A multilevel Jacobi-Davidson method for polynomial eigenvalue pde problems

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Research Training Group “Dynamic of hot plasmas”

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Outline

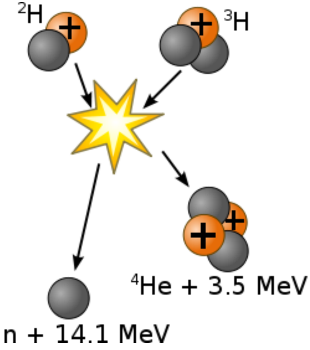
Physical background

Multilevel Jacobi-Davidson method

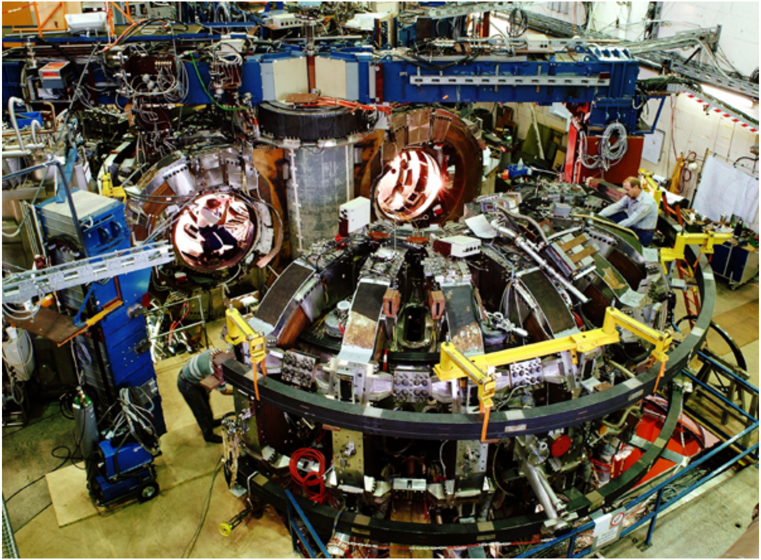
Summary and perspectives

Energy gain by nuclear fusion

- fusion of deuterium and tritium to helium
- ignition of fusion:
  - overcome Coulomb barrier
  - high temperature and high density required for a long time
  - gas is in plasma state (atoms fully ionized)
- magnetic confinement
  - high energy loss if particles hit wall

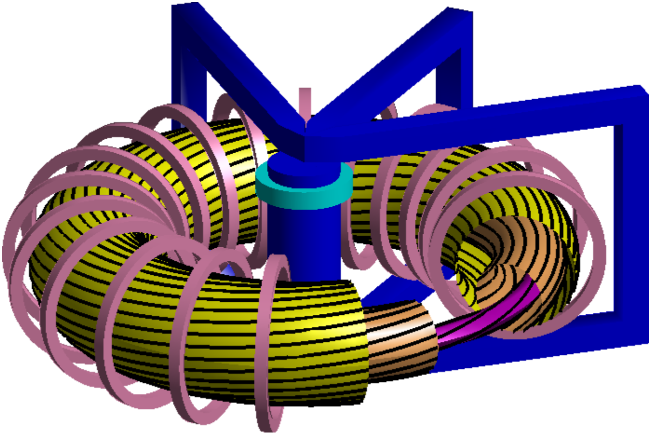


TEXTOR at Research Center Jülich



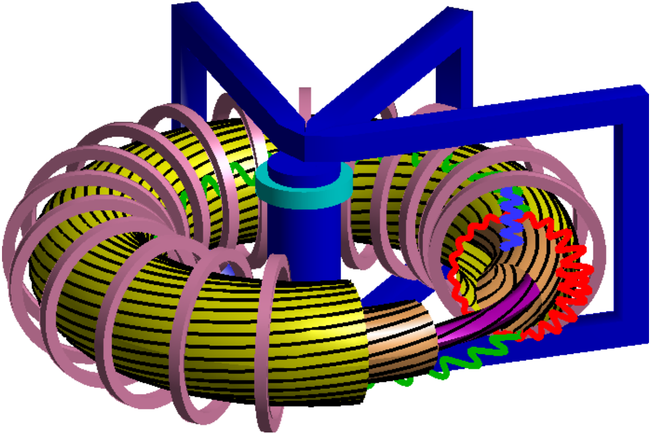
Tokamak Experiment for Technology Oriented Research

Tokamak



- toroidal coil
- magnetic field lines within the flux surface
- primary coil
- transformer iron

Drift instabilities



Fourier analysis

$$\Phi(\theta, t) = \phi(\theta) \cdot \exp(\mathbf{i} k_r r + \mathbf{i} k_\perp y - \mathbf{i}\omega t), \qquad \mathrm{Im}(\omega) \text{ maximal}$$

Eigenvalue pde problem

$$\frac{\partial^2 \phi}{\partial \theta^2} = \frac{\omega(\widehat{\beta} + z\gamma_3 \widehat{\mu} K_\perp^2) - (1+\widehat{\lambda})\widehat{\beta} K_\perp + \mathbf{i} z \gamma_3 \widehat{C} K_\perp^2}{\gamma_1^3 z \left(K_\perp - \omega\left(1 + z\gamma_3(1+\widehat{\alpha})K_\perp^2\right)\right)}$$

$$\cdot \left((1+\widehat{\alpha}) \frac{\gamma_2}{\gamma_3} L_{\mathrm{B}} (1 - z\gamma_3 \omega K_\perp) + z\omega(\omega + \widehat{\alpha} K_\perp) \right) \phi$$

generic form:

$$\left[\omega^3 a_3 + \omega^2 a_2 + \omega \left(a_1 + b_1 \frac{\partial^2}{\partial \theta^2} \right) + a_0 + b_0 \frac{\partial^2}{\partial \theta^2} \right] \phi = 0$$

a_j, b_j, ϕ: $[0, 2\pi[\longmapsto \mathbb{C}$, 2π-periodic smooth functions in θ

sought: eigenpair (ω, ϕ) with maximum growth rate $\mathrm{Im}(\omega)$

Löchel, Tokar, H., Reiser, PoP 2009

Spatial discretization

polynomial pde eigenvalue problem

$$\left[\omega^3 a_3 + \omega^2 a_2 + \omega \left(a_1 + b_1 \frac{\partial^2}{\partial\theta^2}\right) + a_0 + b_0 \frac{\partial^2}{\partial\theta^2}\right] \phi = 0$$

discretization

- $[0, 2\pi[\mapsto \vec{\theta}$
- $a_j(\theta) \to \mathrm{diag}(a_j(\vec{\theta})), \quad b_j(\theta) \to \mathrm{diag}(b_j(\vec{\theta}))$
- finite differences or pseudo-spectral-method (periodic b.c.)

