The *spectre* initial data solver

Nils Vu, Caltech

SXScon 2024, Aug 9 at ICERM, Providence RI

Recap: XCTS initial data

Two black holes in orbit

Einstein constraint equations: 5 coupled, nonlinear, elliptic PDEs

$$
\begin{aligned}
\bar{\nabla}^2\psi &= \frac{1}{8}\psi\bar{R} + \frac{1}{12}\psi^5K^2 - \frac{1}{8}\psi^{-7}\bar{A}_{ij}\bar{A}^{ij} - 2\pi\psi^5\rho \\
\bar{\nabla}^2(\alpha\psi) &= \alpha\psi\left(\frac{7}{8}\psi^{-8}\bar{A}_{ij}\bar{A}^{ij} + \frac{5}{12}\psi^4K^2 + \frac{1}{8}\bar{R}\right. \\
&\qquad \left. + 2\pi\psi^4\left(\rho + 2S\right)\right) - \psi^5\partial_t K + \psi^5\beta^i\bar{\nabla}_i K \\
\bar{\nabla}_i(\bar{L}\beta)^{ij} &= (\bar{L}\beta)^{ij}\bar{\nabla}_i\ln(\bar{\alpha}) + \bar{\alpha}\bar{\nabla}_i\left(\bar{\alpha}^{-1}\bar{u}^{ij}\right) \\
&\qquad + \frac{4}{3}\bar{\alpha}\psi^6\bar{\nabla}^jK + 16\pi\bar{\alpha}\psi^{10}S^j
\end{aligned}
$$

Excision: nonlinear boundary conditions represent black holes

$$
\begin{aligned}
n^k\partial_k\psi &= \frac{\psi^3}{8\alpha}n_in_j(\bar{L}\beta)^{ij} \\
&\qquad - \frac{\psi}{4}\bar{m}^{ij}\bar{\nabla}_in_j - \frac{1}{6}K\psi^3 \\
\beta^i &= -\frac{\alpha}{\psi^2}n^i
\end{aligned}
$$

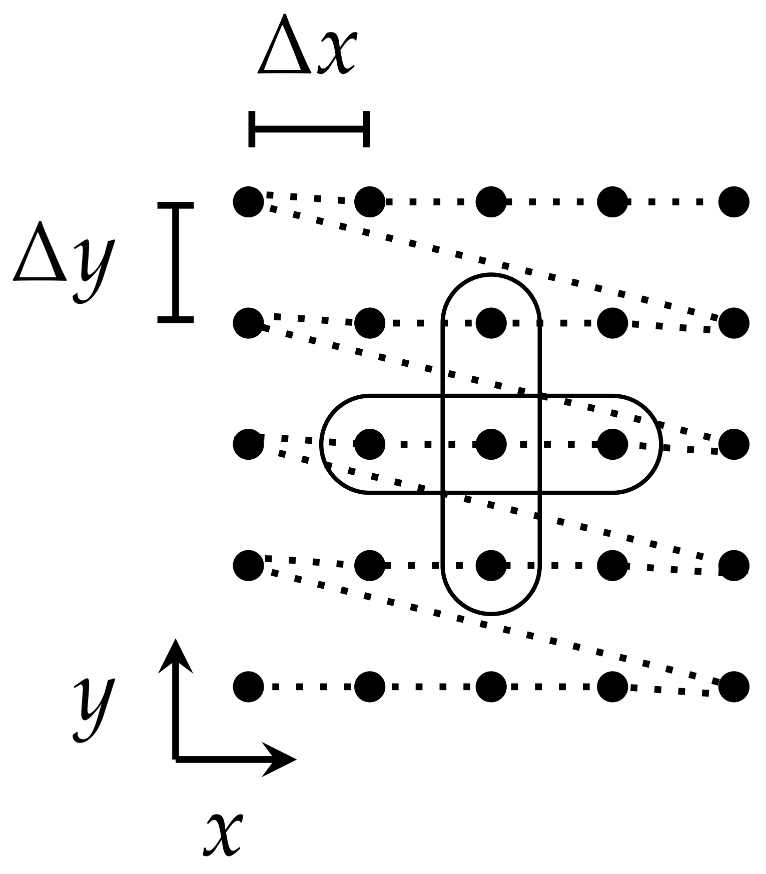
Solving elliptic equations

Discretize and invert!

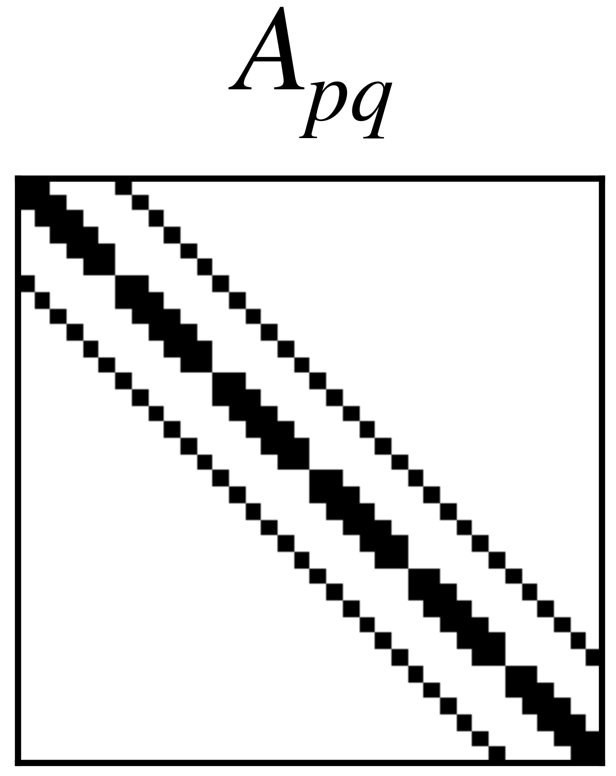
1. Discretize: $-\Delta u = f(x) \quad \rightarrow \quad A_{pq}\, u_q = b_p$

   Example: 2nd order finite difference stencil in 2D

$$-\frac{u_{(p_x+1,p_y)} - 2u_p + u_{(p_x-1,p_y)}}{\Delta x^2} - \frac{u_{(p_x,p_y+1)} - 2u_p + u_{(p_x,p_y-1)}}{\Delta y^2} = f_p$$



$\longrightarrow$



2. Invert matrix: $u_p = A_{pq}^{-1}\, b_q$

Solving elliptic equations

Discretize and invert!

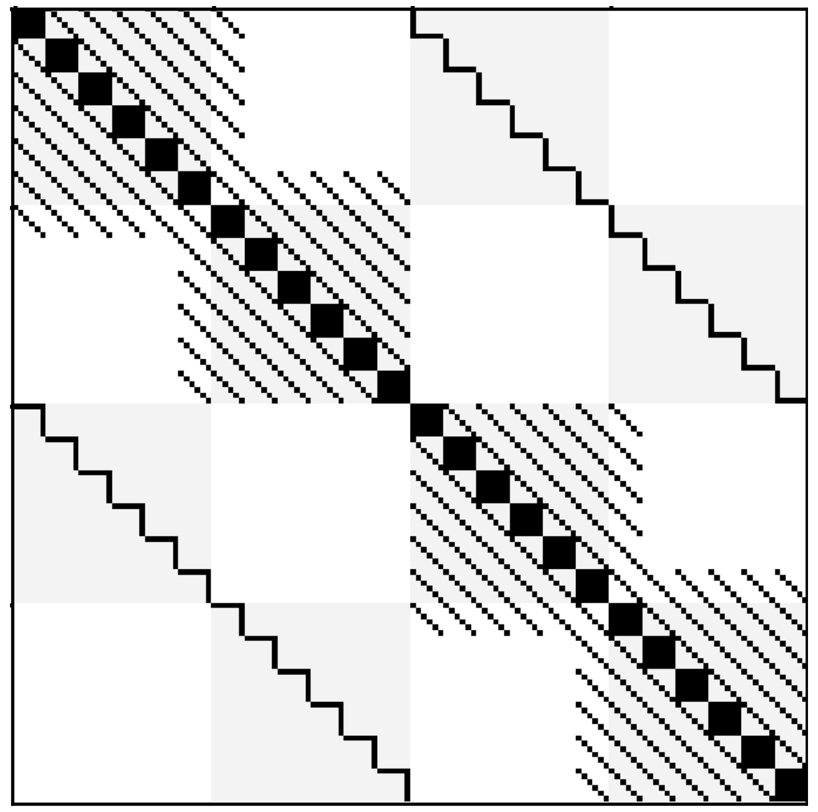
1. Discretize: $$-\Delta u = f(x) \quad \rightarrow \quad A_{pq} u_q = b_p$$

