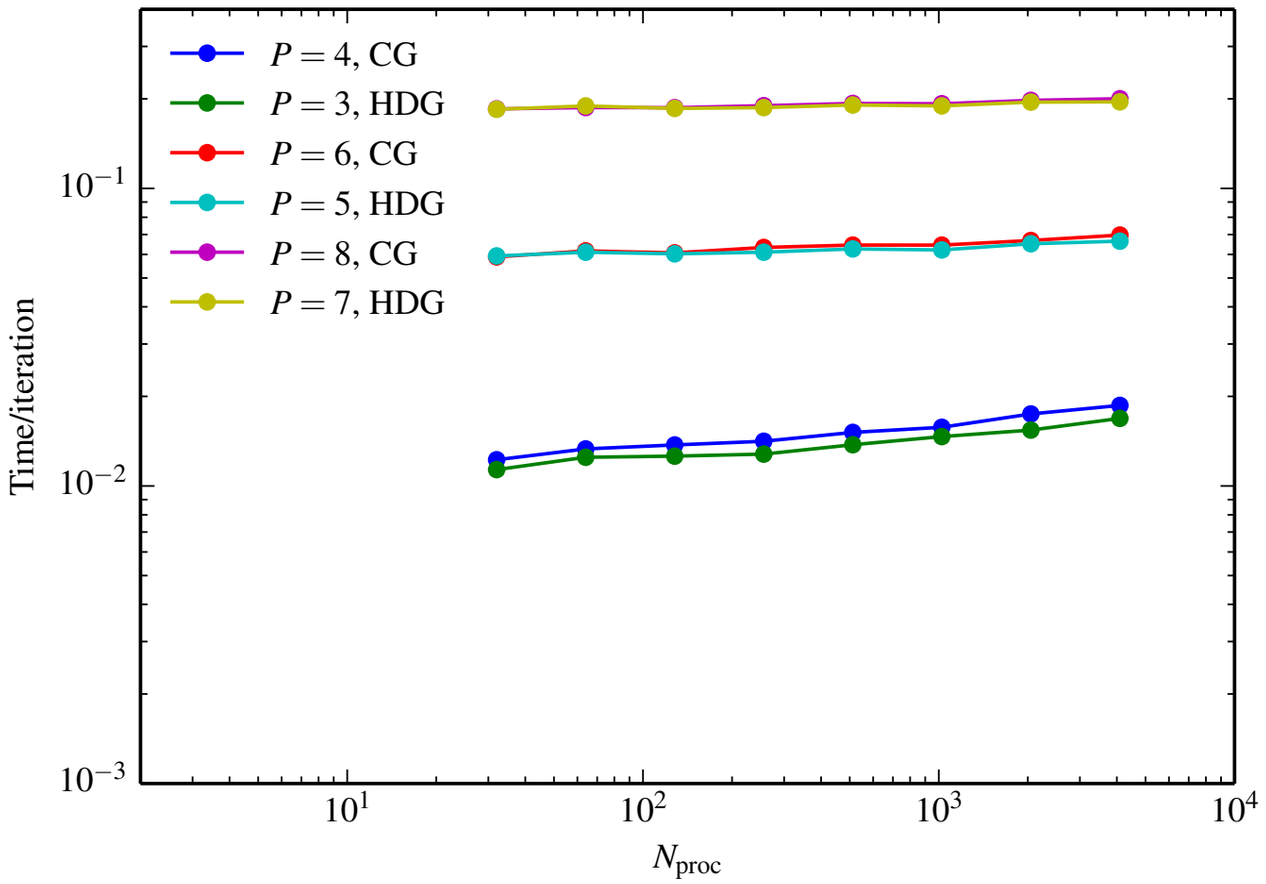
- Measure # iterations for unsteady diffusion equation
- **HDG/CG block:** invert block representing each trace face (HDG) or vertex/edge/face blocks (CG)
- **CG low energy:** basis transform
- **CG linear space:** LE + coarse space precon