$$\frac{\partial^2}{\partial\theta^2}\phi \mapsto D_2 \vec{\phi}$$

- cubic matrix eigenvalue problem

$$P(\omega)\vec{\phi} := \left(\omega^3 M_3 + \omega^2 M_2 + \omega M_1 + M_0\right)\vec{\phi} = 0$$

Linearization – companion form

$$\left(\omega^3 M_3 + \omega^2 M_2 + \omega M_1 + M_0\right)\vec{\phi} = 0$$

$$\Leftrightarrow \left(\omega \begin{bmatrix} M_3 & & \\ & I & \\ & & I \end{bmatrix} + \begin{bmatrix} M_2 & M_1 & M_0 \\ -I & & \\ & -I & \end{bmatrix} \right) \begin{bmatrix} \omega^2 \vec{\phi} \\ \omega \vec{\phi} \\ \vec{\phi} \end{bmatrix} = 0.$$

$$\Leftrightarrow \omega B x = -A x, \qquad \text{(generalized eigenvalue problem)}$$

Higham, D.S.+N. Mackey, Mehl, Mehrmann, Tisseur, ...

Linearization – symmetric form

- $P(\omega)$ is complex symmetric (for equidistant grids)
- symmetric linearization

$$\left(\omega \begin{bmatrix} M_3 & & \\ & -M_1 & -M_2 \\ & -M_0 & \end{bmatrix} + \begin{bmatrix} M_2 & M_1 & M_0 \\ M_1 & M_0 & \\ M_0 & & \end{bmatrix}\right) \begin{bmatrix} \omega^2 \vec{\phi} \\ \omega \vec{\phi} \\ \vec{\phi} \end{bmatrix} = 0$$

- advantage: left and right eigenvectors coincide except for complex conjugation

Higham, Li, Tisseur, Mackey (2006–2007)

Standard methods

- $N = 1024$. QZ-algorithm: 1 hour.
- simulations with 100 000 eigenvalue equations: 10 years
- only interested in one eigenpair: subspace method

Jacobi-Davidson algorithm

(0.) choose search space $V \in \mathbb{C}^{N \times k}$, $k \ll N$

loop

- **(1.)** orthonormalize V
- **(2.)** calculate eigenpairs (ν, y) of $V^H P(\nu) V y = 0$
- **(3.)** select Ritz pair $(\nu, u := Vy)$.
- **(4.)** calculate residual $r := P(\nu)u$.
- **if** $\|r\|$ small enough **do** Stop **end if**
- **(5.)** find new expansion vector t by solving the correction equation
- **(6.)** expand search space to $[V, t]$.

end loop

Sleijpen et al. 1996, 1998

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Sleijpen et al. 1996, 1998

Solution of correction equation

$$\left(I - \frac{P'(\nu)uu^H}{u^H P'(\nu)u}\right) P(\nu)(I - uu^H)t = -r, \quad t \perp u$$

corresponds to one Newton step for

$$F(\lambda, x) := \begin{pmatrix} P(\lambda)x \\ x^H x - 1 \end{pmatrix} = 0.$$

one step approximation

$$t = \frac{u^H Q(\nu) r}{u^H Q(\nu) P'(\nu) u} Q(\nu) P'(\nu) u - Q(\nu) r, \qquad Q(\nu)P(\nu) = I$$

Sleijpen 1998

Solution of correction equation – preconditioning

one step approximation

$$t = \frac{u^H Q(\nu) r}{u^H Q(\nu) P'(\nu) u} Q(\nu) P'(\nu) u - Q(\nu) r, \qquad Q(\nu)P(\nu) = I$$

requires solution of two linear systems

$$Q(\nu) r = z \Leftrightarrow P(\nu) z = r, \qquad Q(\nu) P'(\nu) u = s \Leftrightarrow P(\nu) s = P'(\nu) u$$

$$P(\nu) = \begin{bmatrix} \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \end{bmatrix} = \begin{bmatrix} \bullet&&&&&&&& \\ \bullet&\bullet&&&&&&& \\ \bullet&\bullet&\bullet&&&&&& \\ \bullet&\bullet&\bullet&\bullet&&&&& \\ \bullet&\bullet&\bullet&\bullet&\bullet&&&& \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&&& \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&& \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet& \\ \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \end{bmatrix} \begin{bmatrix} \bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ &\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ &&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ &&&\bullet&\bullet&\bullet&\bullet&\bullet&\bullet \\ &&&&\bullet&\bullet&\bullet&\bullet&\bullet \\ &&&&&\bullet&\bullet&\bullet&\bullet \\ &&&&&&\bullet&\bullet&\bullet \\ &&&&&&&\bullet&\bullet \\ &&&&&&&&\bullet \end{bmatrix}$$

Voss, 2007; Heuveline, Bertsch 2000

Solution of correction equation – preconditioning

one step approximation

$$t = \frac{u^H Q(\nu) r}{u^H Q(\nu) P'(\nu) u} Q(\nu) P'(\nu) u - Q(\nu) r, \qquad Q(\nu) P_{\mathbf{f}}(\nu) = I$$

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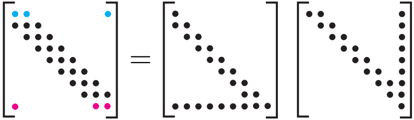
$$Q(\nu) r = z \Leftrightarrow P_{\mathbf{f}}(\nu) z = r, \qquad Q(\nu) P'(\nu) u = s \Leftrightarrow P_{\mathbf{f}}(\nu) s = P'(\nu) u$$

