Polar Discretization for the Spatially Homogeneous Boltzmann equation

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The Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = Q(f, f),$$

for $f := f(t, \boldsymbol{x}, \boldsymbol{v})$ with

- $t \in [0, T]$ (time evolution problem)
- $\boldsymbol{x} \in \Omega \subset \mathbb{R}^d$ (spatial coordinate)
- $\boldsymbol{v} \in \mathbb{R}^d$ (velocity space)

f is *particle density* in phase space. What is Q?

$$Q(f, h)(\boldsymbol{v}) = \int_{\mathbb{R}^d} \int_{S^{d-1}} B(|\boldsymbol{v} - \boldsymbol{v}_*|, \cos\theta)(h'_* f' - h_* f)\, \mathrm{d}\boldsymbol{\sigma}\, \mathrm{d}\boldsymbol{v}_*$$

Let's pick apart this expression.

Binary collisions

Two particles with

- pre-collision velocities $\boldsymbol{v}, \boldsymbol{v}_*$,
- post-collision velocities $\boldsymbol{v}', \boldsymbol{v}'_*$.

Elastic collisions $\Longrightarrow$

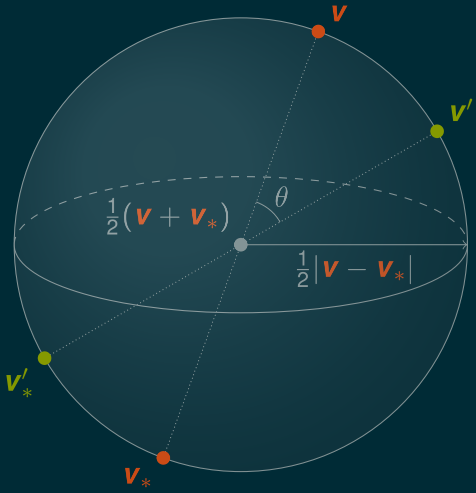
$$\underbrace{\boldsymbol{v}' + \boldsymbol{v}'_* = \boldsymbol{v} + \boldsymbol{v}_*,}_{\text{momentum}} \qquad \underbrace{|\boldsymbol{v}'|^2 + |\boldsymbol{v}'_*|^2 = |\boldsymbol{v}|^2 + |\boldsymbol{v}_*|^2,}_{\text{energy}}$$

solutions are parametrised by $\boldsymbol{\sigma} \in S^{d-1}$:

$$\boldsymbol{v}', \boldsymbol{v}'_* = \frac{1}{2}\left(\boldsymbol{v} + \boldsymbol{v}_* \pm |\boldsymbol{v} - \boldsymbol{v}_*|\boldsymbol{\sigma}\right)$$

Note the dualism

$$(\boldsymbol{v}, \boldsymbol{v}_*) \mapsto (\boldsymbol{v}', \boldsymbol{v}'_*) \mapsto (\boldsymbol{v}, \boldsymbol{v}_*)$$



$\mathbf{v}$
$\mathbf{v}'$
θ
$\frac{1}{2}(\mathbf{v} + \mathbf{v}_*)$
$\frac{1}{2}|\mathbf{v} - \mathbf{v}_*|$
$\mathbf{v}'_*$
$\mathbf{v}_*$

The Boltzmann Collision Operator

$$\int_{\mathbb{R}^d}\int_{S^{d-1}} \underbrace{B(|\boldsymbol{v}-\boldsymbol{v}_*|,\cos\theta)}_{\text{kernel}}\big(\underbrace{h(\boldsymbol{v}'_*)f(\boldsymbol{v}')}_{\text{gain term}}-\underbrace{h(\boldsymbol{v}_*)f(\boldsymbol{v})}_{\text{loss term}}\big)\,\mathrm{d}\sigma\,\mathrm{d}\boldsymbol{v}_*$$

The kernel B derives from physical particle interaction models (i.e. inverse power laws). Usually:

$$B \propto |\boldsymbol{v}-\boldsymbol{v}_*|^{\lambda} b(\cos\theta).$$

Spatial homogeneity

Focus on $\boldsymbol{v} \in \mathbb{R}^d$.