   Finite difference, spectral, ***discontinuous Galerkin****, …*

2. Invert matrix: $$u_p = A^{-1}_{pq} b_q$$

   Direct, ***iterative****, hyperbolic relaxation, …*

- **In parallel on supercomputers!**

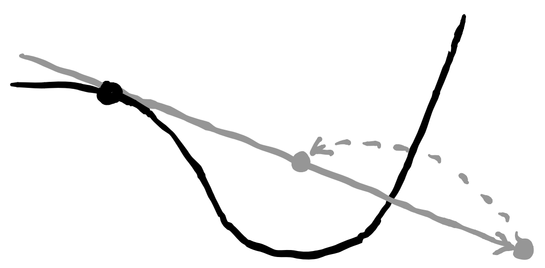


- **NV** & H. Pfeiffer (2022), U*nified discontinuous Galerkin scheme for a large class of elliptic equations,* Phys. Rev. D **105**, 024034, arXiv:2108.05826
- **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code,* Phys. Rev. D **105**, 084027, arXiv:2111.06767

The *spectre* elliptic solver

- **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767

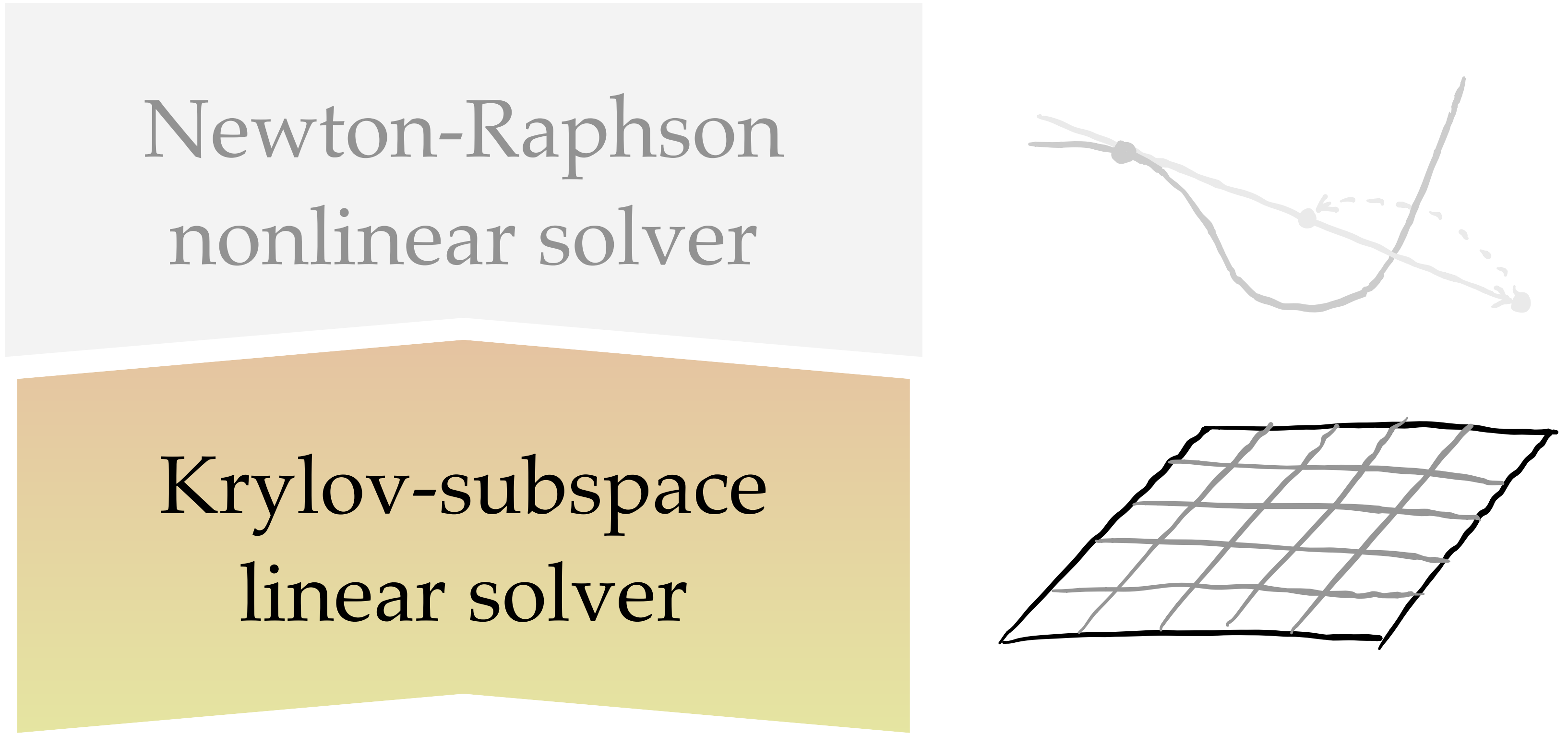
Newton-Raphson nonlinear solver



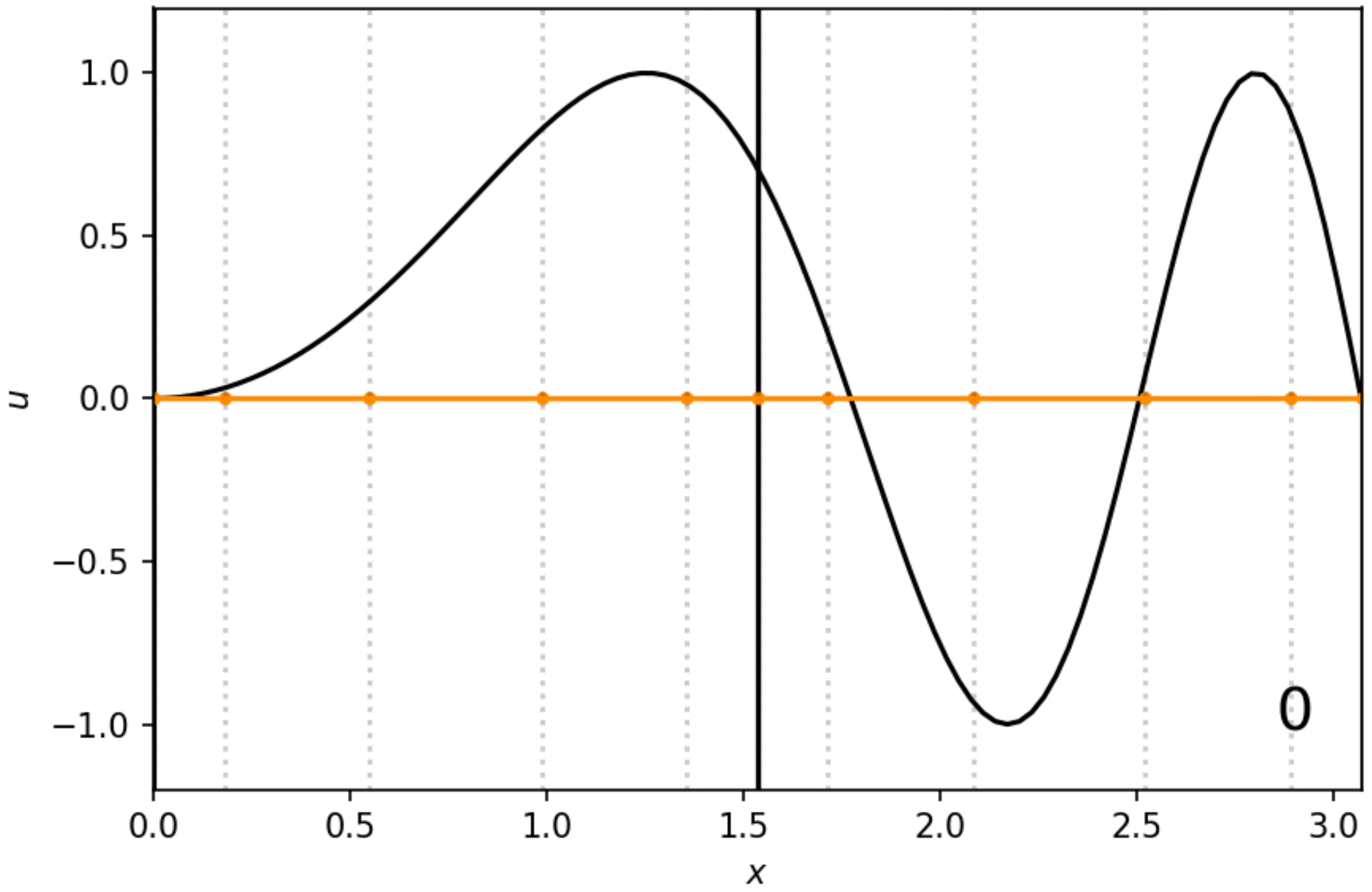
- Repeatedly solve linearization: $\frac{\delta A}{\delta u}(\underline{u})\,\Delta\underline{u} = \underline{b} - A(\underline{u})$
- Line-search globalization to avoid overshoots