$P_{\mathbf{f}}(\nu) =$

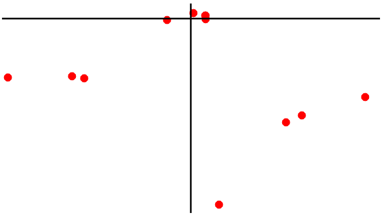


Voss, 2007; Heuveline, Bertsch 2000

Selection of Ritz pair

wanted: eigenpair with strongest growth rate $\mathrm{Im}(\omega)$.

experiment ($N = 4$): $V = [v^1]$, v^1 with random vectors v^1



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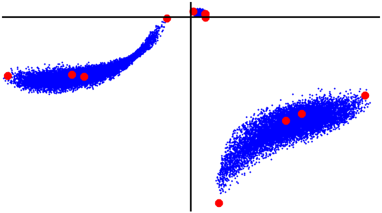

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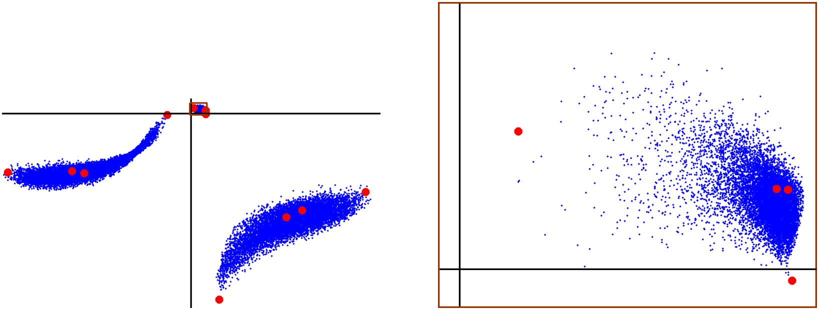

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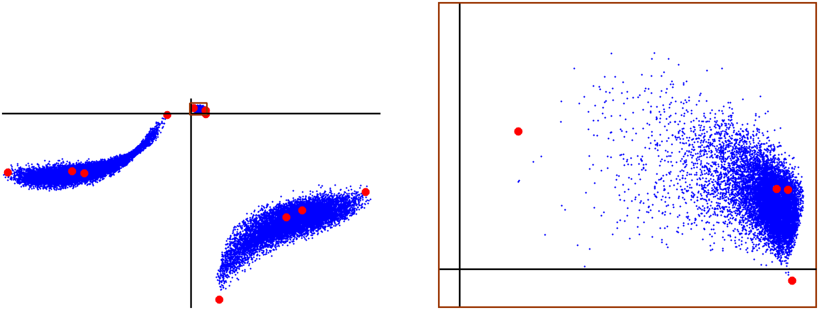


- big chance to miss desired eigenpair

Finding a good initial search space

- random vector
  $\longrightarrow$ not reliable
- Fourier modes $V = \big(\exp(\mathbf{i}j\theta)\big)_{j=-m,\dots,m}$
  $\longrightarrow$ useful for very smooth eigenfunctions only
- new idea: multilevel approach

Finding a good initial search space

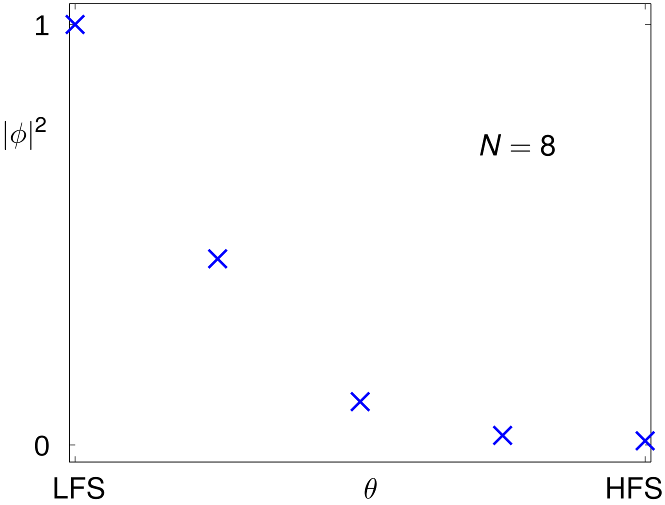
multilevel approach

compute (cheap) approximation on coarse grid

- QZ algorithm on coarsest grid (e.g. $N = 8$)
- crucial: reliable selection of eigenpair
- can expect good approximation if eigenfunction is smooth (for pseudo-spectral method or fd on adaptive grid)
- refinement of eigenpair: prolongation to finer grid $+$ Jacobi-Davidson method
- selection of Ritz pair by similarity to coarse grid approximation.

Multilevel Jacobi-Davidson approach

Example:



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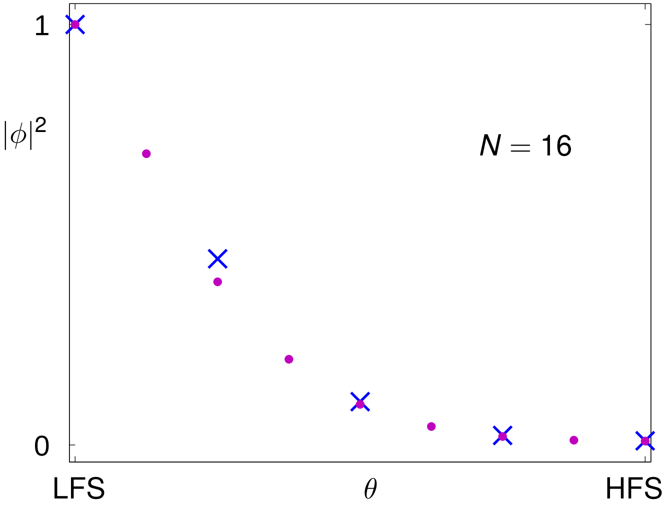

