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UKAEA NEPTUNE Mathematical Support Project

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Who we are

Hussam

STFC

Rutherford Appleton Laboratory (RAL)

Hartree Centre

Sue

Numerical Linear Algebra

Data analytics

AI

HPC

Large-scale optimisation

Niall

Tyrone

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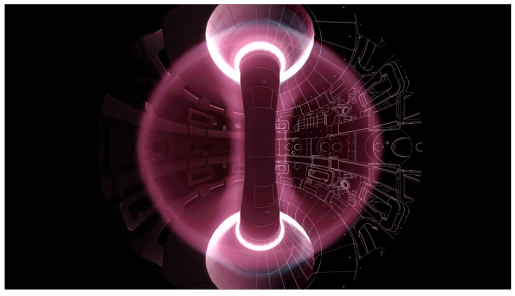
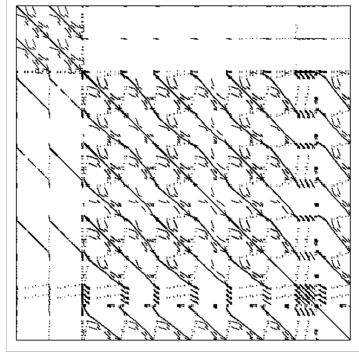
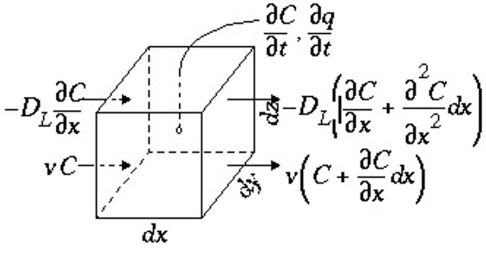
The big picture

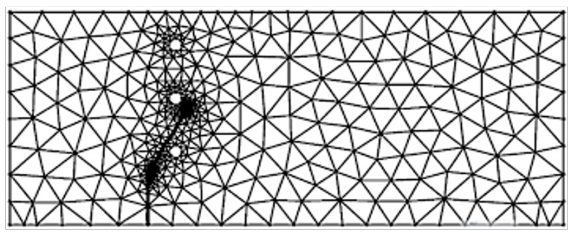


$$\frac{du_1}{dx} = \frac{-3u_1 + 4u_2 - u_3}{2h}$$
$$\frac{du_i}{dx} = \frac{-u_{i+1} + u_{i+1}}{2h},\ i = 2(1)N-2$$
$$\frac{du_{N-1}}{dx} = \frac{u_{N-3} - 4u_{N-2} + 3u_{N-1}}{2h}.$$



Mathematical Model → Discretisation → Solve Linear Systems





```
procedure pcg(A, Θ^k, b̄)
1    Compute Δy_0 as a guess of Δy^k;
2    r_0 := b̄ − AΘ^k A^⊤ Δy_0;
3    solve M z_0 = r_0;
4    p_0 := z_0;
5    i := 0;
6    do stopping criterion not satisfied →
7        q_i := AΘ^k A^⊤ p_i;
8        α_i := z_i^⊤ r_i / p_i^⊤ q_i;
9        Δy_{i+1} := Δy_i + α_i p_i;
10       r_{i+1} := r_i − α_i q_i;
11       solve M z_{i+1} = r_{i+1};
12       β_i := z_{i+1}^⊤ r_{i+1} / z_i^⊤ r_i;
13       p_{i+1} := z_{i+1} + β_i p_i;
14       i := i + 1
15   od;
16   Δy^k := Δy_i
end pcg;
```