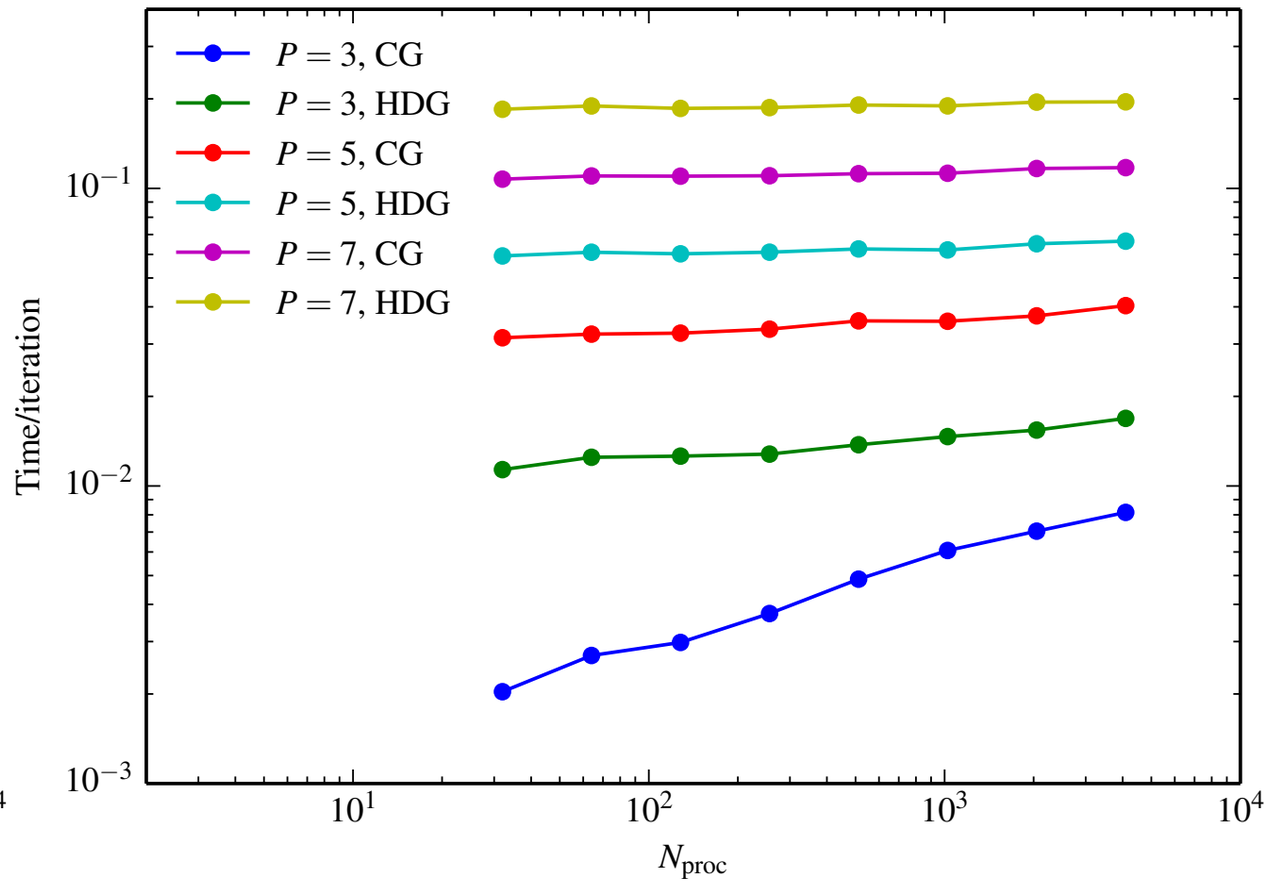
Matrix block sizes



HDG local blocks are far larger unless