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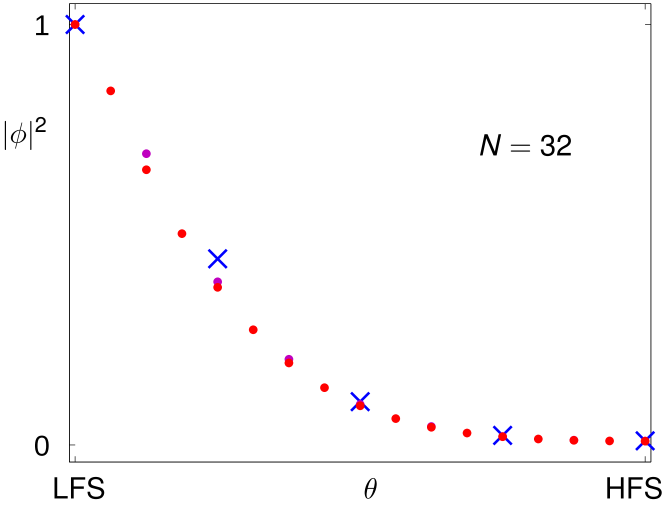

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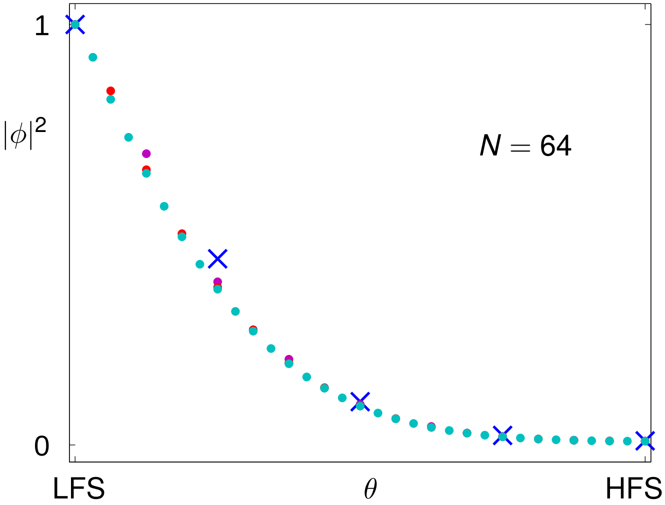

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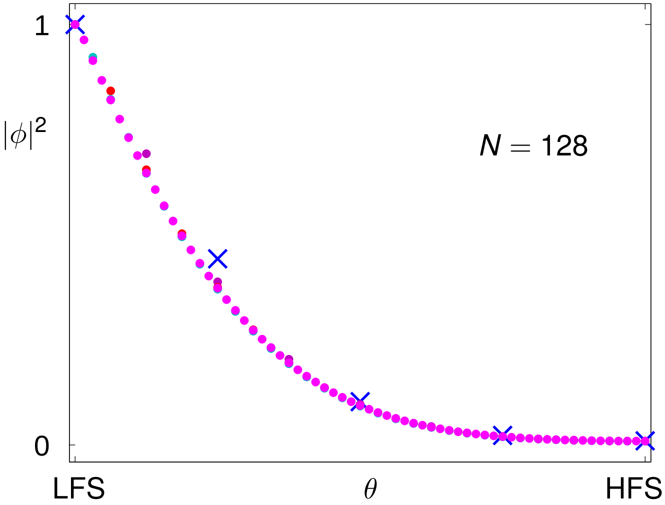

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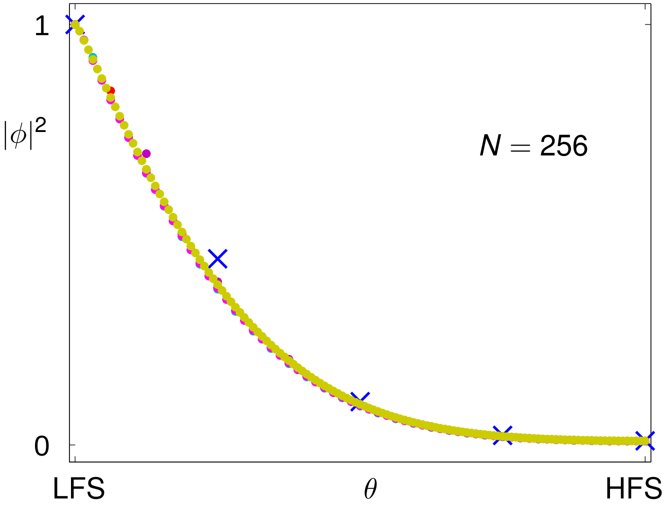

Multilevel Jacobi-Davidson approach

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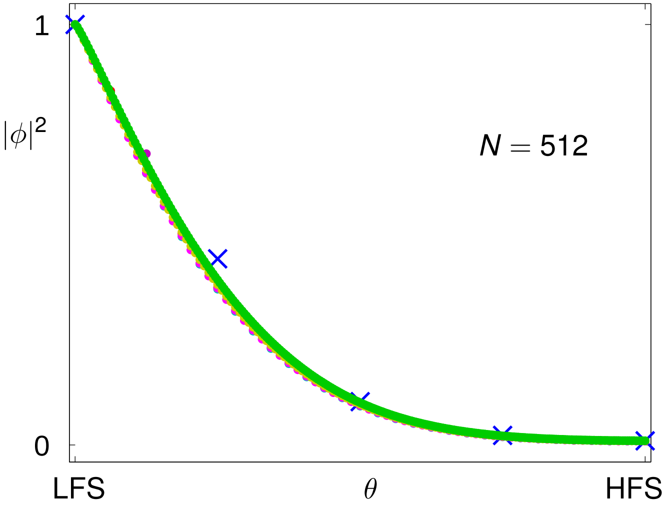