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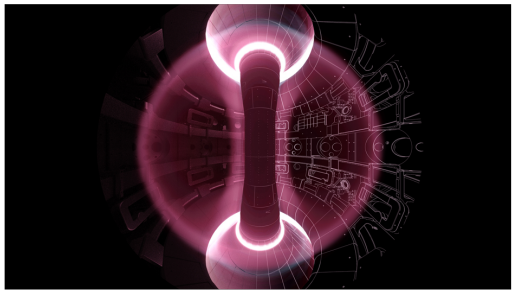
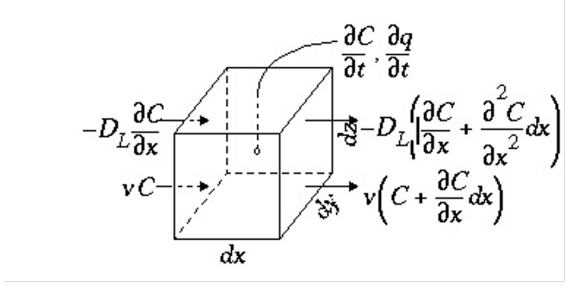
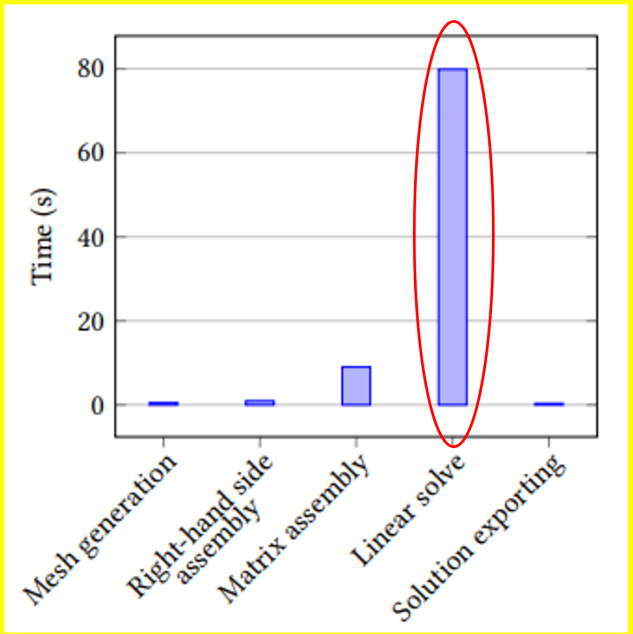
The big picture