$$f(t, \boldsymbol{x}, \boldsymbol{v}) := f(t, \boldsymbol{v}) \implies \frac{\partial f}{\partial t} = Q(f, f)$$

Conserved quantities (observables):

$$\rho(f) = \int f \qquad \text{mass}$$

$$(\boldsymbol{u}\rho)(f) = \int f\, \boldsymbol{v} \qquad \text{momentum}$$

$$(E\rho)(f) = \int f\, |\boldsymbol{v}|^2 \qquad \text{energy}$$

Equilibrium

Solutions "always" converge to Gaussian distributions

$$\mu(\boldsymbol{v}) = \frac{\rho}{(2\pi T)^{d/2}} \exp\left[-\frac{|\boldsymbol{v}-\boldsymbol{u}|^2}{2T}\right]$$

where T is temperature,

$$T = \frac{1}{d}\left(E - |\boldsymbol{u}|^2\right) = \frac{1}{d\rho}\int f(\boldsymbol{u}+\boldsymbol{v})\,|\boldsymbol{v}|^2$$

Fourier discretization

- ☹ Requires truncation of Q. Introduces aliasing.
- ☺ Quite fast, good convergence.

$$Q\left(e^{i\boldsymbol{k}\cdot\boldsymbol{v}}, e^{i\boldsymbol{\ell}\cdot\boldsymbol{v}}\right) = \hat{\beta}(\boldsymbol{k}, \boldsymbol{\ell})\, e^{i(\boldsymbol{k}+\boldsymbol{\ell})\cdot\boldsymbol{v}}$$

- ☹ Not well-suited to typical solutions f.
- ☹ Cannot conserve momentum and energy.

Polar discretization

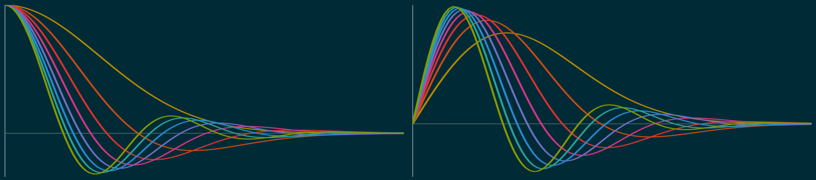
$\xi_l(\theta) = \mathrm{e}^{\mathrm{i}\ell\theta}$	angular BF
$\psi_k^{\mathrm{S}}(r) = \mathrm{e}^{-r^2/\beta} L_k^{(0)}(r^2)$	radial symmetric BF
$\psi_k^{\mathrm{K}}(r) = \mathrm{e}^{-r^2/\beta} r\, L_k^{(1)}(r^2)$	radial antisymmetric BF*

where $\beta > 0$ to be chosen later, and $L_k^{(0)}, L_k^{(1)}$ are generalized Laguerre polynomials. Combinations:

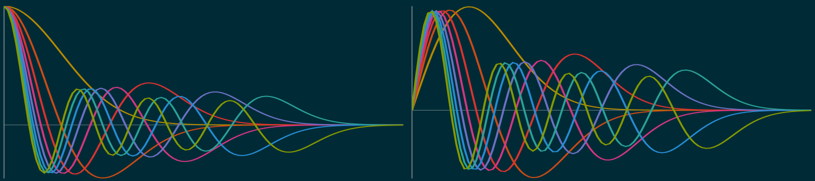
$\psi_k^{\mathrm{S}}\xi_\ell$	for ℓ even
$\psi_k^{\mathrm{K}}\xi_\ell$	for ℓ odd

Radial basis functions

$\beta = 1$



$\beta = 2$



Orthogonality

Renumbering for convenience

$$\varphi_k = \begin{cases} \psi^{\mathrm{S}}_{k/2}, & k \equiv 0 \pmod 2, \\ \psi^{\mathrm{K}}_{(k-1)/2}, & k \equiv 1 \pmod 2 \end{cases}$$

$$\implies \varphi_k \xi_\ell \ \text{for} \ k \equiv \ell \pmod 2.$$

Theorem (β-orthogonality)