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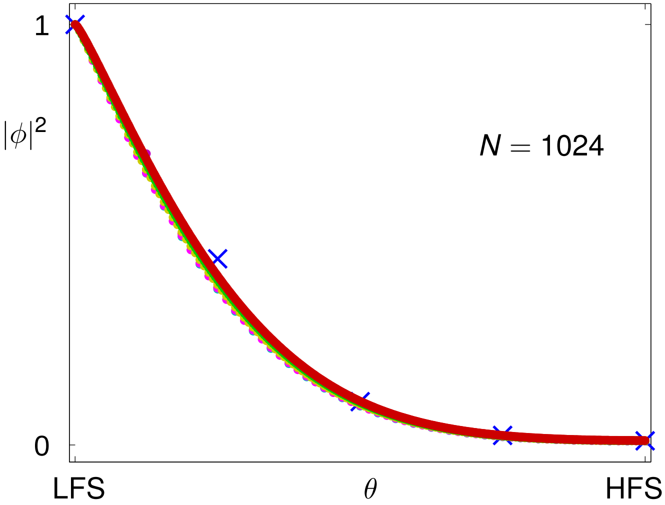

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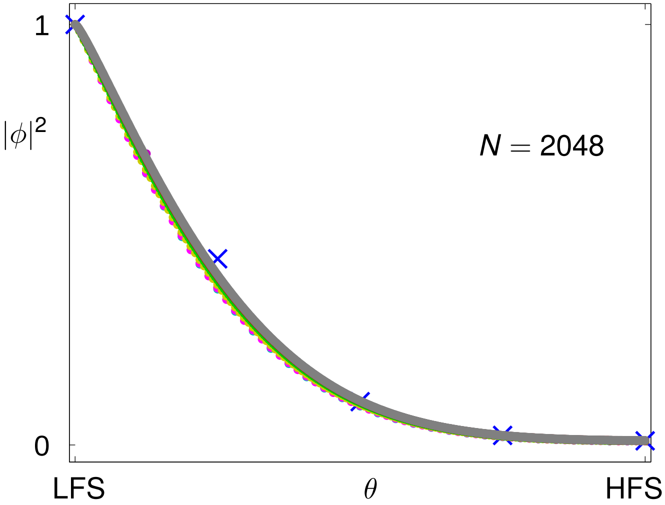

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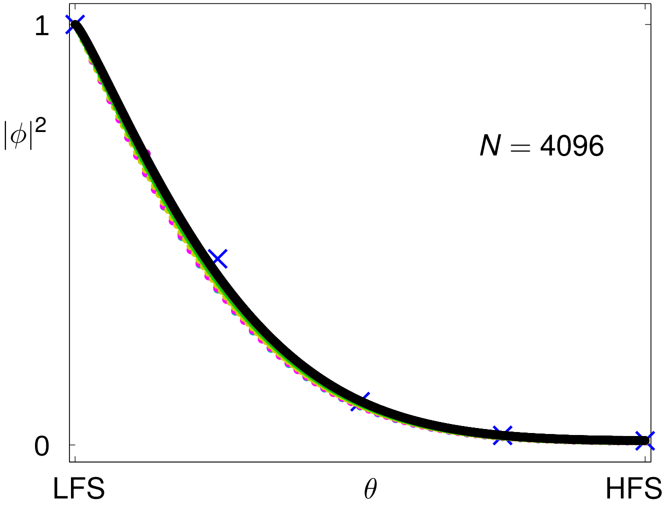

Error control

- Tisseur 00: normwise backward error of $(\widetilde{\lambda}, \widetilde{x})$

$$\eta(\widetilde{\lambda}, \widetilde{x}) := \min_{\epsilon}\Big\{ \big(P(\widetilde{\lambda}) + \Delta P(\widetilde{\lambda})\big)\widetilde{x} = 0,\ \|\Delta M_j\| \le \epsilon \|E_j\| \Big\}$$

$$= \frac{\|P(\widetilde{\lambda})\widetilde{x}\|_2}{\widetilde{\alpha}\|\widetilde{x}\|_2}, \qquad \widetilde{\alpha} = \sum_{j=0}^{d} |\widetilde{\lambda}|^j \|E_j\|_2$$

- normwise condition number of exact eigentriple (y, λ, x)

$$\kappa(\lambda, P) = \frac{\alpha\|y\|_2\|x\|_2}{|\lambda||y^H P'(\lambda)x|}, \qquad \alpha = \sum_{j=0}^{d} |\lambda|^j \|E_j\|_2 \qquad (1)$$

- forward error estimate: $(y, \lambda, x) \approx (\widetilde{y}, \widetilde{\lambda}, \widetilde{x})$

$$\eta(\widetilde{\lambda}, \widetilde{x})\kappa(\widetilde{\lambda}, P) = \frac{\|P(\widetilde{\lambda})\widetilde{x}\|_2\|\widetilde{y}\|_2}{|\widetilde{\lambda}||\widetilde{y}^H P'(\widetilde{\lambda})\widetilde{x}|}.$$

- stop if forward error estimate $\le$ tol

Scaling of eigenvalues

- original problem: $P(\omega)x = 0$
- choose scaling parameter α, $\widehat{\omega}$ scaled eigenvalue

$$P(\omega) = P(\alpha\widehat{\omega}), \qquad \alpha = |\omega|$$

- problem: requires unkown eigenvalue ω
- impact on companion linearization

$$\left(\omega \begin{bmatrix} M_3 & & \\ & I & \\ & & I \end{bmatrix} + \begin{bmatrix} M_2 & M_1 & M_0 \\ -I & & \\ & -I & \end{bmatrix} \right) \begin{bmatrix} \omega^2 \vec{\phi} \\ \omega \ \vec{\phi} \\ \vec{\phi} \end{bmatrix} = 0$$

$$\left(\widehat{\omega} \begin{bmatrix} \alpha^3 M_3 & & \\ & I & \\ & & I \end{bmatrix} + \begin{bmatrix} \alpha^2 M_2 & \alpha M_1 & M_0 \\ -I & & \\ & -I & \end{bmatrix} \right) \begin{bmatrix} \widehat{\omega}^2 \vec{\phi} \\ \widehat{\omega} \ \vec{\phi} \\ \vec{\phi} \end{bmatrix} = 0$$

