Scalable Solvers for Multicomponent Flows

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Scalable solvers: parallelisable on modern computer hardware.

Section 2

Onsager–Stefan–Maxwell equations

Let's start with the simplest case of the OSM equations: **multicomponent diffusion of ideal gaseous mixtures**. Furthermore, we assume isothermal, isobaric, and steady-state conditions.

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Steady, isothermal, isobaric, and ideal gaseous OSM problem

For given v_{bulk} and $\{r_i\}_{i=1}^n$, find $\{c_i\}_{i=1}^n$ and $\{v_i\}_{i=1}^n$ such that

$$-c_i \nabla \mu_i = \sum_j \boldsymbol{M}_{ij} v_j \qquad \forall i \in \{1, \dots, n\}, \qquad (\star)$$

$$\nabla \cdot (c_i v_i) = r_i \qquad \forall i \in \{1, \dots, n\},$$

$$v_{\text{bulk}} = \frac{\sum_i M_i c_i v_i}{\rho}, \qquad (\star\star)$$

where $\rho := \sum_{i=1}^n M_i c_i$ is the density and $\boldsymbol{M}$ is the Onsager transport matrix defined as

$$\boldsymbol{M}_{ij} = \begin{cases} -\frac{RTc_ic_j}{\mathcal{D}_{ij}c_T} & \text{if } i \neq j, \\ \sum_{k \neq i}^n \frac{RTc_ic_k}{\mathcal{D}_{ik}c_T} & \text{if } i = j. \end{cases}$$

We add the mass-average constraint $(\star\star)$ to $(\star)$ as an augmentation term, and rewrite the OSM equations in terms of the mass fluxes $\{J_i\}_{i=1}^n$ and chemical potentials $\{\mu_i\}_{i=1}^n$

$$\begin{aligned} J_i &= M_i c_i v_i && \forall i \in \{1, \ldots, n\}, \\ \mu_i &= e^{c_i} && \forall i \in \{1, \ldots, n\}. \end{aligned}$$

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$$

We can derive a weak formulation with $J_i \in H(\mathrm{div})$ and $\mu_i \in L^2$ for each i, and discretise using conforming FEM with arbitrary polynomial degree.

For a **Picard linearisation** of the OSM problem we can prove continuous well-posedness and discrete well-posedness and quasi-optimality. Empirically, the Picard linearisation can be solved at each step of a fixed point iteration to obtain a solution to the fully nonlinear problem.

In practice, we employ **Newton's method** because of its superior convergence.

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Hence, we need to use an iterative solver. We start with a stationary iterative method for $Ax = b$ with splitting $A = M - N$

$$Mx^{k+1} = Nx^k + b.$$

where M is usually chosen to resemble A but easier to solve.

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The stationary iterative method can be improved by the Generalised Minimum RESidual method (GMRES) which finds $y^{k+1} \in \text{span}(\{x^0, \ldots, x^{k+1}\})$ such that the residual $\|b - Ay^{k+1}\|_2$ is minimised.

In this setting, GMRES is referred to as the iterative solver and the stationary iterative method is the preconditioner.

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In this setting, GMRES is referred to as the iterative solver and the stationary iterative method is the preconditioner. **This talk is essentially about good choices for M.**

At each step of Newton's method we have to solve a linear system with the Jacobian. To determine a good choice for M we should look at the matrix structure of the Jacobian

$$\mathcal{J} = \begin{array}{c c} & \begin{array}{cc} \bar{J} & \bar{\mu} \end{array} \\ \begin{array}{c} \bar{\tau} \\ \bar{w} \end{array} & \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & \end{pmatrix} \end{array},$$

where we have used bar notation to denote n-tuples, e.g. $\bar{J} = (J_1, \ldots, J_n)$, and $\bar{\tau}$ and $\bar{w}$ are corresponding test functions.

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- monolithic preconditioner, i.e. M considers $\mathcal{J}$ completely,
- block preconditioner, i.e. $M = \begin{pmatrix} D_1 & \\ & D_2 \end{pmatrix}$ and D_1, D_2 are solved iteratively.

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Goal

The preconditioner exhibits bounded GMRES iterations for arbitrary mesh refinements and polynomial degree, as well as parallelisation of its most costly operation.

Section 3

Monolithic multigrid preconditioner

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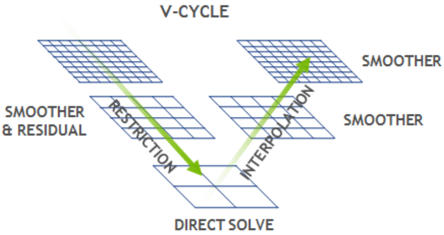
Multigrid moves the iterate between meshes with different refinements to reduce all frequencies.