postprocessing taken into account

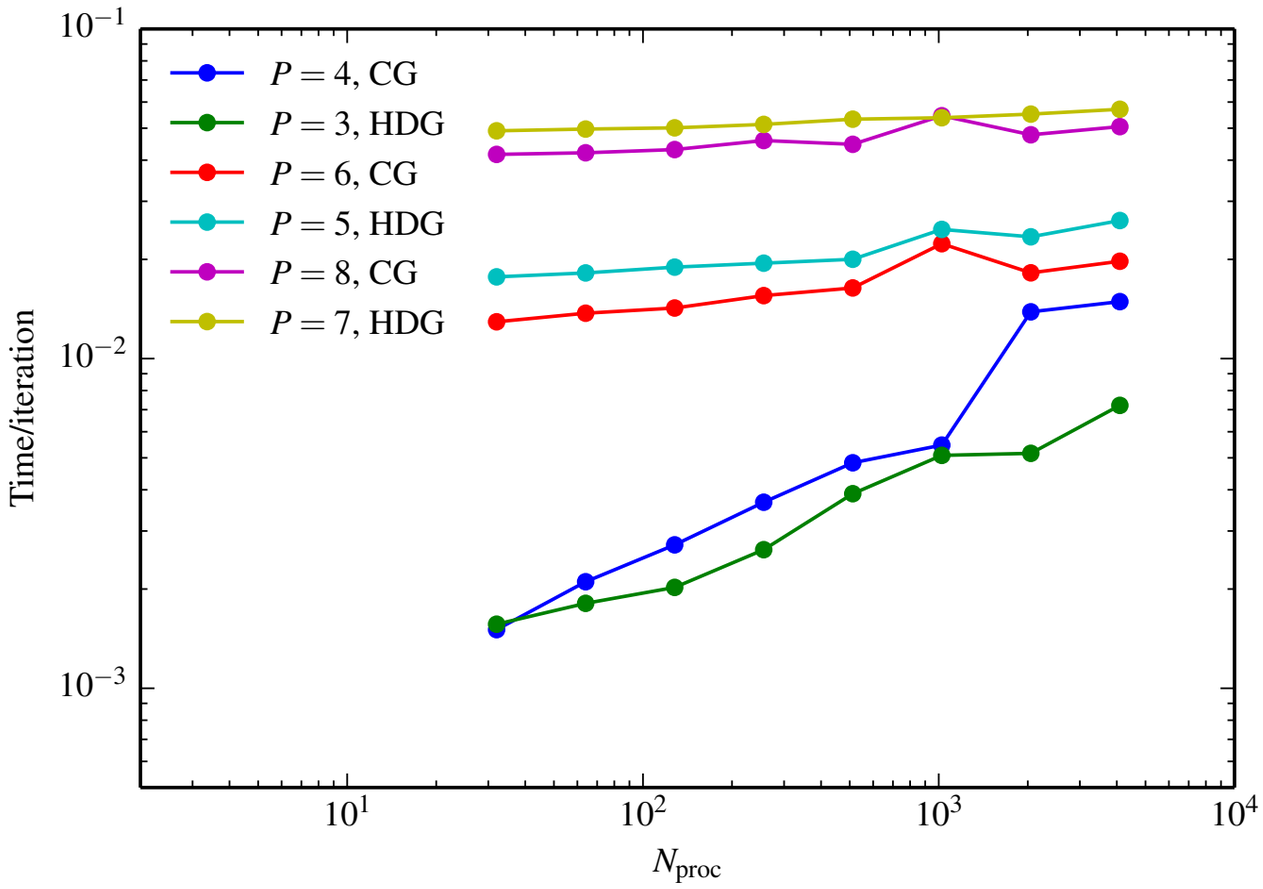
Weak scaling (hex)