The *spectre* elliptic solver

- **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767



- GMRES or Conjugate Gradients
- Builds up a basis of $K_n = \mathrm{span}\{b, Ab, \dots, A^{n-1}b\}$
- Struggles with large-scale modes

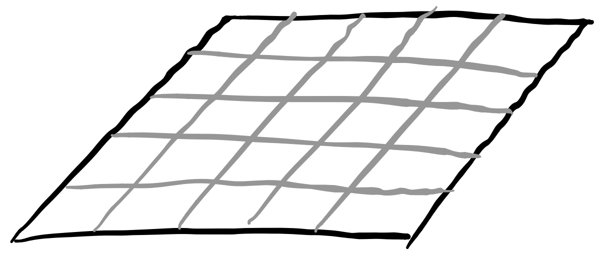


The *spectre* elliptic solver

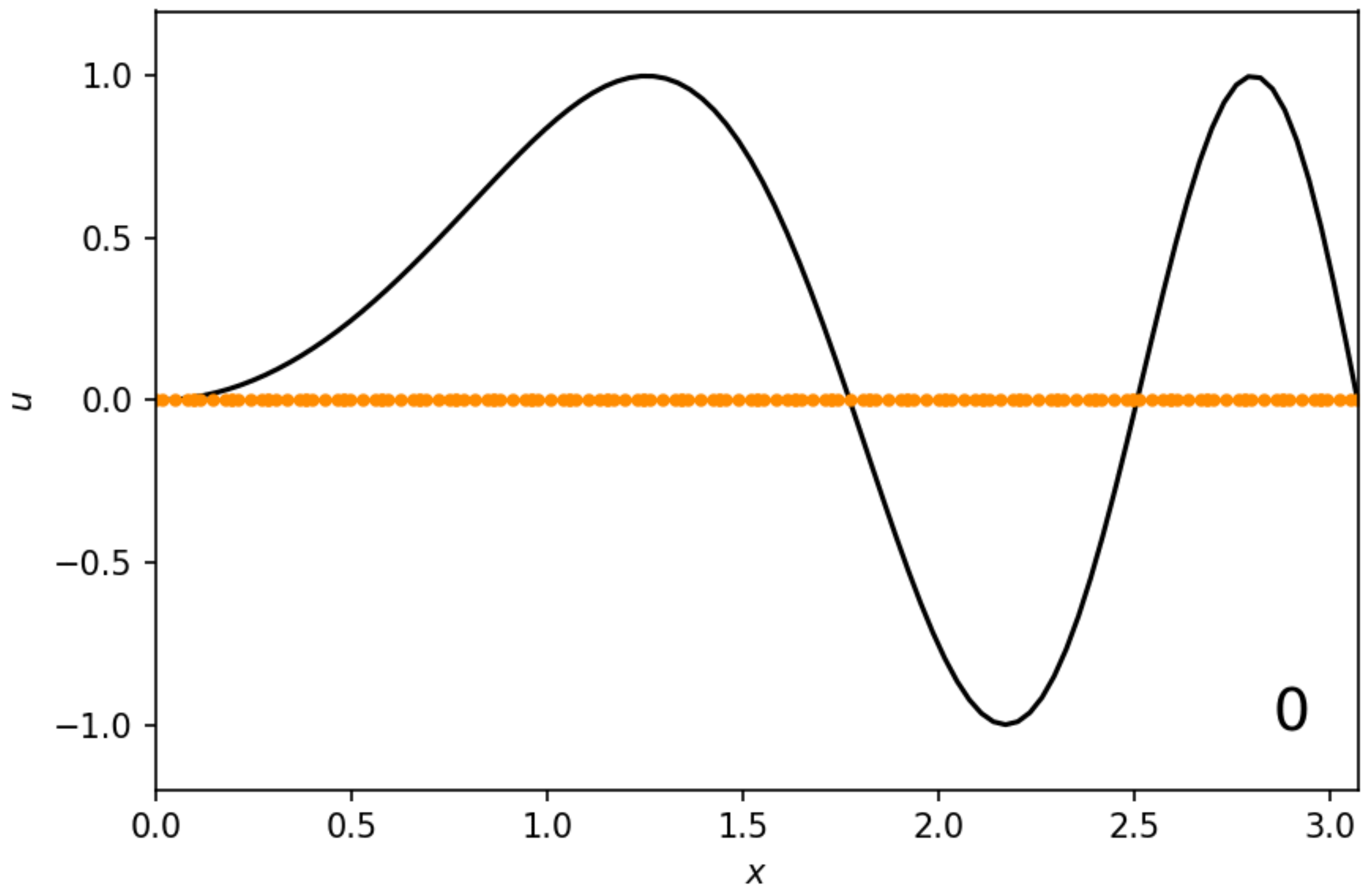
- **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767

Newton-Raphson nonlinear solver

Krylov-subspace linear solver

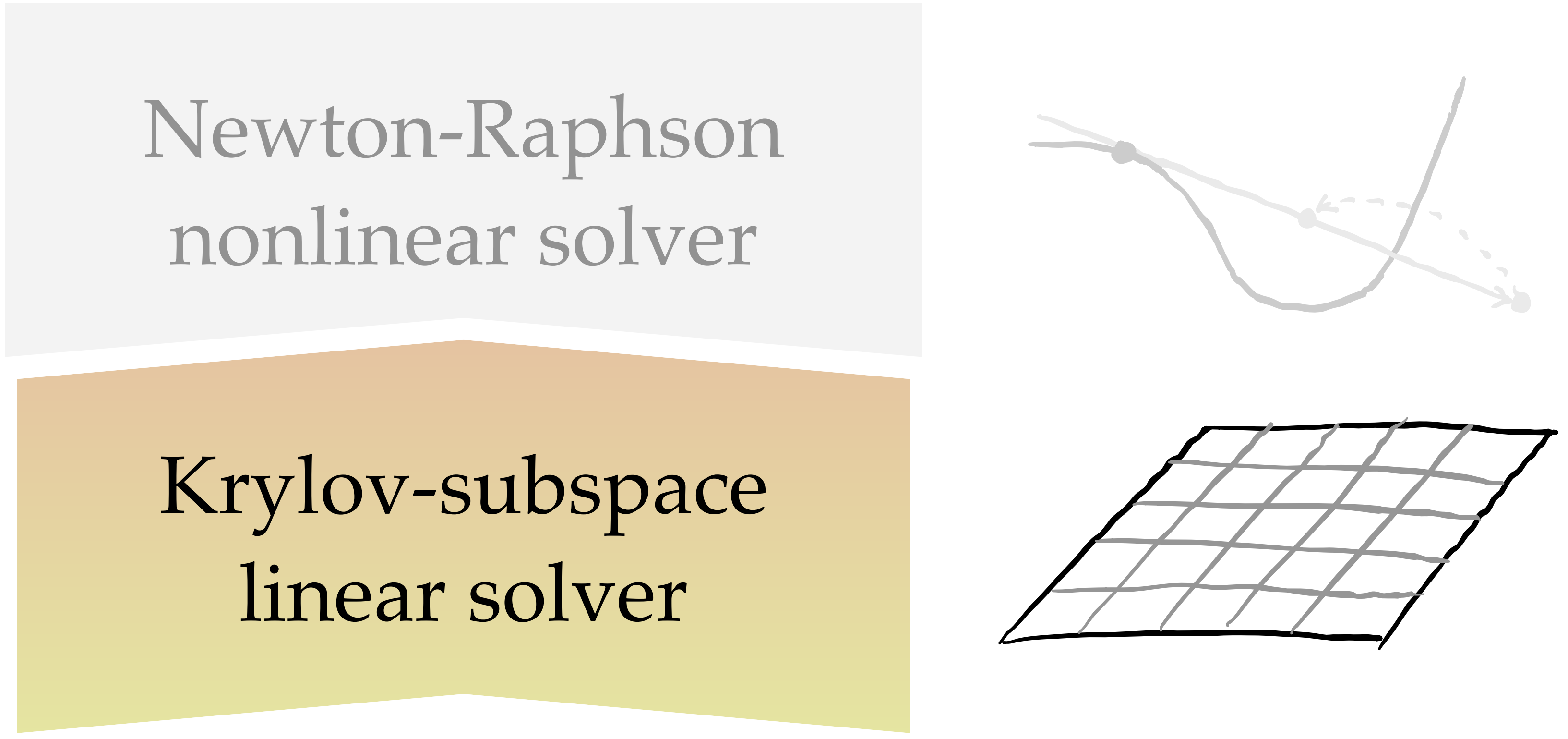


- GMRES or Conjugate Gradients
- Builds up a basis of $K_n = \mathrm{span}\{b, Ab, \ldots, A^{n-1}b\}$
- Struggles with large-scale modes