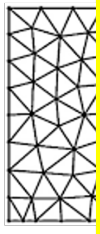


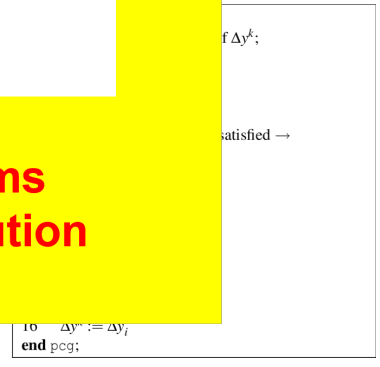
Mathematical Model

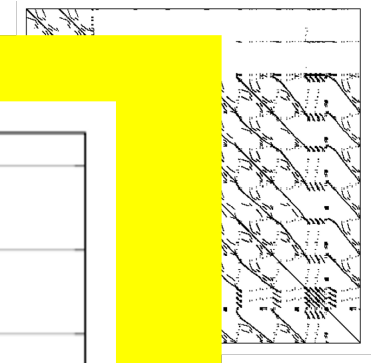




Solving linear systems dominates time to solution







inear
ms

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Time dependent solvers

We consider fully IRK methods

- high order accuracy
- require solving classic LS as in backward Euler

Solving linear systems – preconditioning

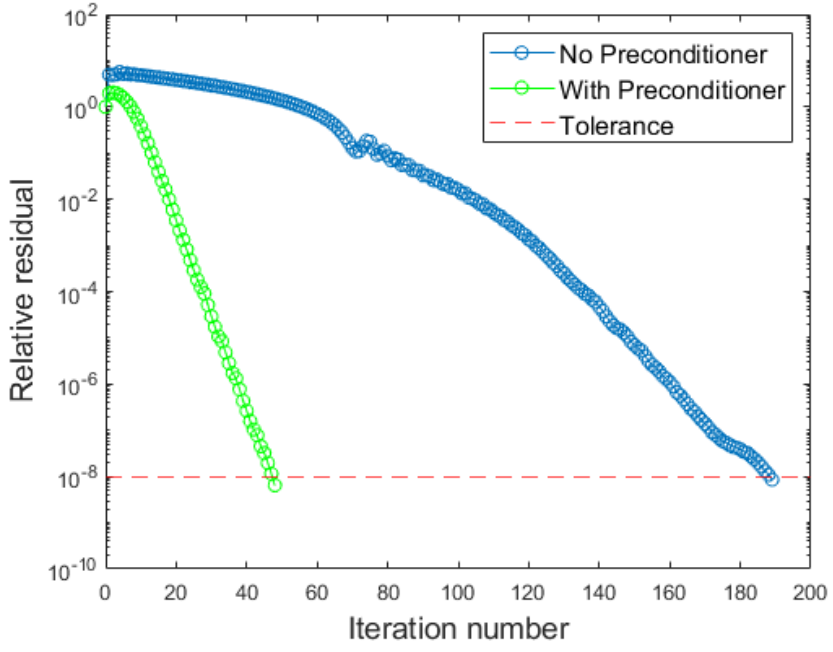
- Linear systems from discretised PDE models are typically very large and sparse
- Iterative methods are best suited to solve them
- However, properties degrade for real problems of interest (ill-conditioning prohibits convergence)
- Poor convergence avoided by having a good **preconditioner**

Solve

$$Ax = b$$

vs

$$\mathbf{P}Ax = \mathbf{P}b$$



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High-order finite elements

Solving is particularly challenging for high-order finite elements

Higher p gives better accuracy (exponential vs linear in # DOFs) but increased cost

	Complexity	Low order ($p = 1$)	High order ($p = 8$)
DOFs per element	$\mathcal{O}(p^d)$	~ 1	$\sim 8^d$
# of couplings	$\mathcal{O}(p^d)$	~ 1	$\sim 8^d$
non-zeros (memory)	$\mathcal{O}(p^{2d})$	~ 1	$\sim 64^d$
matrix-free memory	$\mathcal{O}(p^d)$	~ 1	$\sim 8^d$
matrix-free action	$\mathcal{O}(dp^{d+1})$	$\sim d$	$\sim d8^{d+1}$

Preconditioners for HO FEM

Leverage well-established preconditioners such as Algebraic Multigrid and Domain Decomposition methods.
Should avoid as possible assembling the HO operator matrix
Options

- use p-hierarchy of grids
- use the low-order operator matrix assembled on a refined mesh

If assembled, static condensation should be used

Synthetic results

Diffusion

Tests on orders up to $p = 13$, anisotropy (coef $10^{-6} - 1$, mesh $0.3 - 1$)

- Homogeneous diffusion: pMG scales perfectly
- Anisotropic diffusion (coef) : LOR AMG scales perfectly
- Anisotropic diffusion (mesh) : LOR AMG scales perfectly
- Anisotropic diffusion (coef&mesh): tough