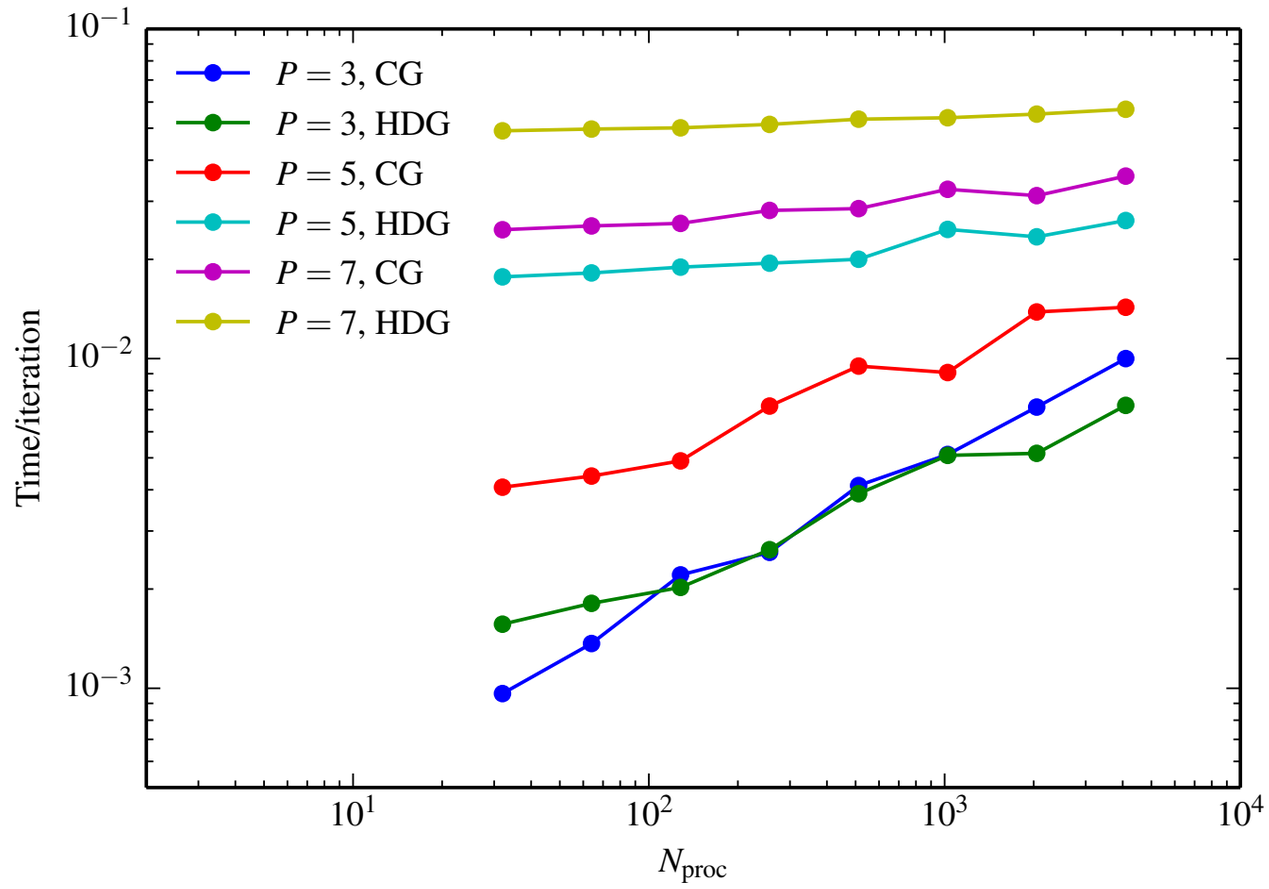




Cube geometry
3^3 hexes per core

Weak scaling (tet)