Scaling of eigenvectors

- choose nonsingular diagonal matrix S
- Betcke 2008: optimal scaling for (ϕ_l, ω, ϕ_r)

$$S_l P(\omega) S_r y = 0, \qquad x = S_r y,$$

with $S_l = \mathrm{diag}(|\phi_l|),\ S_r = \mathrm{diag}(|\phi_r|)$

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Scaling of eigenvectors

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  with $S_l = \mathrm{diag}(|\phi_l|),\ S_r = \mathrm{diag}(|\phi_r|)$
- problem: requires unknown left and right eigenvectors
- solution by multilevel approach
  - interpolate coarse grid solution to approximate S_l, S_r
  - ϕ_l can be computed from (ω, ϕ_r), since

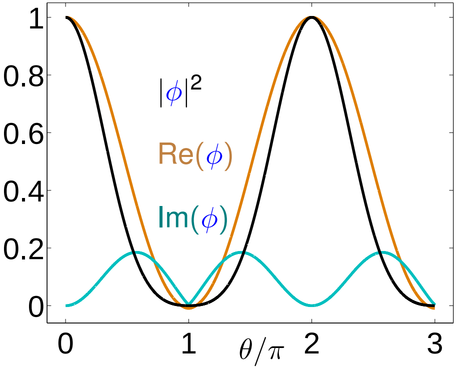
$$0 = P(\omega)\phi = \left(a(\omega) + b(\omega)\frac{\partial^2}{\partial\theta^2}\right)\phi_r$$

    with complex symmetric (diagonal) $a(\omega)$, $b(\omega)$

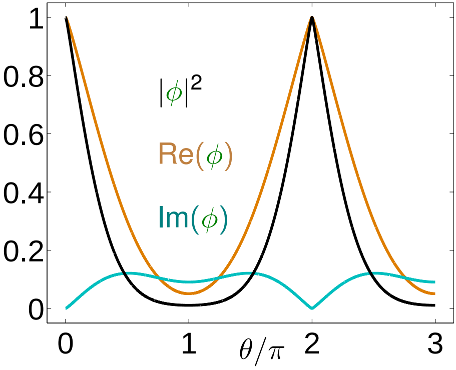
$$\phi_l = \overline{b(\omega)^{-1}\phi_r}$$

Numerical examples

Example 1
$\omega = -0.074 + 0.332\mathrm{i}$



Example 2
$\omega = -0.001 + 0.135\mathrm{i}$



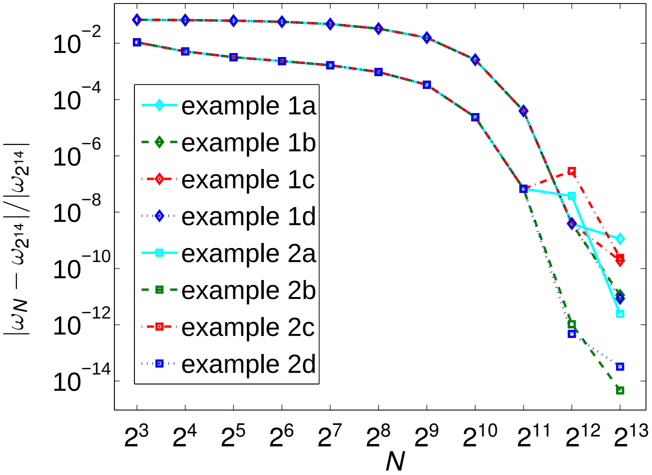
Example 1, results

linearization	scaling	comp		comp		sym		sym	
		no		yes		no		yes	
ℓ	N	$\dim V$	t/sec	$\dim V$	t/sec	$\dim V$	t/sec	$\dim V$	t/sec
11	2^{14}	1	0.08	1	0.07	1	0.08	1	0.06
10	2^{13}	17	5.10	4	0.68	4	0.69	4	0.66
9	2^{12}	11	1.31	9	0.94	7	0.67	8	0.81
8	2^{11}	15	0.95	9	0.45	9	0.45	9	0.45
7	2^{10}	9	0.23	10	0.27	9	0.24	10	0.27
6	2^{9}	10	0.15	10	0.15	9	0.13	10	0.14
5	2^{8}	9	0.08	9	0.08	9	0.08	9	0.08
4	2^{7}	9	0.06	9	0.05	9	0.05	9	0.06
3	2^{6}	8	0.04	8	0.05	8	0.04	8	0.03
2	2^{5}	7	0.01	7	0.02	7	0.03	7	0.03
1	2^{4}	6	0.03	6	0.02	6	0.02	6	0.01
	total	102	8.04	82	2.78	78	2.48	81	2.60

Example 2, results

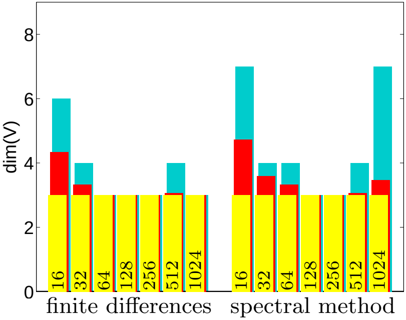
linearization	scaling	comp		comp		sym		sym	
		no		yes		no		yes	
ℓ	N	dim V	t/sec	dim V	t/sec	dim V	t/sec	dim V	t/sec
11	2^{14}	1	0.06	1	0.08	1	0.07	1	0.07
10	2^{13}	3	0.45	3	0.51	3	0.47	3	0.49
9	2^{12}	≥ 64	32.79	7	0.71	≥ 64	33.86	7	0.74
8	2^{11}	15	0.92	9	0.45	10	0.52	9	0.49
7	2^{10}	≥ 64	14.61	10	0.27	10	0.26	10	0.30
6	2^{9}	27	0.86	10	0.15	10	0.16	10	0.16
5	2^{8}	19	0.28	10	0.10	10	0.09	10	0.09
4	2^{7}	10	0.07	10	0.07	10	0.07	10	0.08
3	2^{6}	10	0.05	10	0.05	10	0.05	10	0.05
2	2^{5}	9	0.04	9	0.03	9	0.04	9	0.05
1	2^{4}	8	0.04	8	0.04	8	0.03	8	0.02
	total	230	50.17	87	2.46	145	35.62	87	2.54