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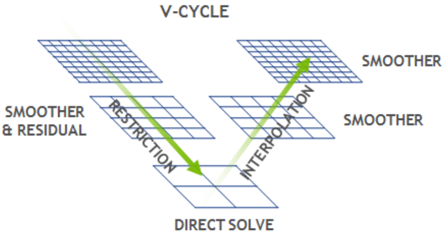

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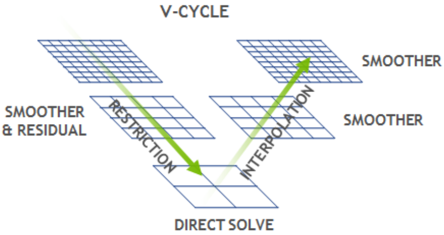

Often, Gaussian elimination is used on the coarsest mesh and a parallel stationary iterative method on the finer meshes. **Empirically multigrid has proven to be a powerful solver for a wide variety of problems.**

Solver diagram for the monolithic multigrid preconditioner.

- Newton's method
  - Preconditioned GMRES
    - Multigrid
      - Coarse grid solver
        - Gaussian elimination
      - Fine grid solver
        - 1 Vertex Vanka iteration
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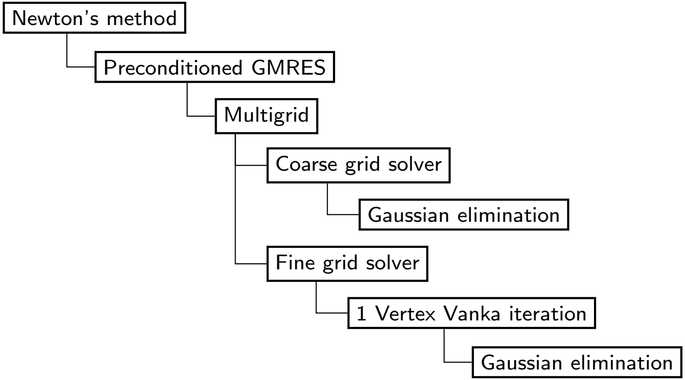
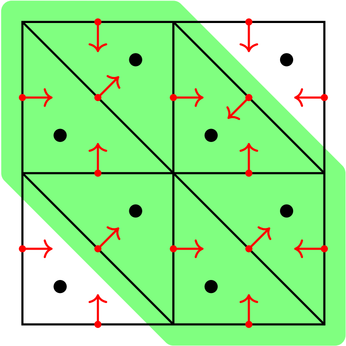


Vertex Vanka patch for RT_1-DG_0 discretisation.



Manufactured test problems: preconditioned GMRES iteration counts for various mesh refinements and polynomial degrees.

refinement\degree	1	2	3	4
0	1.0	1.0	1.0	1.0
1	10.0	7.0	6.5	7.0
2	11.67	7.33	7.0	7.0
3	12.0	6.5	7.5	7.0

Coarse 4×4 unit square mesh.

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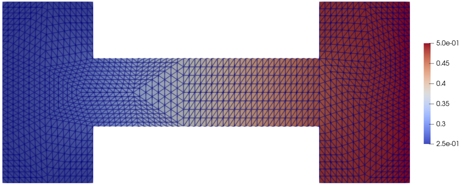
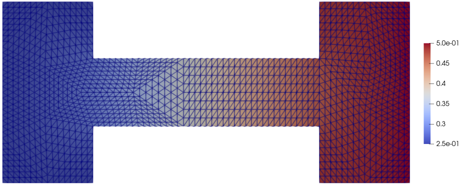
Coarse 4×4 unit square mesh.

refinement\degree	1	2	3	4
0	1.0	1.0	1.0	1.0
1	8.67	6.67	6.0	6.0
2	11.33	7.5	7.5	

Coarse $4 \times 4 \times 4$ unit cube mesh.



Gas separation chamber: mole fraction of helium in ternary mixture of He-Ar-Kr in the presence of a temperature gradient.



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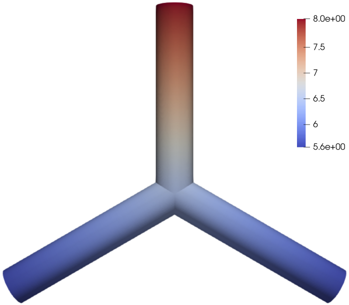

Human airways: concentration of oxygen in mixture of H_2O-O2-CO_2-N_2.

Section 4

Augmented Lagrangian block preconditioner

The augmented Lagrangian preconditioning approach adds $\kappa(\nabla \cdot (c_i v_i) - r_i, \nabla \cdot \tau_i)$ where $\kappa > 0$ to the weak formulation of $(\star)$. If $\nabla \cdot (c_i v_i) = r_i$ can be satisfied exactly in the finite element space for each i, e.g. when $r_i = 0$ for each i, then the solution doesn't change.