Let $\mu(r) = e^{-r^2}$. *Then*

$$\langle \varphi_{k_1}\xi_{\ell_1}, \varphi_{k_2}\xi_{\ell_2} \rangle_{L^2(\mathbb{R}^2,\beta)} = \int \mu^{2/\beta - 1} \varphi_{k_1}\xi_{\ell_1}\varphi_{k_2}\xi_{-\ell_2}$$

$$= \pi\, \delta_{k_1,k_2}\, \delta_{\ell_1,\ell_2}.$$

Choosing β

Theorem (Stability w.r.t. observables)

$$\rho(\xi_0\psi_k^{\mathsf{S}}) = \beta\pi(1-\beta)^k,$$

$$(\boldsymbol{u}\rho)(\xi_{-1}\psi_k^{\mathsf{K}}) = \beta^2\pi(k+1)(1-\beta)^k,$$

$$(E\rho)(\xi_0\psi_k^{\mathsf{S}}) = \begin{cases} \beta^2\pi[1-(k+1)\beta](1-\beta)^{k-1}, & k>0 \\ \beta^2\pi, & k=0. \end{cases}$$

Choosing β

Corollary:

☺ For $0 < \beta < 2$, observables are $\mathcal{O}(|\beta - 1|^k)$.

☺☺ For $\beta = 1$, observables become zero $\implies$ conservation.

☹ For $\beta = 2$, observables are $\mathcal{O}(k)$.

☹☹ For $\beta > 2$, observables are $\mathcal{O}(|\beta - 1|^k)$.

Other considerations:

- Higher β usually gives better convergence (both norms).
- $\beta > 2$ gives unbounded basis functions.
- For $\beta = 2$, we have orthogonality w.r.t. Lebesgue measure.

We have run experiments with $\beta \in \{1, 2\}$.

- $(2, \infty)$: Exponentially unstable, unbounded, growing weight
- 2: Polynomially unstable, bounded, fast convergence, constant weight
- $(0, 2) \setminus \{1\}$: Stable, bounded, fast convergence for larger β, decaying weight
- 1: Conservative, bounded, decaying weight

Equilibrium, conformity

Function space contains

$$\varphi_0\xi_0 = \mathrm{e}^{-r^2/\beta} = \mu^{1/\beta},$$

which is an equilibrium solution with

$$\rho = \beta\pi, \qquad \boldsymbol{u} = \boldsymbol{0}, \qquad T = \frac{\beta}{2}. \tag{1}$$

Definition (β-conformity)

A function f is β-conforming if it satisfies (1).

Conformity

Theorem (Transforming solutions)

Assume $f(t, \mathbf{v})$ solves (6). Let

$$\gamma = \sqrt{\frac{2T}{\beta}}, \qquad \alpha = \frac{2\pi T}{\rho}, \qquad \eta = \frac{\alpha}{\gamma^{\lambda+2}}$$

and define $g(t, \mathbf{v}) = \alpha f(\eta t, \gamma \mathbf{v} + \mathbf{u})$. Then g is a β-conforming solution to (6).

Evaluating collisions

$$f = F_k^\ell \varphi_k \xi_\ell \implies Q(f,f) = S_{k_1,k_2,\ell_1,\ell_2}^{k,\ell} F_{k_1}^{\ell_1} F_{k_2}^{\ell_2} \varphi_k \xi_\ell$$

where

$$S_{k_1,k_2,\ell_1,\ell_2}^{k,\ell} = \frac{1}{\pi} \langle Q(\varphi_{k_1}\xi_{\ell_1}, \varphi_{k_2}\xi_{\ell_2}), \varphi_k \xi_\ell \rangle_{L^2(\mathbb{R}^2,\beta)}$$

- ☹ Expensive.
- ☺ $S_{k_1,k_2,\ell_1,\ell_2}^{k,\ell} = 0$ unless $\ell = \ell_1 + \ell_2$. We're "only" one order behind Fourier: $\mathcal{O}(N^{2d+1})$ vs. $\mathcal{O}(N^{2d})$.
- ☺ Adaptivity will help for large times.
- ☺ Easily parallelizable.