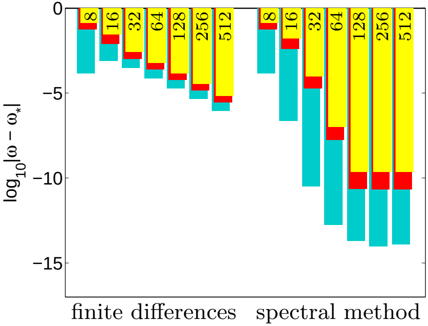
Eigenvalue error



Prolongation by linear interpolation

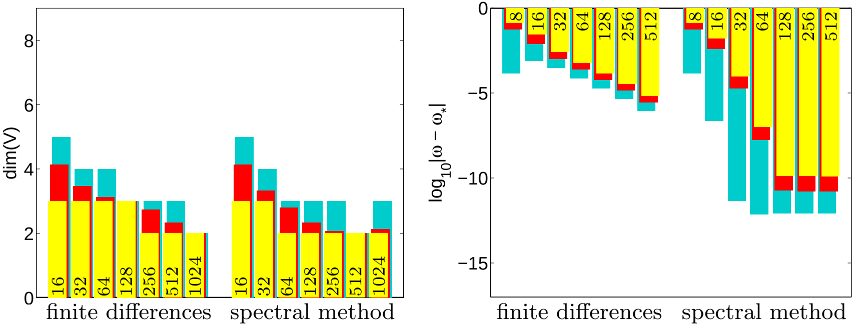
minimum, average, maximum





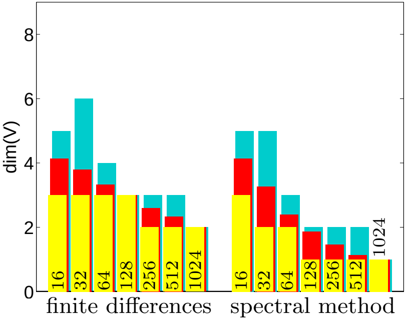
Prolongation by splines

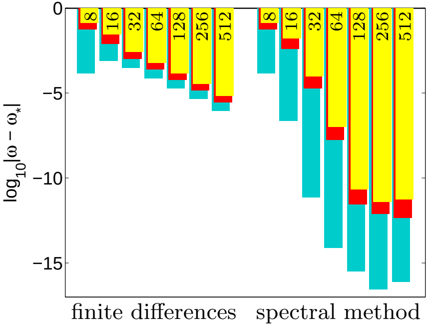
minimum, average, maximum



Prolongation by trigonometric interpolation

minimum, average, maximum





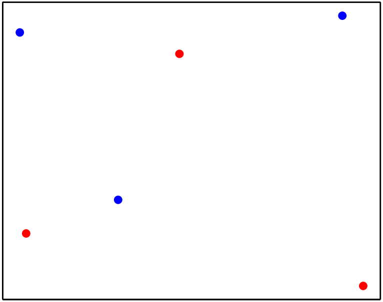
Wave number $K_\perp$

$$\frac{\partial^2 \phi}{\partial \theta^2} = \frac{\omega(\widehat{\beta} + z\gamma_3 \widehat{\mu} K_\perp^2) - (1+\widehat{\lambda})\widehat{\beta} K_\perp + iz\gamma_3 \widehat{C} K_\perp^2}{\gamma_1^3 z \left(K_\perp - \omega\left(1 + z\gamma_3(1+\widehat{\alpha})K_\perp^2\right)\right)}$$
$$\cdot \left((1+\widehat{\alpha}) \frac{\gamma_2}{\gamma_3} L_{\mathrm{B}} (1 - z\gamma_3 \omega K_\perp) + z\omega(\omega + \widehat{\alpha} K_\perp) \right) \phi$$

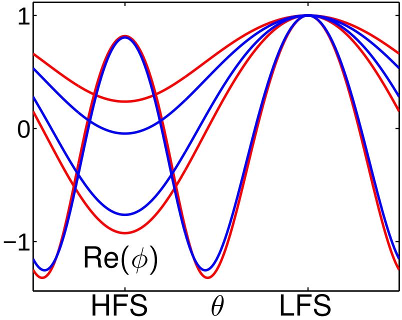
- discrete representation of wave number range
- define modes $(\omega(K_\perp), \phi(K_\perp))$
- trace modes and find wave number of maximal growth rate

Tracing eigenpairs – similarity measure

$K_\perp = 0.4$, $K_\perp = 0.5$



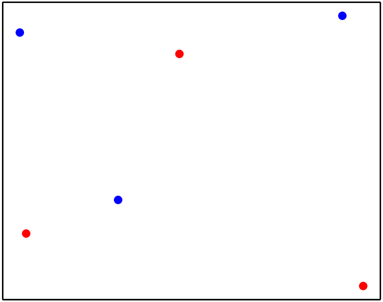
$$\mathrm{sim}(\omega, \omega) = \exp(-|\omega - \omega|)$$

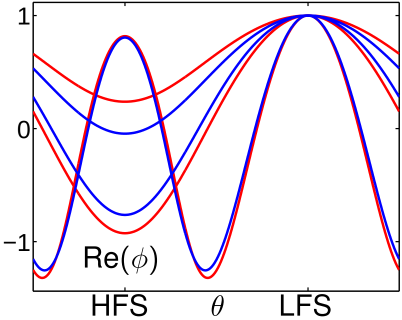


$$\mathrm{sim}(\phi, \phi) = |\phi^H \phi|$$

Tracing eigenpairs – similarity measure

$K_\perp = 0.4$, $K_\perp = 0.5$



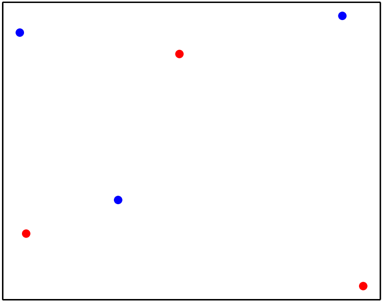


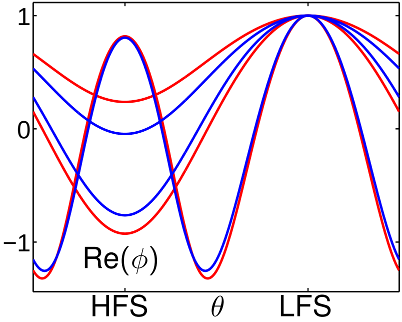
$$\mathrm{sim}(\omega,\omega) = \exp(-|\omega - \omega|) \qquad \mathrm{sim}(\phi,\phi) = |\phi^H\phi|$$

$$\mathrm{sim}(\omega,\omega) = \begin{pmatrix} 0.99 & 0.99 & 1.00 \\ 0.97 & 1.00 & 1.00 \\ 1.00 & 0.96 & 0.98 \end{pmatrix}, \quad \mathrm{sim}(\phi,\phi) = \begin{pmatrix} 0.47 & 0.87 & 0.99 \\ 0.28 & 0.99 & 0.87 \\ 1.00 & 0.34 & 0.45 \end{pmatrix}$$