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However, the Jacobian changes to

$$\mathcal{J} = \begin{array}{c c} & \begin{array}{cc} \bar{J} & \bar{\mu} \end{array} \\ \begin{array}{c} \bar{\tau} \\ \bar{w} \end{array} & \begin{pmatrix} A_{00}^{\kappa} & A_{01} \\ A_{10} & \end{pmatrix} \end{array} \approx \begin{array}{c c} & \begin{array}{cc} \bar{J} & \bar{\mu} \end{array} \\ \begin{array}{c} \bar{\tau} \\ \bar{w} \end{array} & \begin{pmatrix} \kappa(\nabla \cdot \bar{J}, \nabla \cdot \bar{\tau}) & (\bar{\mu}, \nabla \cdot \bar{\tau}) \\ (\nabla \cdot \bar{J}, \bar{w}) & \end{pmatrix} \end{array}.$$

For large κ the augmented Lagrangian term dominates the top left block of the Jacobian.

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For large κ the augmented Lagrangian term dominates the top left block of the Jacobian. It can be shown that a good approximation for the Schur complement is $\tilde{S} = (\bar{\mu}, \bar{w})$. Hence we will use the preconditioner

$$M = \begin{pmatrix} A_{00}^{\kappa} & \\ & \hat{S} \end{pmatrix}.$$

Solver diagram for the augmented Lagrangian preconditioner.

- Newton's method
  - Preconditioned GMRES
    - Block preconditioner
      - Multigrid on A_{00}^{κ} block
        - Coarse grid solver
          - Gaussian elimination
        - Fine grid solver
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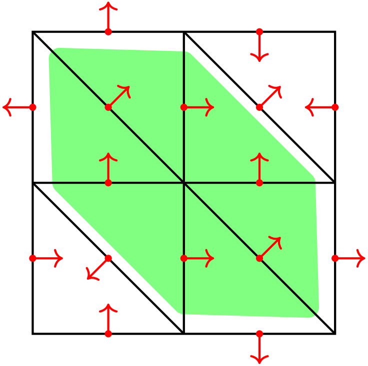
Vertex star patch for RT_1 discretisation.



Manufactured test problems: preconditioned GMRES iteration counts for various mesh refinements and polynomial degrees. $\kappa = 10$.

refinements \degree	1	2	3	4
1	9.75	9.75	9.75	9.75
2	20.67	20.5	23.5	20.5
3	21.67	19.0	23.0	19.0
4	20.5	18.5	20.5	18.0

Coarse 4×4 unit square mesh.

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Coarse 4×4 unit square mesh.

refinements \degree	1	2	3	4
0	10.0	20.5	24.5	28.25
1	47.4	30.33	25.33	22.0
2	41.5	26.0	25.33	

Coarse $4 \times 4 \times 4$ unit cube mesh.

Section 5

Conclusions

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Monolithic multigrid preconditioner:

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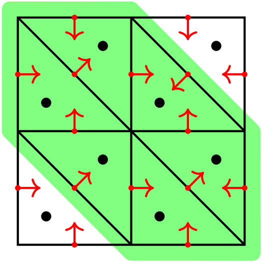
- straightforward implementation.



Vertex Vanka patch for RT_1-DG_0 discretisation.

We have two scalable solvers for multicomponent diffusion of ideal gaseous mixtures.

Monolithic multigrid preconditioner:

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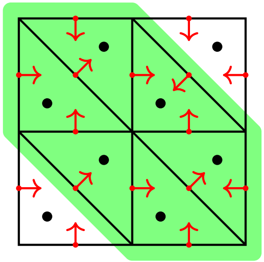
Augmented Lagrangian preconditioner:

- small patch problems,
- more challenging implementation.



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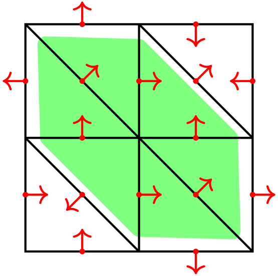

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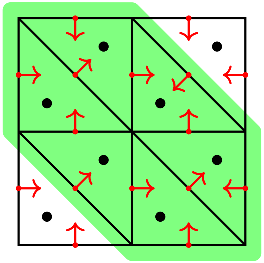

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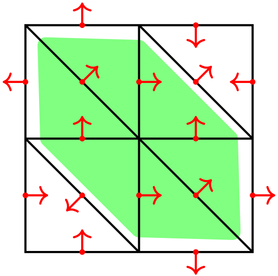

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In the future we hope to extend these preconditioners to more multicomponent problems!

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Thank you for listening!