The *spectre* elliptic solver

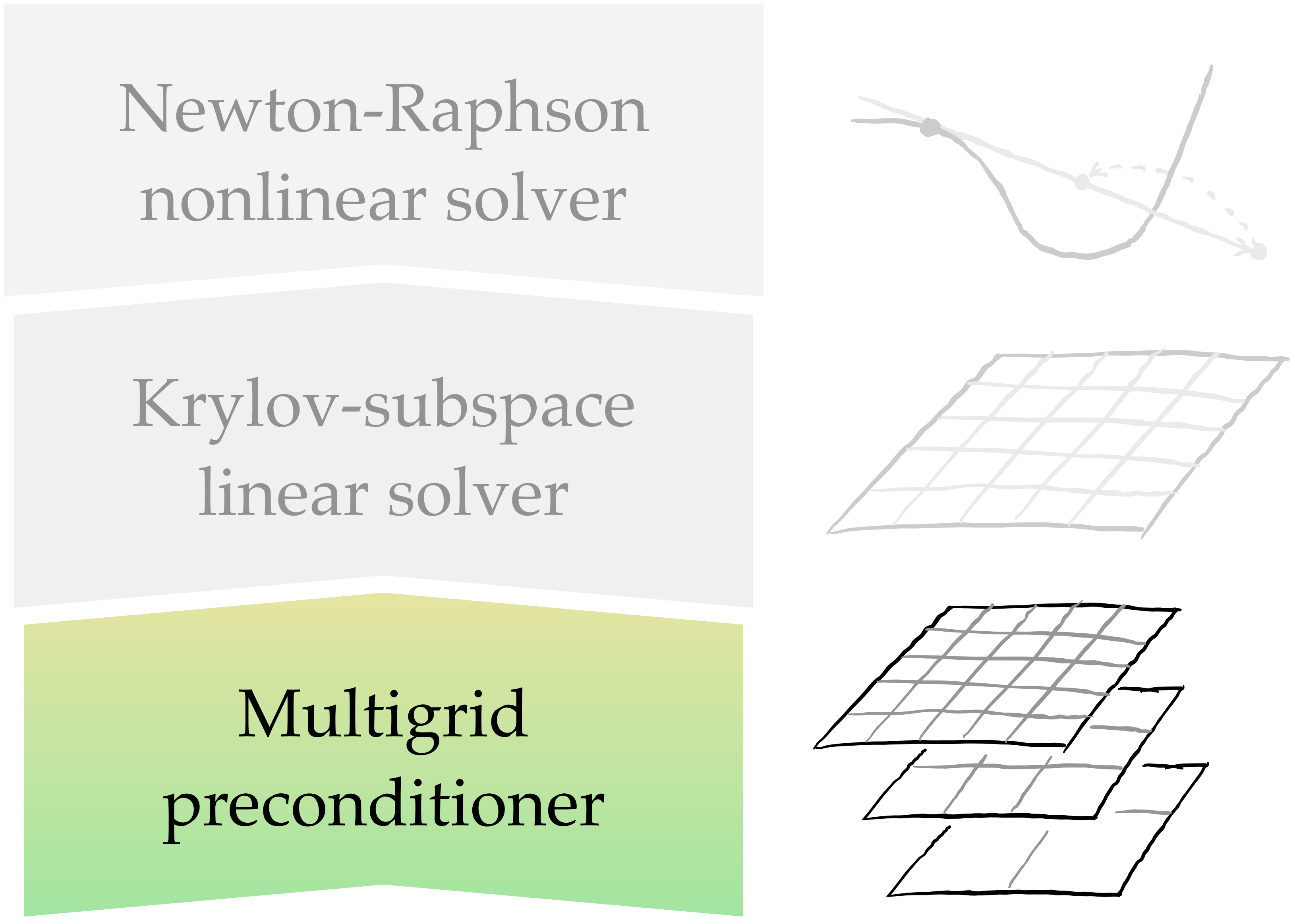
- **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767

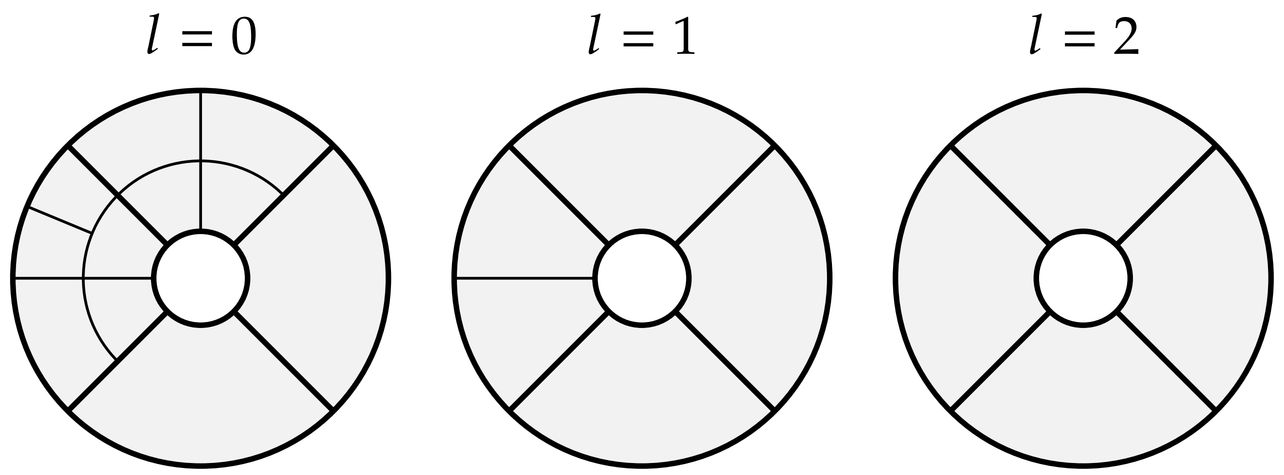


- GMRES or Conjugate Gradients
- Builds up a basis of $K_n = \mathrm{span}\{b, Ab, \ldots, A^{n-1}b\}$
- Struggles with large-scale modes
- Poor parallelization

The *spectre* elliptic solver

- **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767





- Interpolates residuals to coarser grids
- Large-scale modes become small-scale
- Coarse-grid solutions correct fine-grid solutions
- A **smoother** runs on every grid

The *spectre* elliptic solver

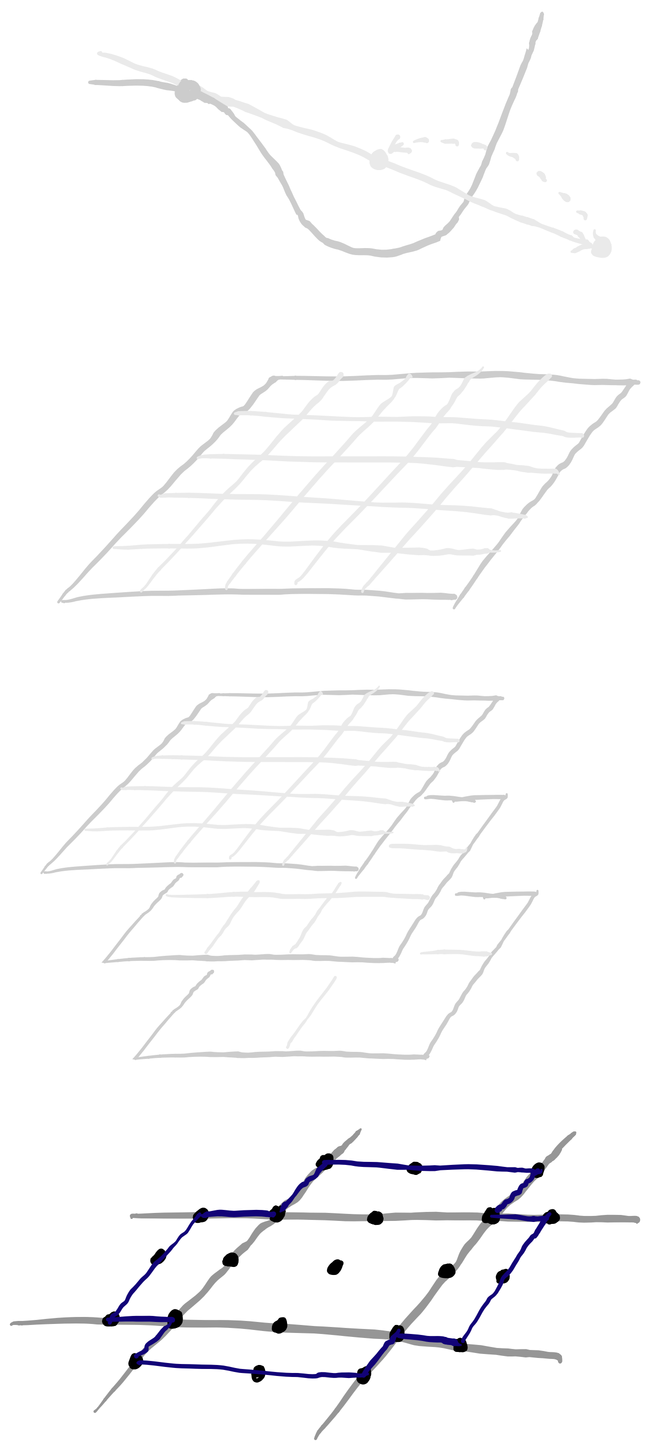
▸ **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767