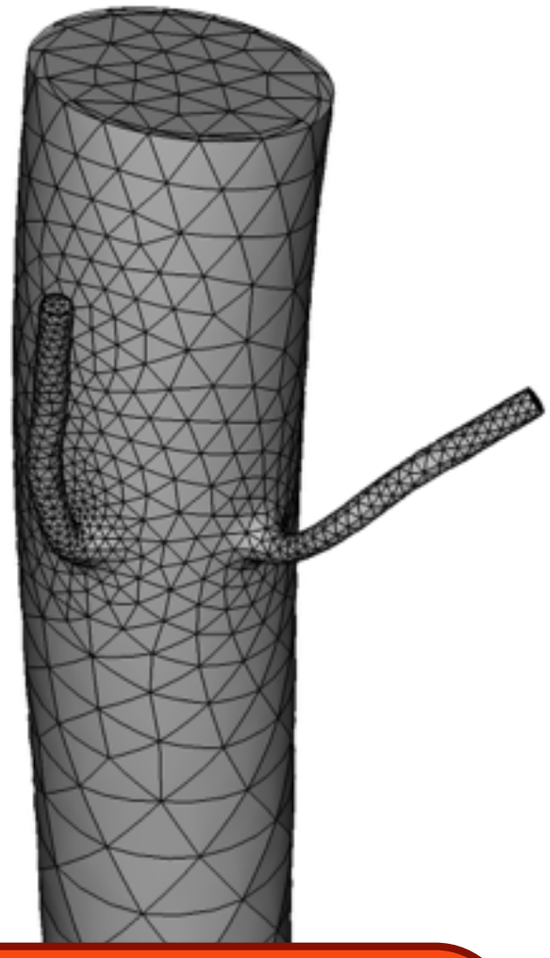


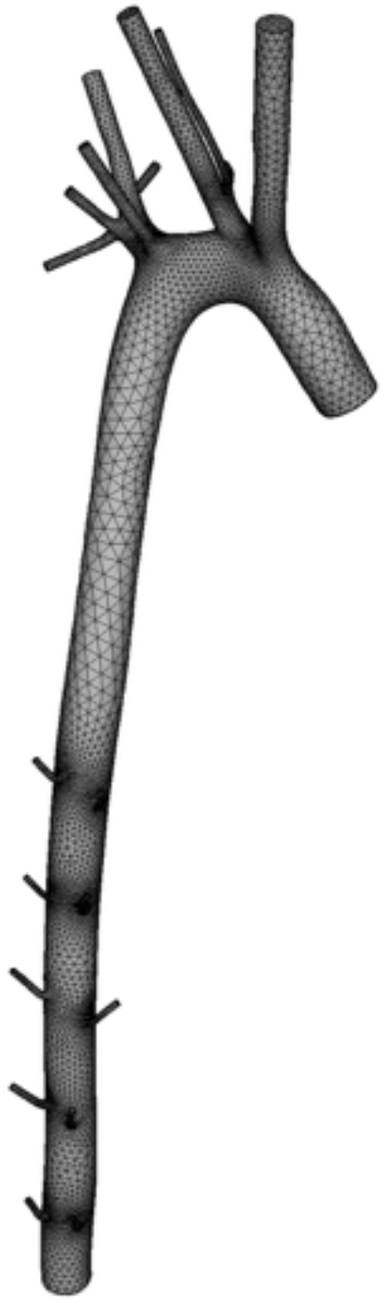


Cube geometry
6 x 2^3 tets per core

Strong scaling

intercostal pair
~8,500 tets
higher P