Advection-diffusion

Tests on orders up to $p = 8$, viscosity $10^{-4} - 1$

- LOR AMG scales well

Numerical experiments

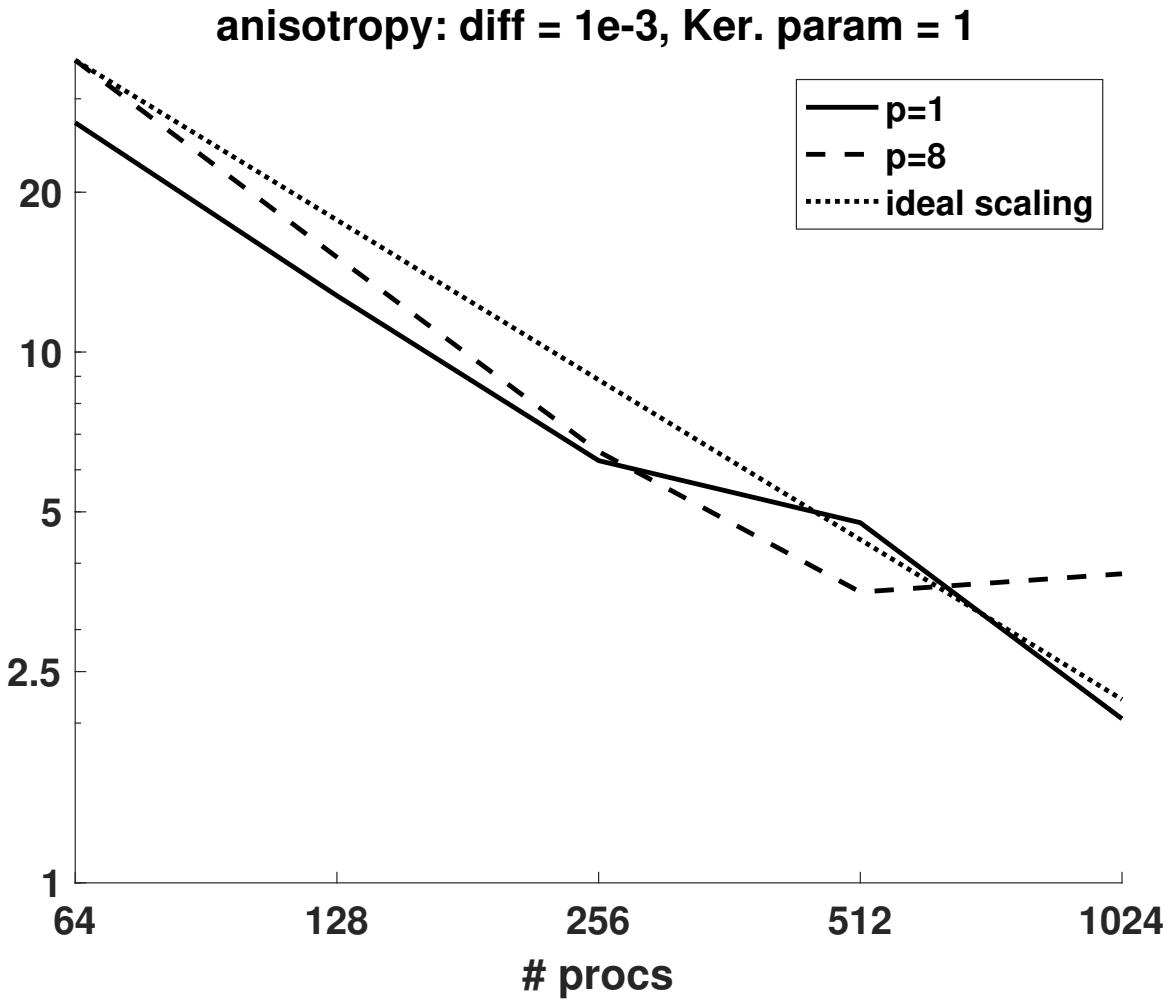

Figure: #DOFs $\approx$ 67M. # iter$_{p=1}$ = 11. # iter$_{p=8}$ = 15

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Numerical experiments