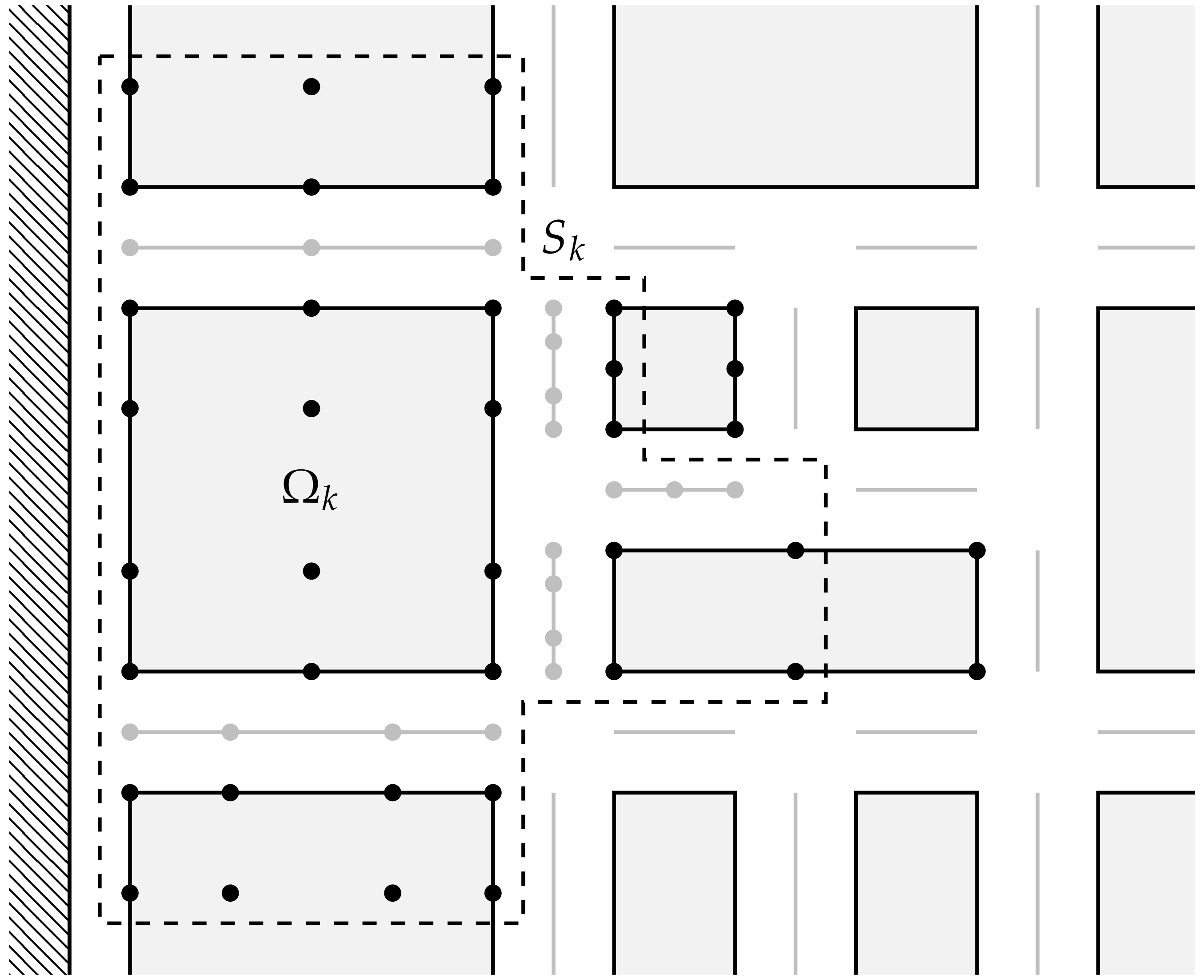
Newton-Raphson nonlinear solver

Krylov-subspace linear solver

Multigrid preconditioner

Schwarz smoother

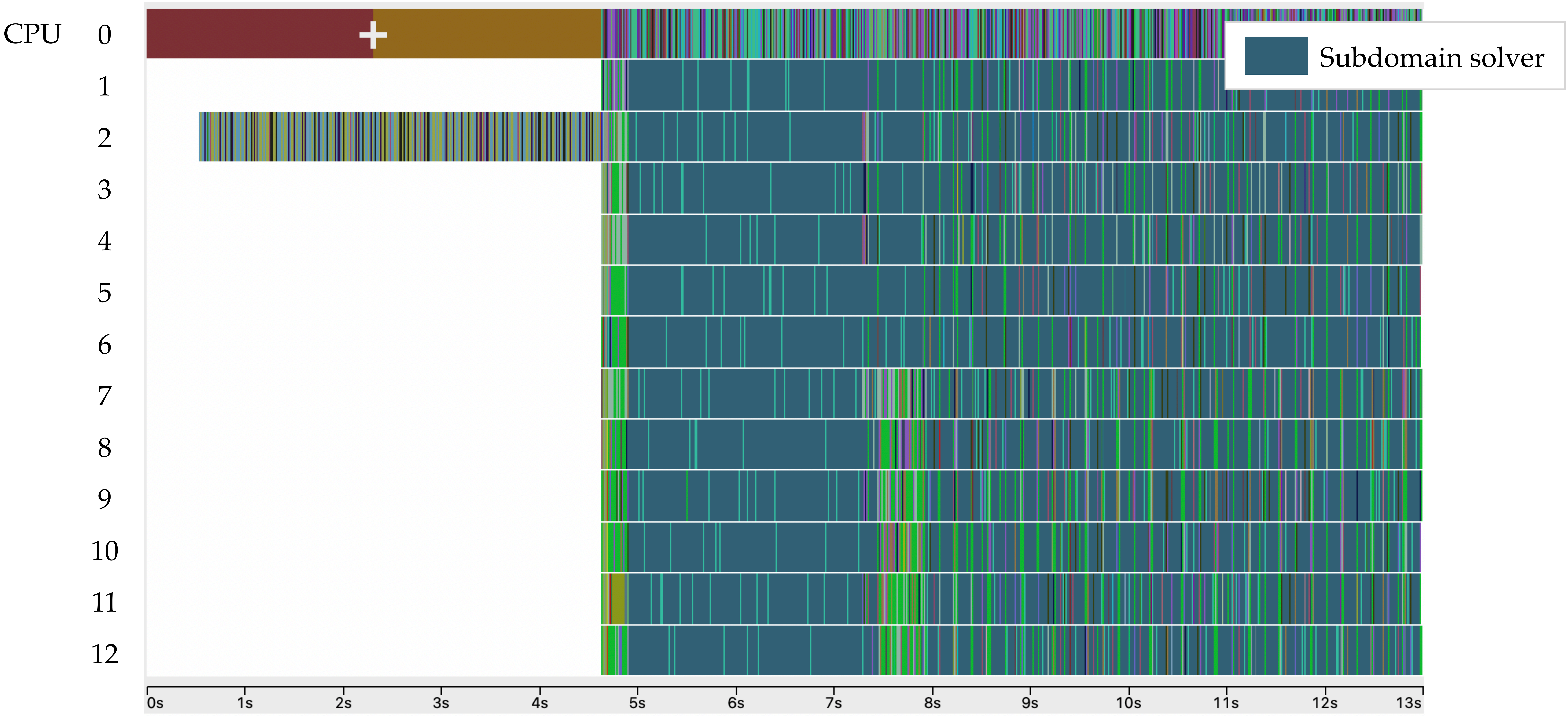




- Restricts problem to overlapping subdomains
- Solves all subdomains in parallel
- Combines subdomain solutions by weighting overlaps