Tracing eigenpairs – similarity measure

$K_\perp = 0.4$, $K_\perp = 0.5$





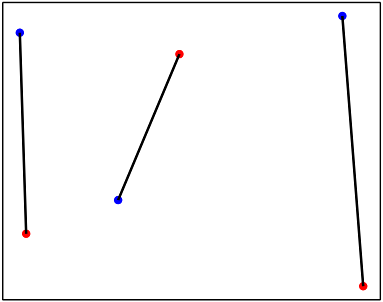
$$\mathrm{sim}(\omega,\omega) = \exp(-|\omega - \omega|)$$

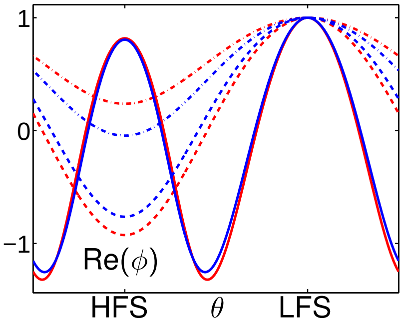
$$\mathrm{sim}(\phi,\phi) = |\phi^H \phi|$$

$$\mathrm{sim}(\omega,\omega) = \begin{pmatrix} 0.99 & 0.99 & 1.00 \\ 0.97 & 1.00 & 1.00 \\ 1.00 & 0.96 & 0.98 \end{pmatrix}, \quad \mathrm{sim}(\phi,\phi) = \begin{pmatrix} 0.47 & 0.87 & 0.99 \\ 0.28 & 0.99 & 0.87 \\ 1.00 & 0.34 & 0.45 \end{pmatrix}$$

Tracing eigenpairs – similarity measure

$K_\perp = 0.4$, $K_\perp = 0.5$





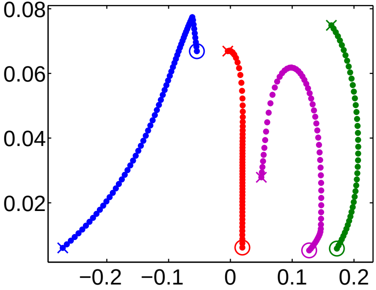
$\mathrm{sim}(\omega, \omega) = \exp(-|\omega - \omega|)$

$\mathrm{sim}(\phi, \phi) = |\phi^H \phi|$

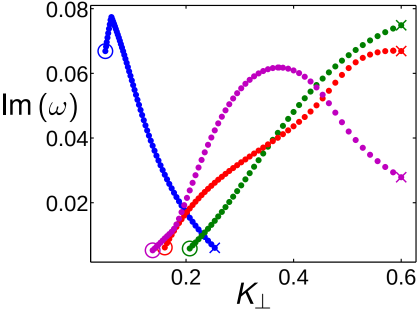
$$\mathrm{sim}\big((\omega, \phi), (\omega, \phi)\big) := \mathrm{sim}(\omega, \omega)\, \mathrm{sim}(\phi, \phi)$$

$$= \begin{pmatrix} 0.47 & 0.86 & 0.99 \\ 0.27 & 0.99 & 0.87 \\ 1.00 & 0.33 & 0.44 \end{pmatrix}$$

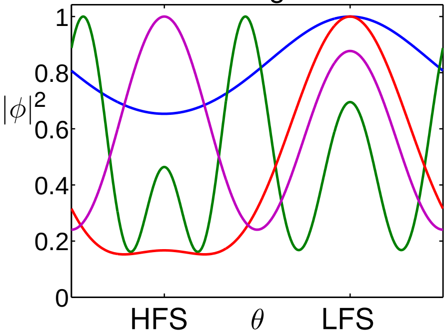
Wave number $K_\perp$



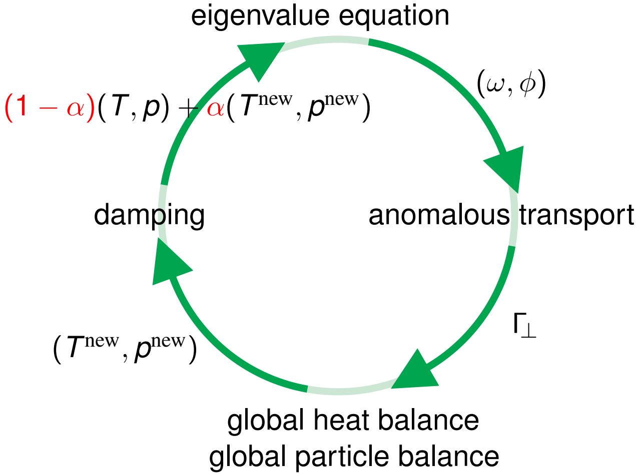
eigenvalues



eigenfunctions for $K_\perp$ which maximizes the growth rate



Self-consistent calculation



Summary and perspectives

- multilevel Jacobi-Davidson eigenvalue solver
  - approximation of search space on coarser grid
  - correction equation by low cost LU decomposition
- tracing eigenpairs with respect to the wave number
- other linearizations
- nonlinear (e.g. rational) eigenvalue problems (in progress)
- transport model needs improvement, especially modeling of heat power from plasma core ($\rightarrow$ 2d model).

References

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Technical Report, University of Düsseldorf, 2009