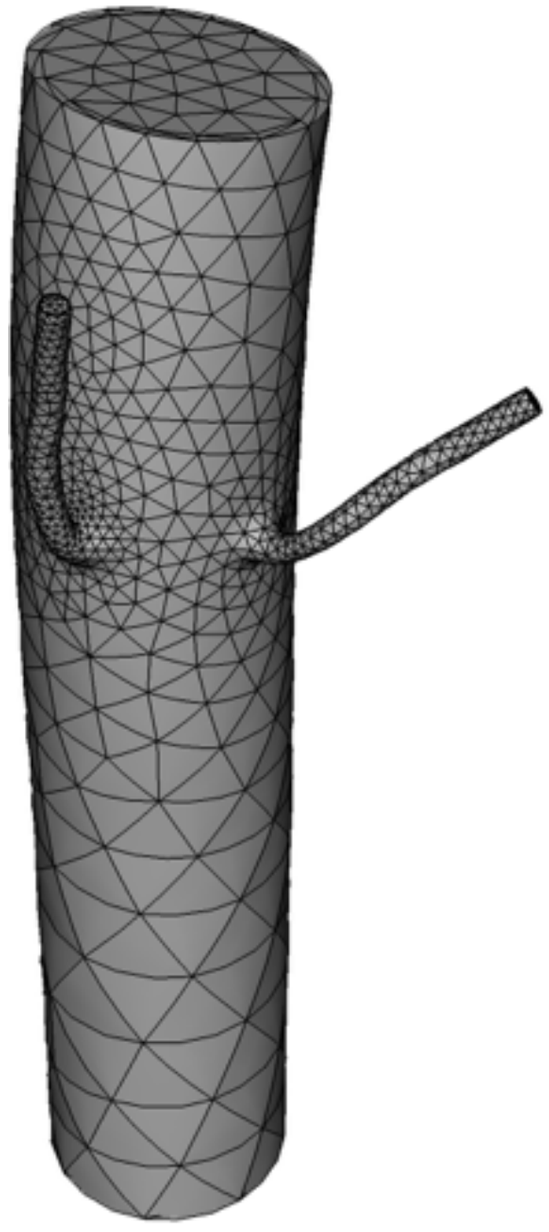


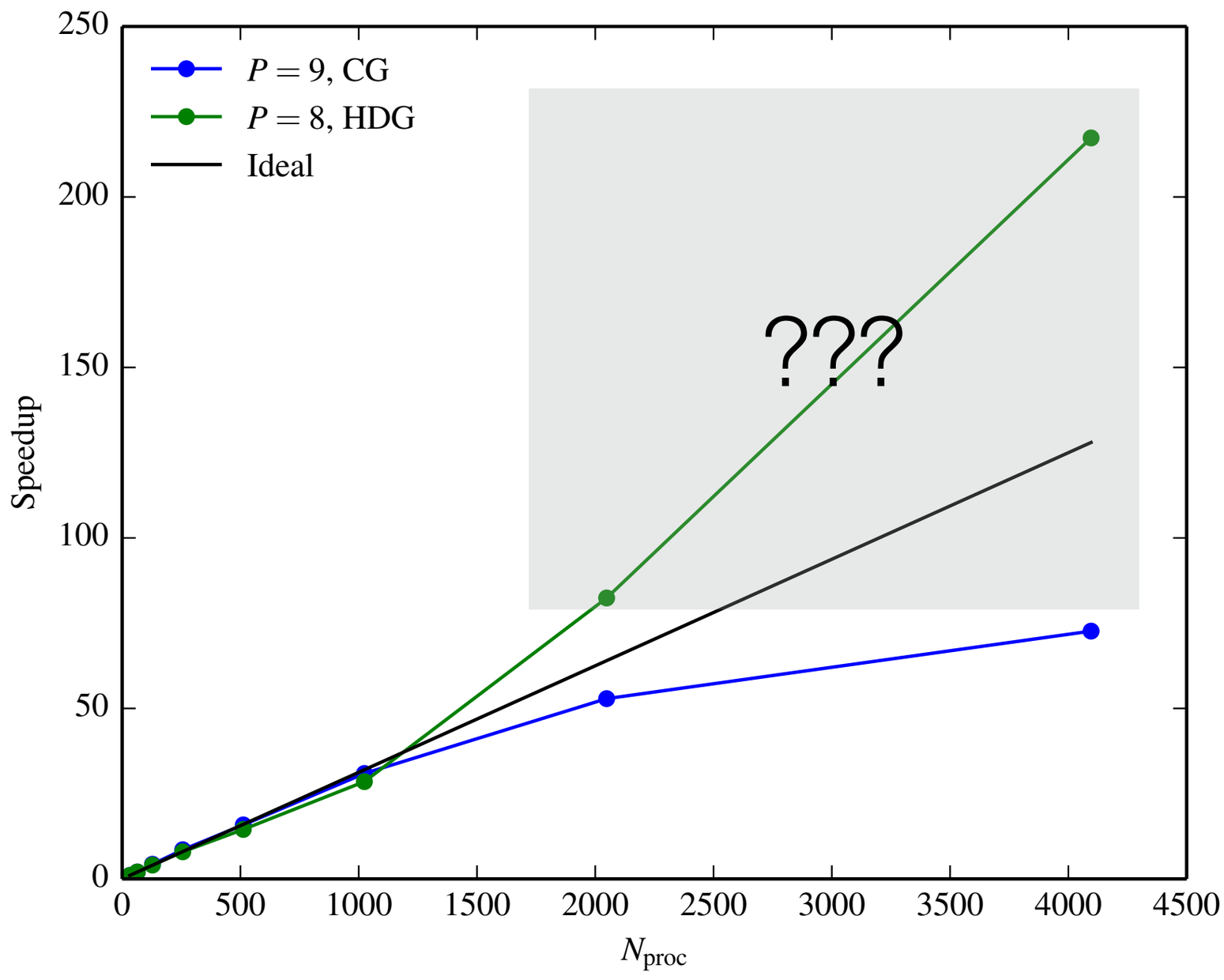


aortic arch
~150,000 tets
lower *P*

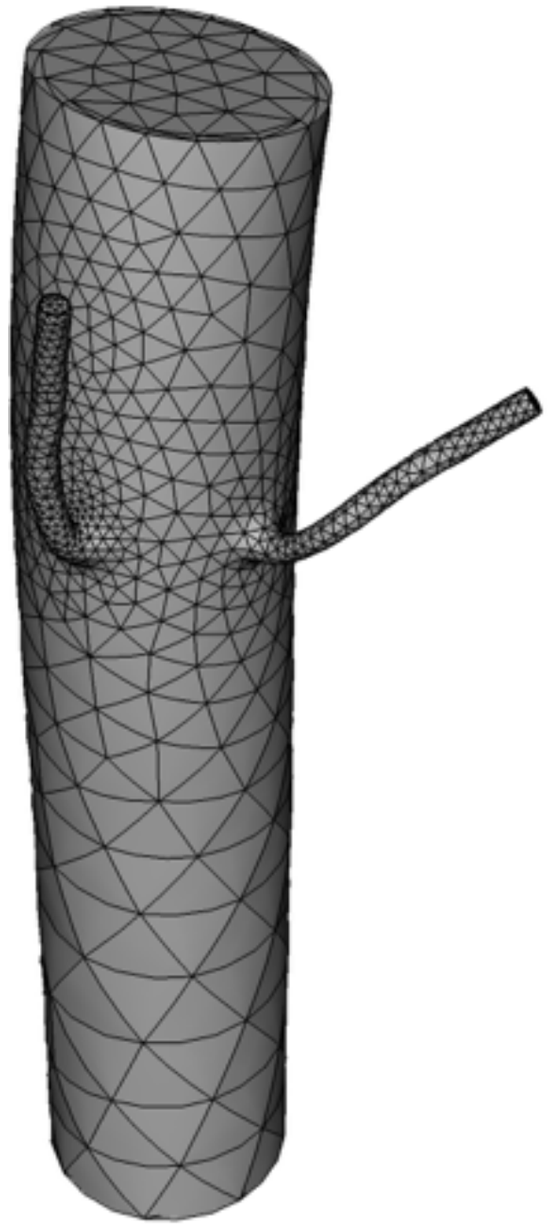
Mean vertex valency: 12
Max vertex valency: 44!