The *spectre* elliptic solver

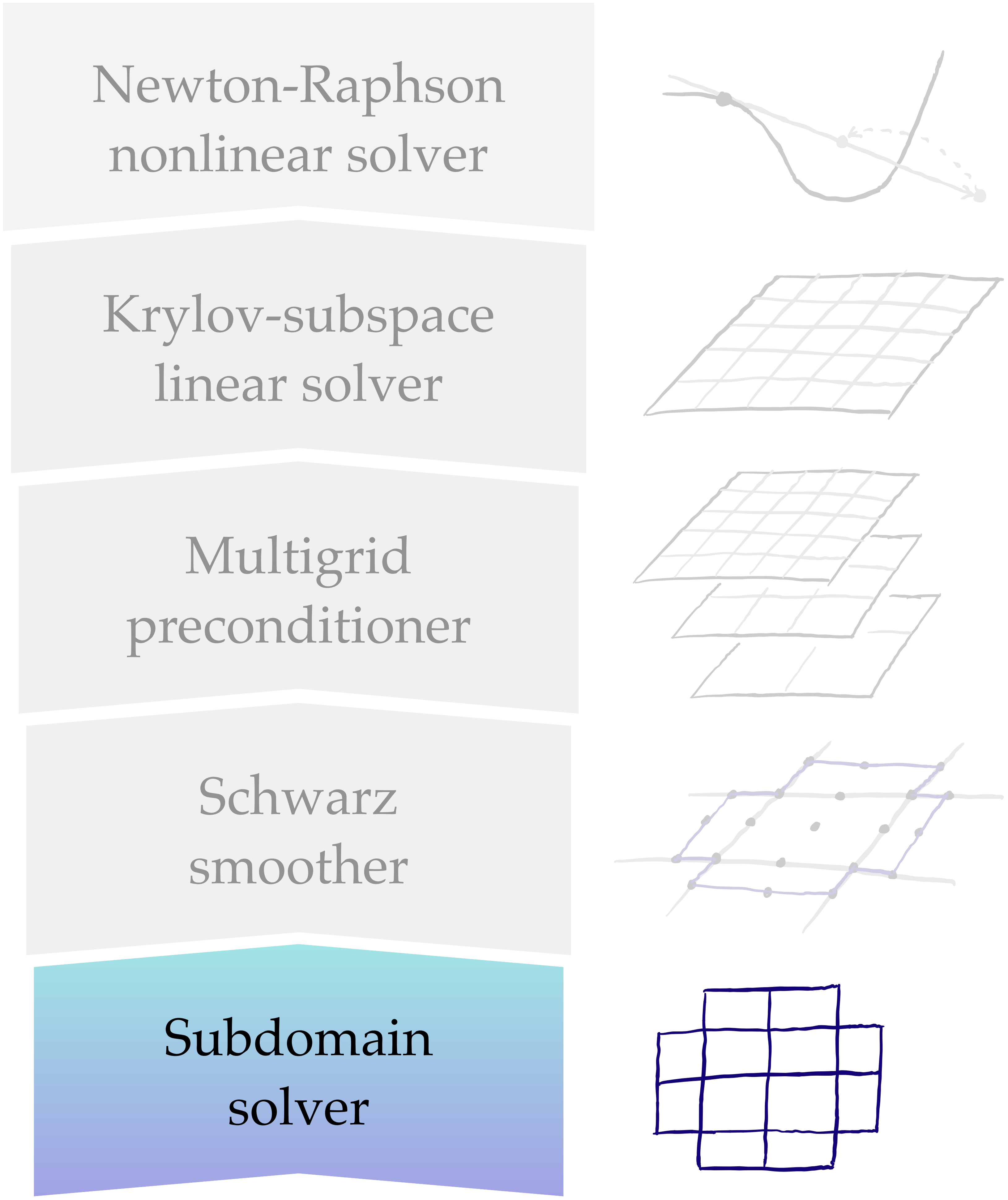
- **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767



- HPCToolkit, hpctoolkit.org

The *spectre* elliptic solver

NV et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767



- Solves the subdomain problem in serial
- Another iterative Krylov-subspace algorithm