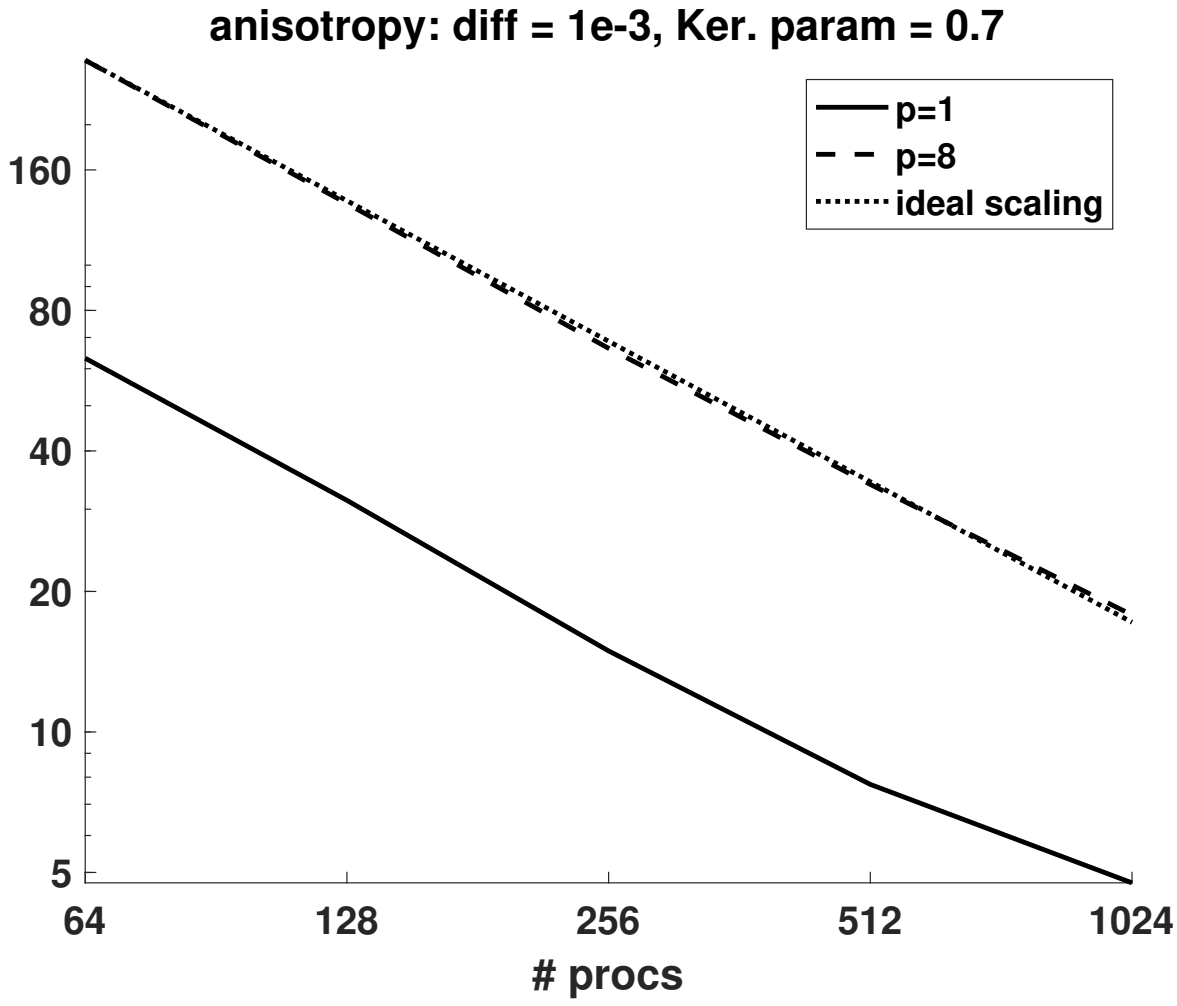

Figure: #DOFs $\approx$ 67M. # iter$_{p=1}$ = 53. # iter$_{p=8}$ = 317

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Numerical experiments

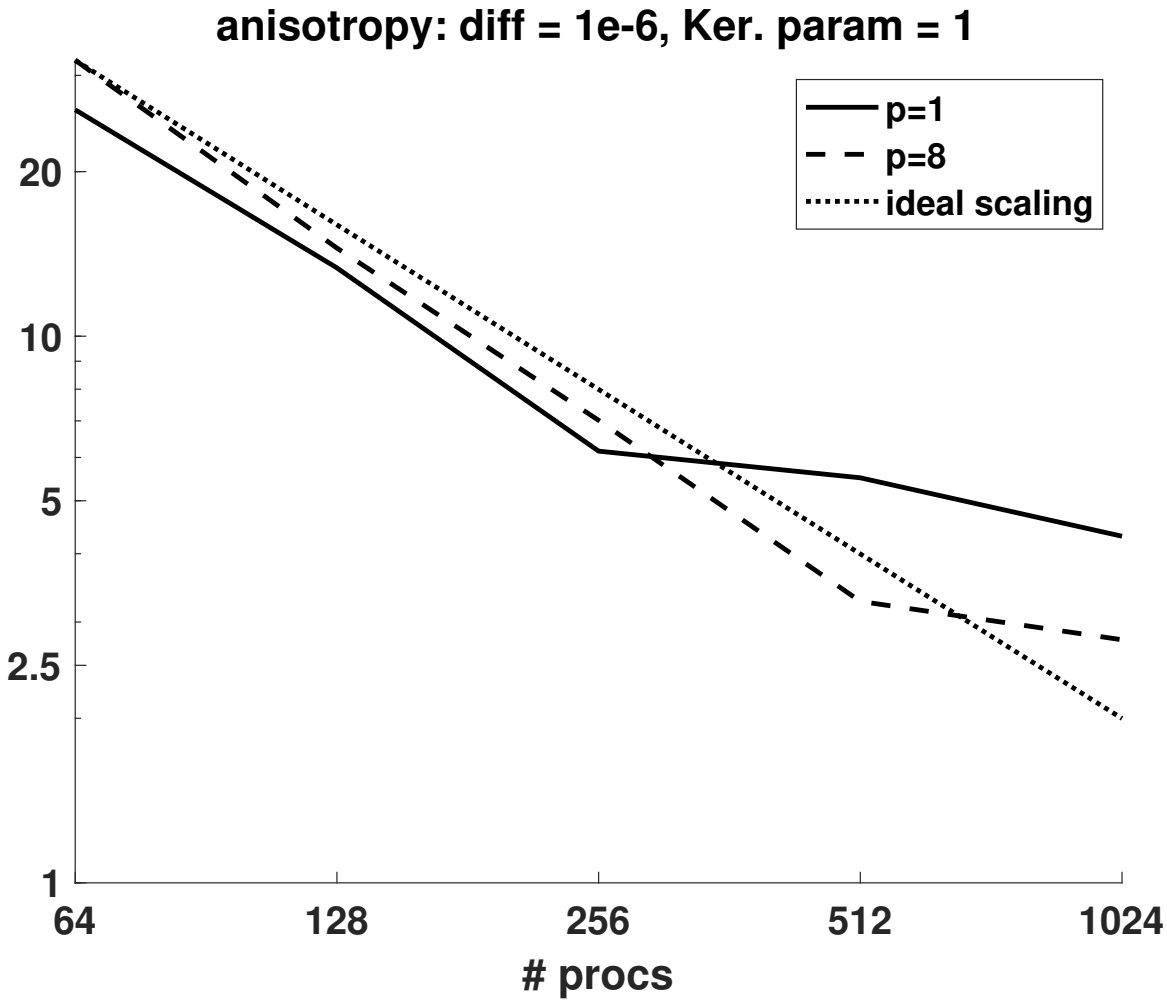

Figure: #DOFs $\approx$ 67M. # iter$_{p=1}$ = 11. # iter$_{p=7}$ = 17