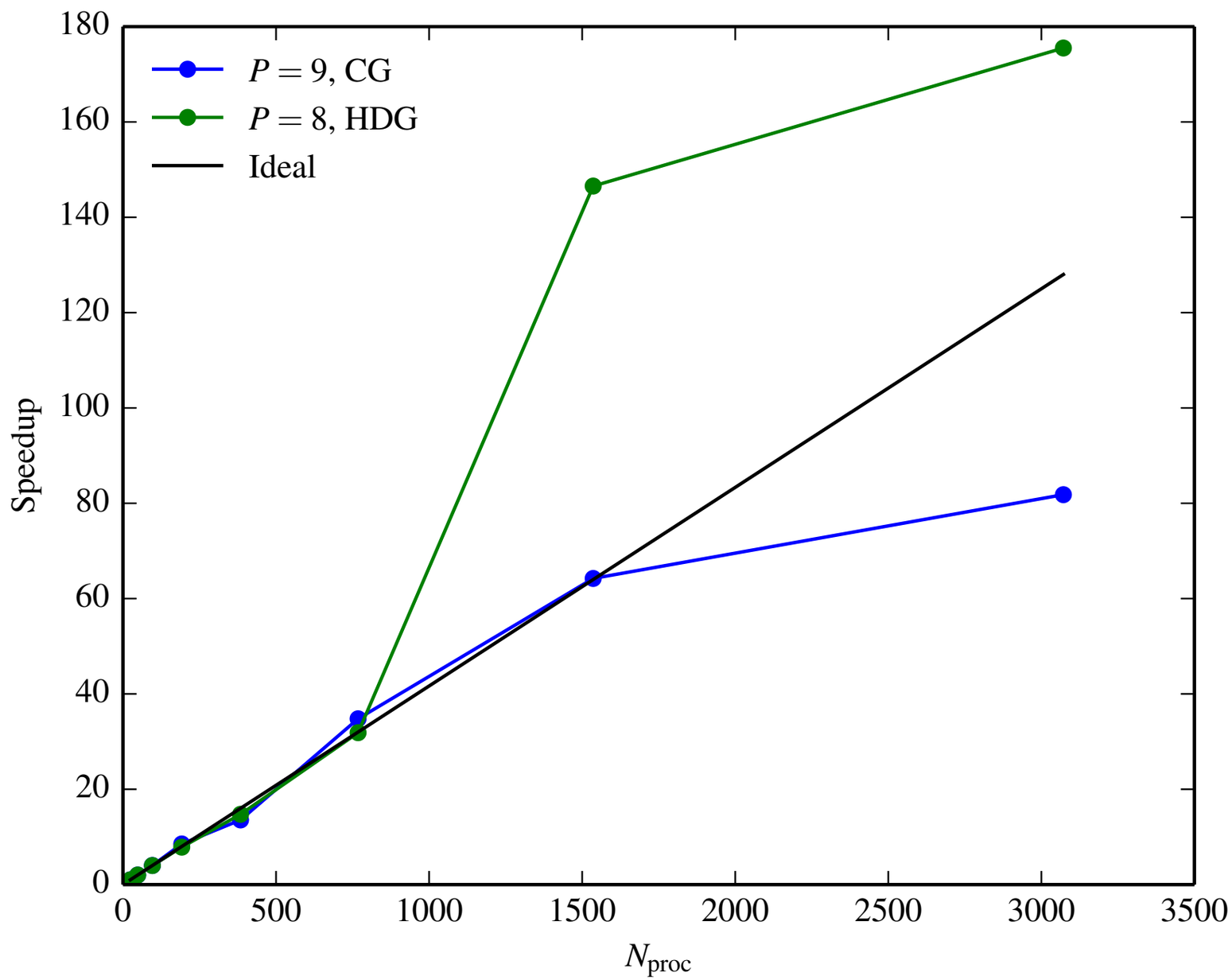
Strong scaling



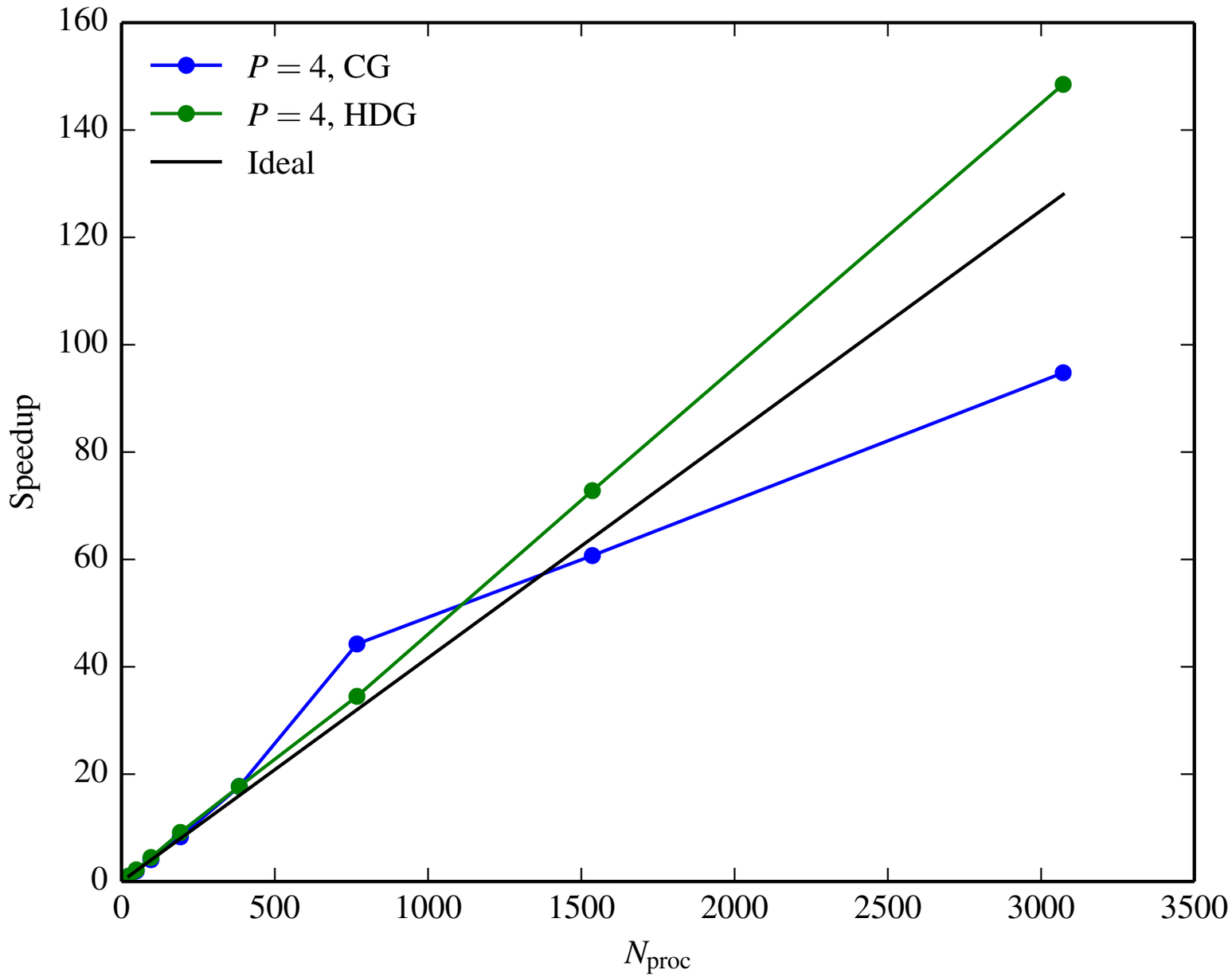


Strong scaling





Strong scaling



Summary

Direct solver + postprocessing

- HDG outperforms CG to various degrees depending on mesh + solver for elliptic problems
- Less pronounced for tetrahedral mesh

Iterative solver

- w/postprocessing: HDG can (barely) match CG
- Still need effective preconditioning strategy

Parallel

- HDG can outperform CG *on per-iteration basis* when communication cost is high
- However scaling is still pretty good for both methods

Nektar++ high-order framework

Framework for spectral(/hp) element method:

- Dimension independent, supports CG/DG/HDG
- Mixed elements (quads/tris, hexes, prisms, tets, pyramids) using hierarchical modal and classical nodal formulations
- Solvers for (in)compressible Navier-Stokes, advection-diffusion-reaction, shallow water equations, ...
- Parallelised with MPI, tested scaling up to ~10k cores

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Thanks for listening!

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