The *spectre* elliptic solver

- **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767

Newton-Raphson nonlinear solver

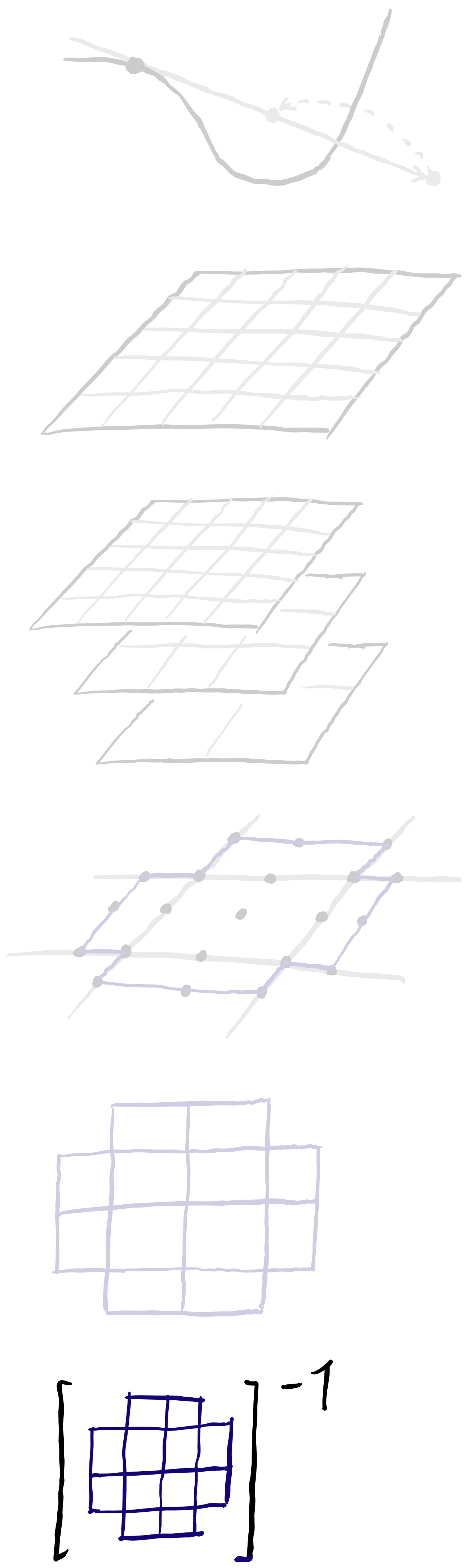
Krylov-subspace linear solver

Multigrid preconditioner

Schwarz smoother

Subdomain solver

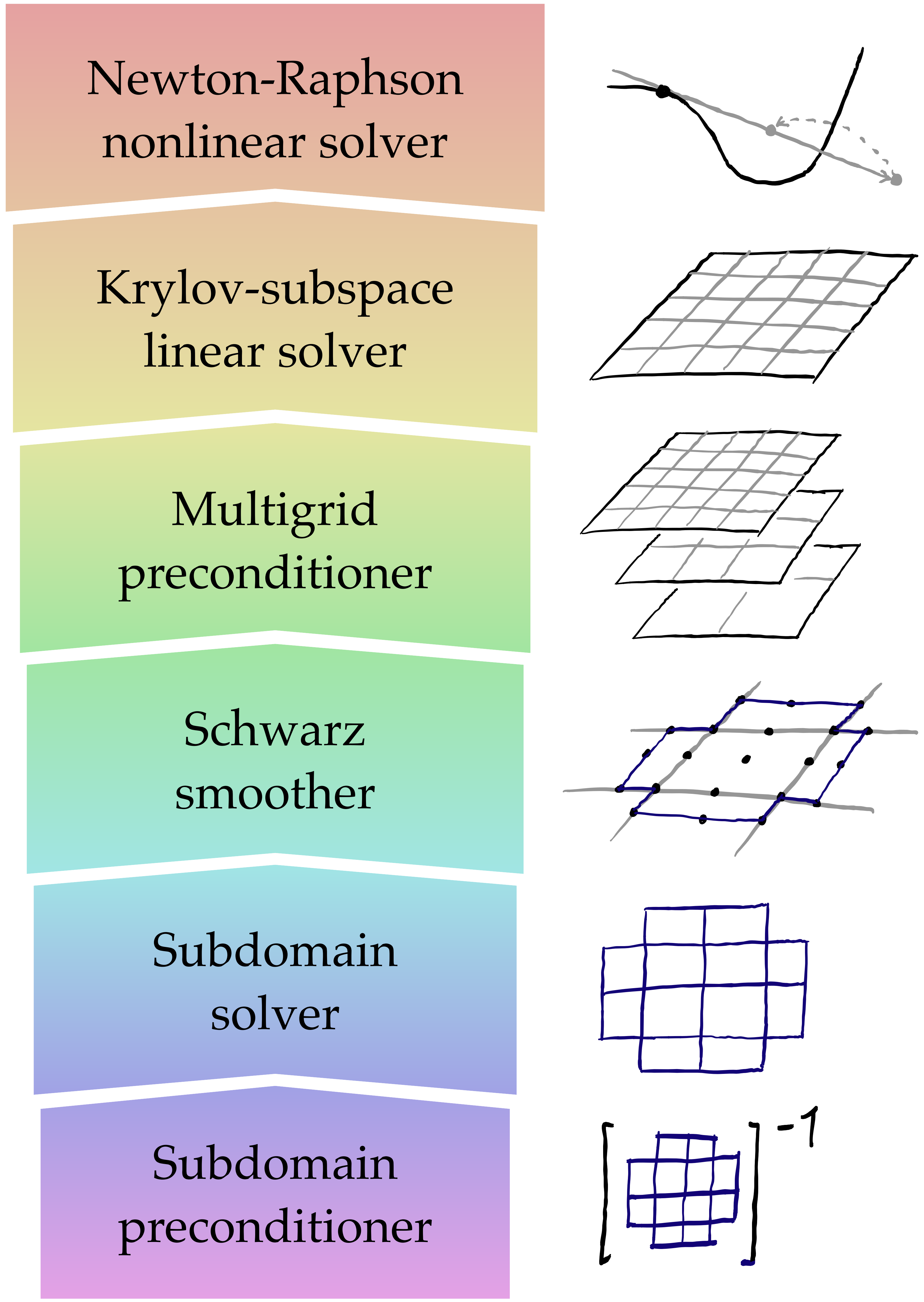
Subdomain preconditioner



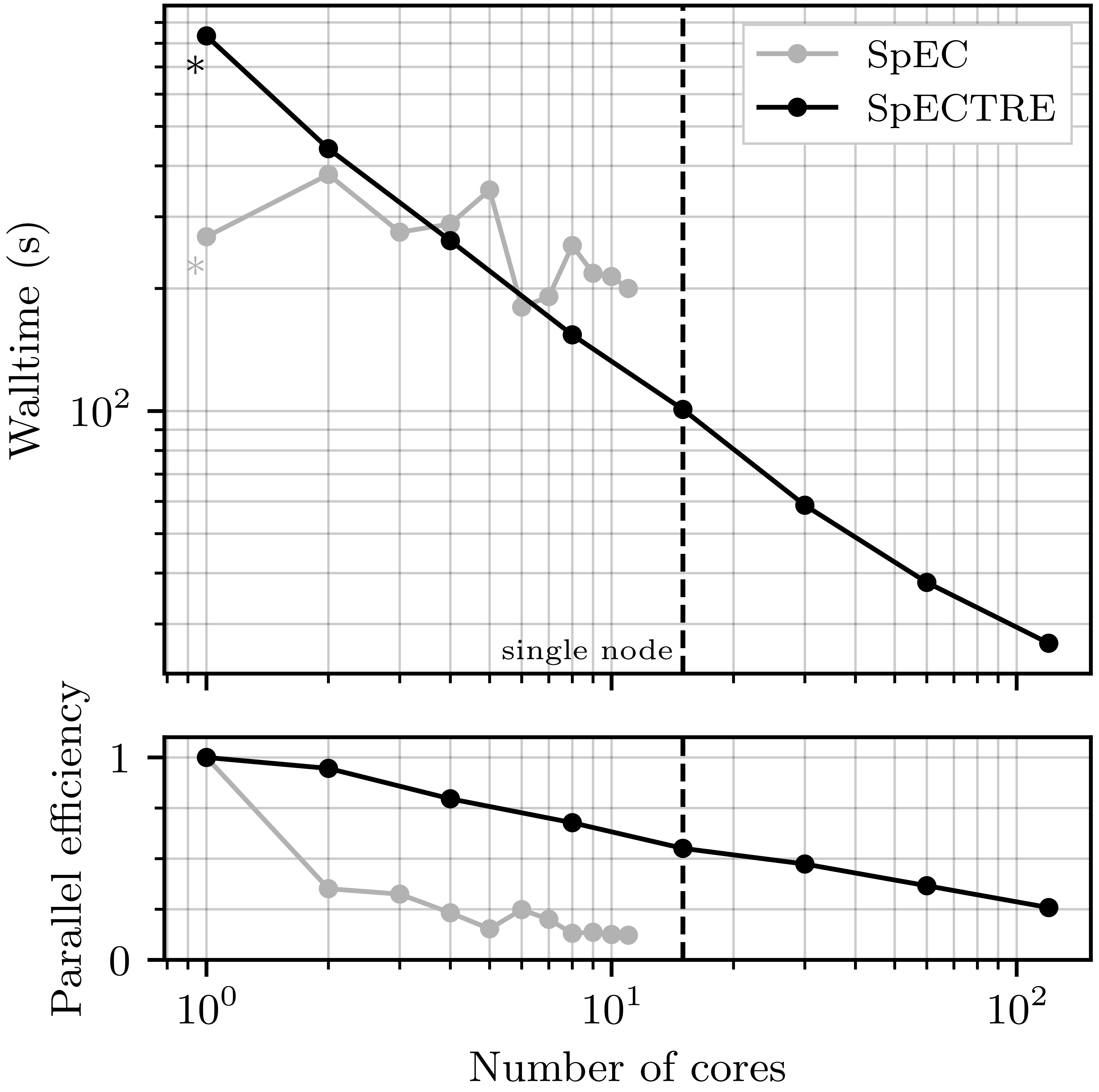
- Laplacian approximation for every equation
- Explicit inverse of Laplacian with ILU

The *spectre* elliptic solver

‣ **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767



BBH initial data: ~10x faster than SpEC on 120 cores



The *spectre* initial data solver

- State-of-the-art SXS initial data + *spectre* elliptic solver

  ➡ **~10x** faster than SpEC & open source

  ➡ Scalable & ready for next-gen numerical relativity

- BBH: public
  - **NV** et al. (2022), *A scalable elliptic solver with task-based parallelism for the SpECTRE code*, Phys. Rev. D **105**, 084027, arXiv:2111.06767

- Scalar Gauss-Bonnet: published & will be open source

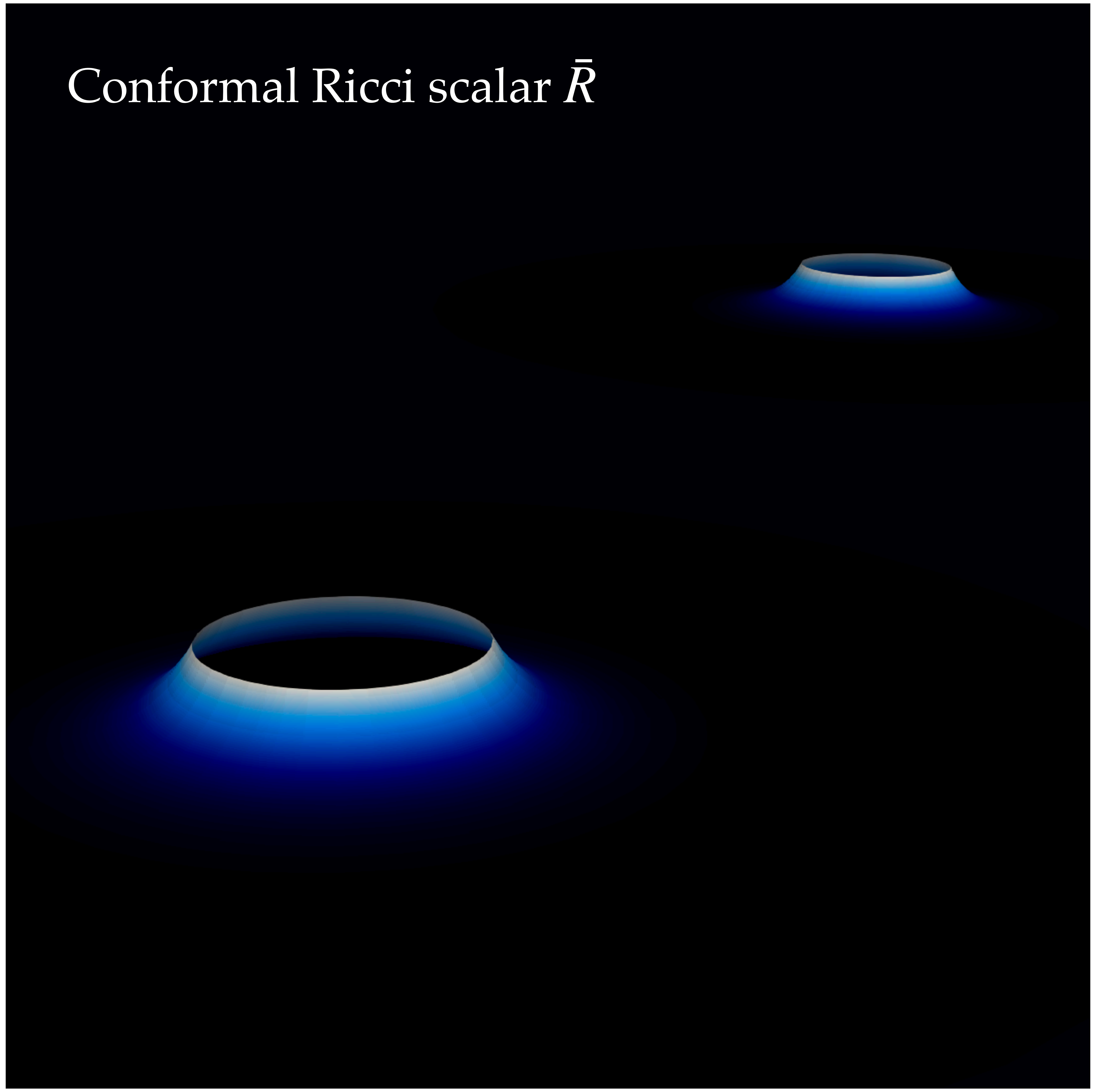
- P.J. Nee (AEI Potsdam), arXiv:2406.08410