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Numerical experiments

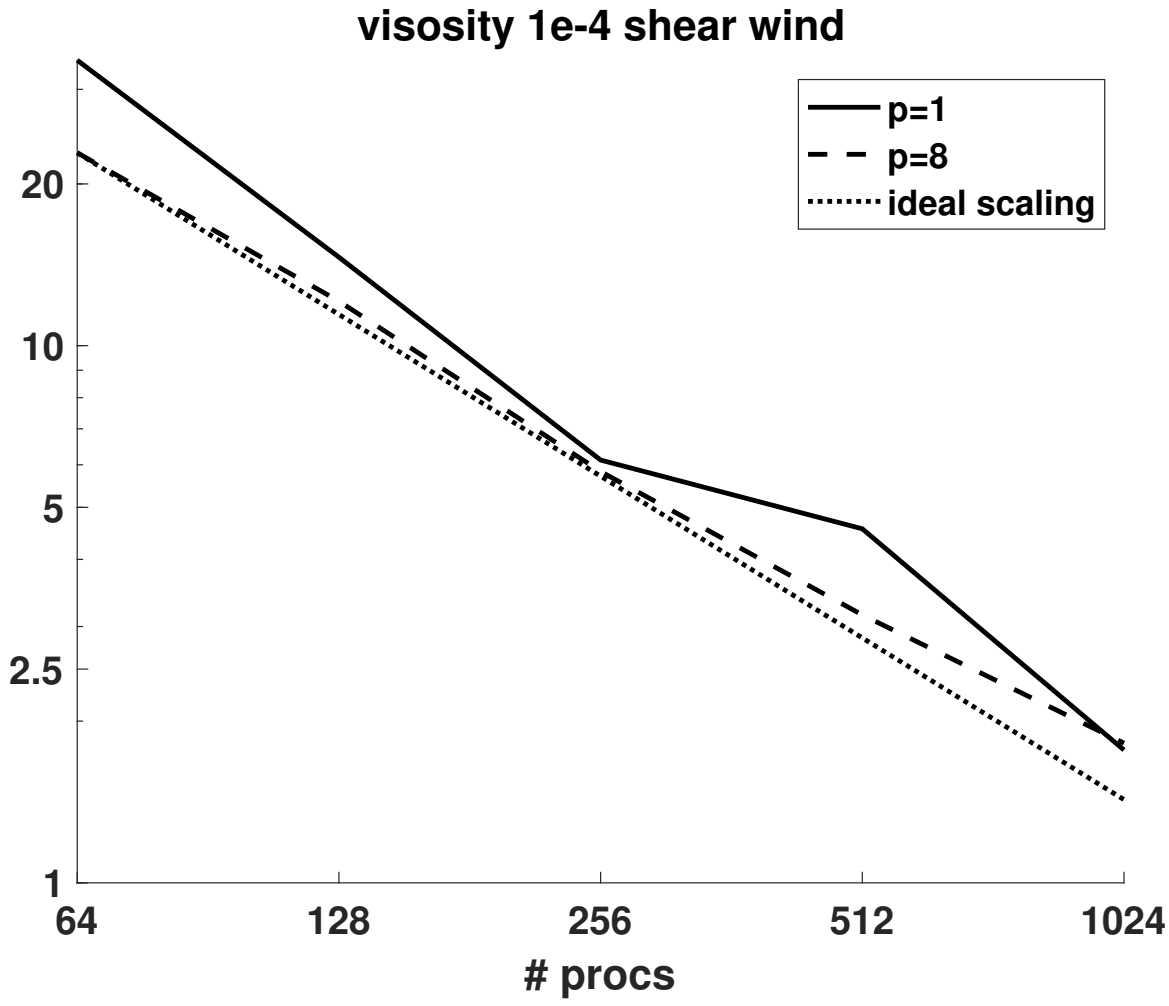

Figure: #DOFs $\approx$ 67M. # iter$_{p=1}$ = 20. # iter$_{p=8}$ = 17

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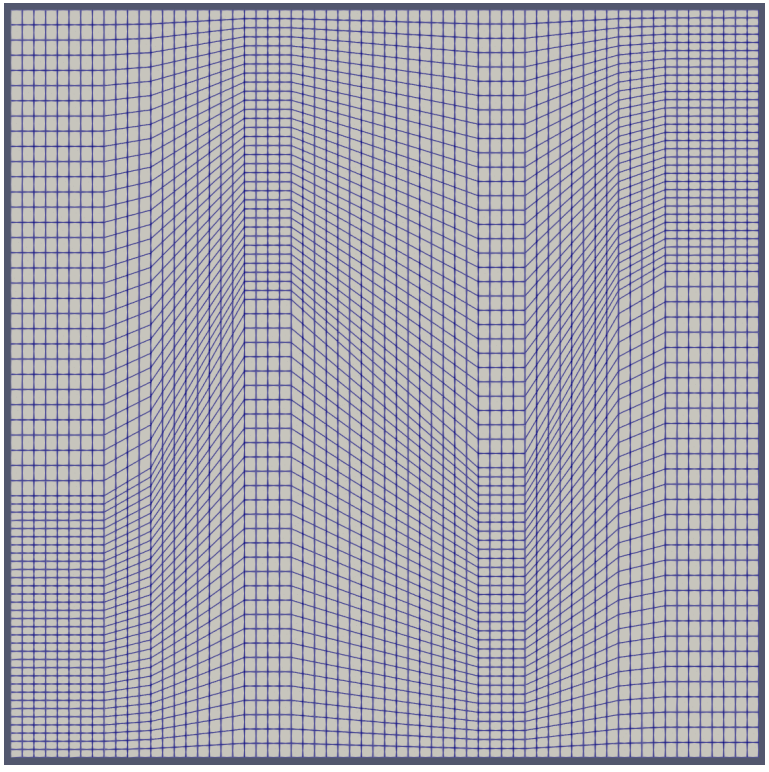
Code coupling Fluid–Particle

- Suggested Spatial Hybridization (SpH) Approach