- BNS+: in development

- I. Legred (Caltech)

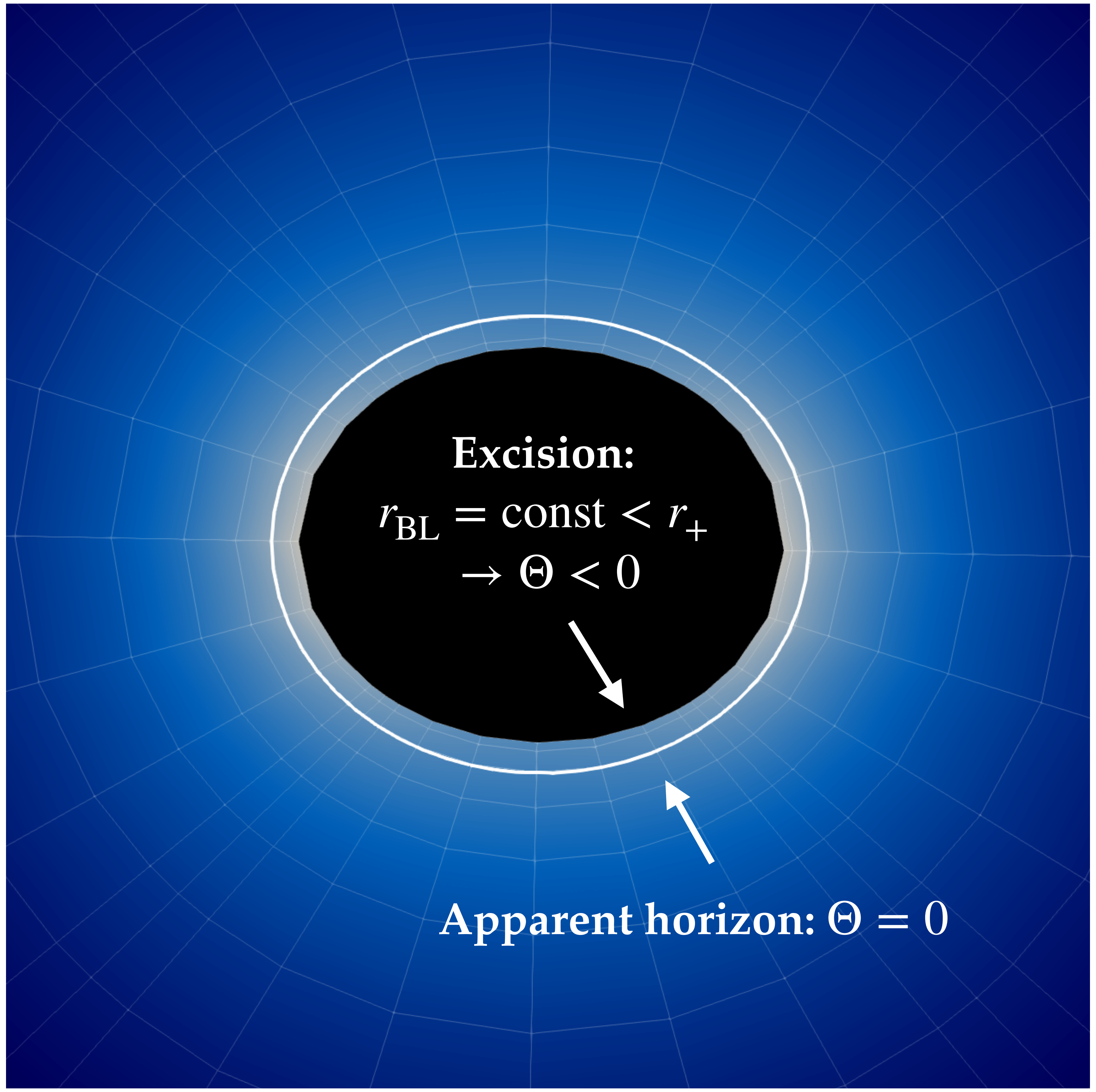
The *spectre* initial data solver

- Non-conformally-flat: **Superposed Kerr variants**
  - ➡ High spins are possible
  - ‣ Lovelace et al. (2008), arXiv:0805.4192



The *spectre* initial data solver

- Non-conformally-flat: **Superposed Kerr variants**
  - ➡ High spins are possible
    - Lovelace et al. (2008), arXiv:0805.4192
- **Black hole excisions**
  - ➡ Exponential convergence with spectral methods
- **Negative-expansion boundary conditions**
  - Varma et al. (2018), arXiv:1808.08228
  - ➡ Horizon is well resolved
  - ➡ Extrapolation into horizon is possible
- No symmetries, parameter control, eccentricity control, …



Running the *spectre* initial data solver

Multiple options:

- Container:

```
$ docker/apptainer run sxscollaboration/spectre bbh generate-id -o ./bbh_id
  -q 1 --chi-A 0 0 0 --chi-B 0 0 0 -D 16 -w 0.015 -a 0
```

- Download static executable from latest release:
  https://github.com/sxs-collaboration/spectre/releases

- Install *spectre*:
  https://spectre-code.org/installation.html

▸ **Tutorial**

More elliptic problems in *spectre*

$$\Delta u = f(x)$$
$$\downarrow$$
$$F^i = \partial_i u$$
$$S = 0$$

1. Formulate in first-order flux form: $-\partial_i F_\alpha{}^i + S_\alpha = f_\alpha(x)$
2. Implement $F_\alpha{}^i$, S_α, $f_\alpha(x)$
3. Implement boundary conditions
4. Use `elliptic::Solver` to compose an executable

More elliptic problems in *spectre*

Thermal noise

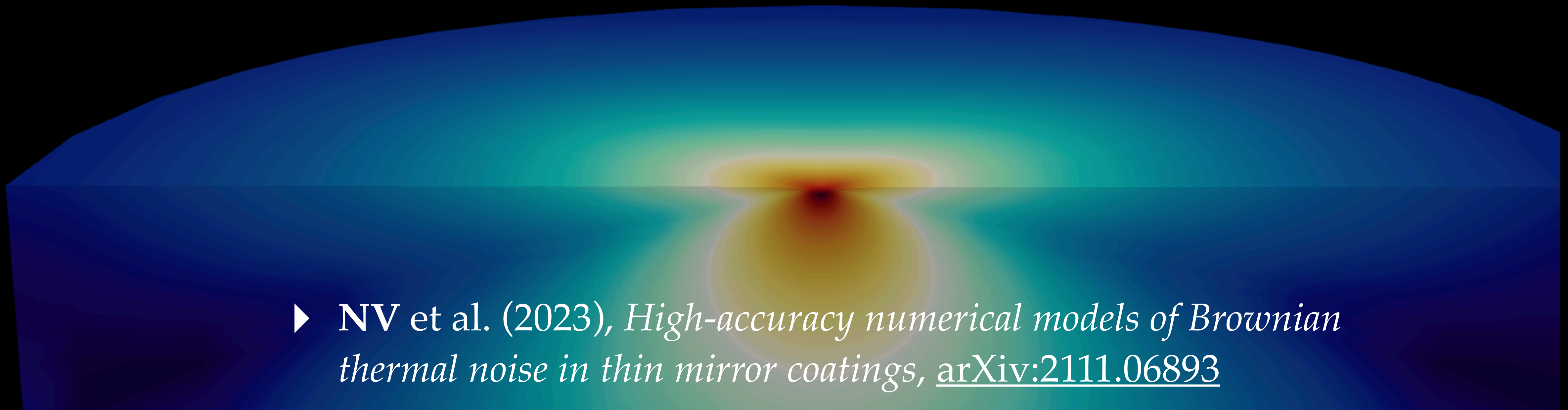
- XCTS momentum constraint is an elasticity equation:

$$\bar\nabla_i (\bar L \beta)^{ij} = \text{(nonlinear sources)}$$

with $\quad \left(\bar L \beta\right)^{ij} = 2\,\bar\nabla^{(i}\beta^{j)} - \frac{2}{3}\bar\gamma^{ij}\bar\nabla_k \beta^k$

- Fluctuation dissipation theorem connects thermal noise to elasticity.

➡ We can simulate thermal noise in LIGO mirrors!



- **NV** et al. (2023), *High-accuracy numerical models of Brownian thermal noise in thin mirror coatings*, arXiv:2111.06893

M-mode self force

- Second-order Kerr self force

➡ EMRI waveforms for LISA

- 1 elliptic PDE per m-mode
  - **Osburn & Nishimura (2022),** *New self-force method via elliptic partial differential equations for Kerr inspiral models,* arXiv:2206.07031