- Identified several lightweight and efficient coupling software (MUI, CWIPI, preCICE)

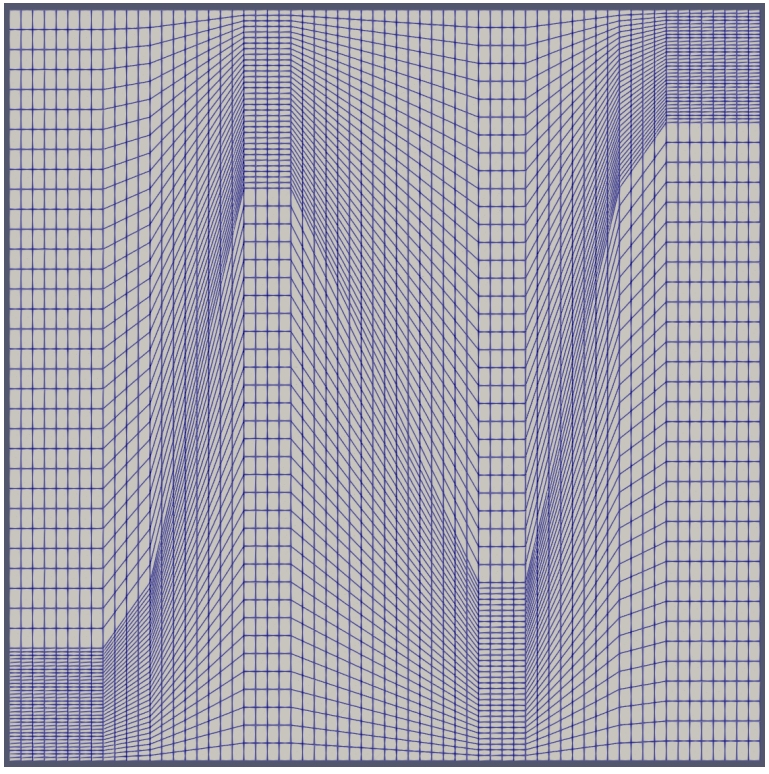
Since NESO particle-in-cell solver not yet available in Nektar++, current proxyapp plan is to represent particle-in-cell solver by sampling a travelling sine wave, the fluid model by an advection equation, in Nektar++

- 1-D model with variable overlap region
- At each timestep combine particle contribution with existing density using an indicator function

Kershaw mesh



(a) Ker. param: 0.7



(b) Ker. param: 0.3

Figure: Anisotropic mesh

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