Evaluating collisions

Theorem (Invariance)

Let $\mathcal{T}$ be a translation operator and $\mathcal{R}$ a rotation operator. Then

$$Q(\mathcal{A}f, \mathcal{A}g) = \mathcal{A}Q(f, g), \qquad \mathcal{A} = \mathcal{T}, \mathcal{R}.$$

Corollary

$$Q\left(\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{v}}, \mathrm{e}^{\mathrm{i}\boldsymbol{\ell}\cdot\boldsymbol{v}}\right) = (\cdots)\mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{\ell})\cdot\boldsymbol{v}},$$

$$Q\left(f(r)\mathrm{e}^{\mathrm{i}k\theta}, g(r)\mathrm{e}^{\mathrm{i}\ell\theta}\right) = (\cdots)(r)\mathrm{e}^{\mathrm{i}(k+\ell)\theta}.$$

The number crunching (loss part)

$$S^- = \frac{1}{\pi}\int_{\boldsymbol{v}} \mu^{2/\beta-1}\varphi_{k_1}\varphi_k\xi_{\ell_1}\xi_{-\ell}\int_{\boldsymbol{v}_*}\varphi_{k_2}\xi_{\ell_2}\int_{\boldsymbol{\sigma}} B$$

The inner integral couples $\boldsymbol{v}$ and $\boldsymbol{v}_*$,

$$\mathcal{I}^-(\boldsymbol{v},\boldsymbol{v}_*) = |\boldsymbol{v}-\boldsymbol{v}_*|^\lambda \underbrace{\int_{\boldsymbol{\sigma}} b(\cos\theta)}_{\text{const.}}$$

If $B \equiv$ const. (Maxwellian kernel):

$$S^- = \delta_{k,k_1}\ \delta_{\ell,\ell_1}\ \delta_{0,\ell_2}\ \rho(\varphi_{k_2}).$$

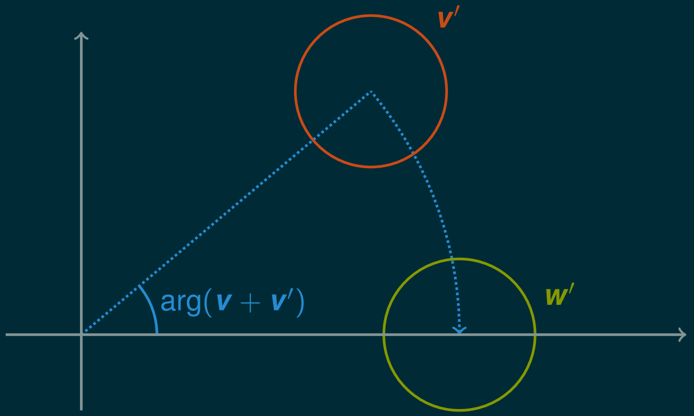
The number crunching (gain part)

$$S^+ = \frac{1}{\pi}\int_{\boldsymbol{v}} \varphi_{k_1}\xi_{\ell_1} \int_{\boldsymbol{v}_*} \varphi_{k_2}\xi_{\ell_2} \int_{\boldsymbol{\sigma}} B\mu^{2/\beta-1}\varphi_k\xi_{-\ell}$$

The inner integral is now (assuming $b \equiv$ const.)

$$\begin{aligned}\mathcal{I}^+(\boldsymbol{v},\boldsymbol{v}_*) &= |\boldsymbol{v}-\boldsymbol{v}_*|^\lambda b \int_{\boldsymbol{\sigma}} \left[\mu^{2/\beta-1}\varphi_k\xi_{-\ell}\right](\boldsymbol{v}') \\ &= |\boldsymbol{v}-\boldsymbol{v}_*|^\lambda b\, \xi_{-\ell}(\boldsymbol{v}+\boldsymbol{v}_*) \int_{\boldsymbol{\sigma}} \left[\mu^{2/\beta-1}\varphi_k\xi_{-\ell}\right](\boldsymbol{w}')\end{aligned}$$

after substituting $\boldsymbol{v}' = \mathrm{e}^{\mathrm{i}\arg(\boldsymbol{v}+\boldsymbol{v}_*)}\boldsymbol{w}'$.

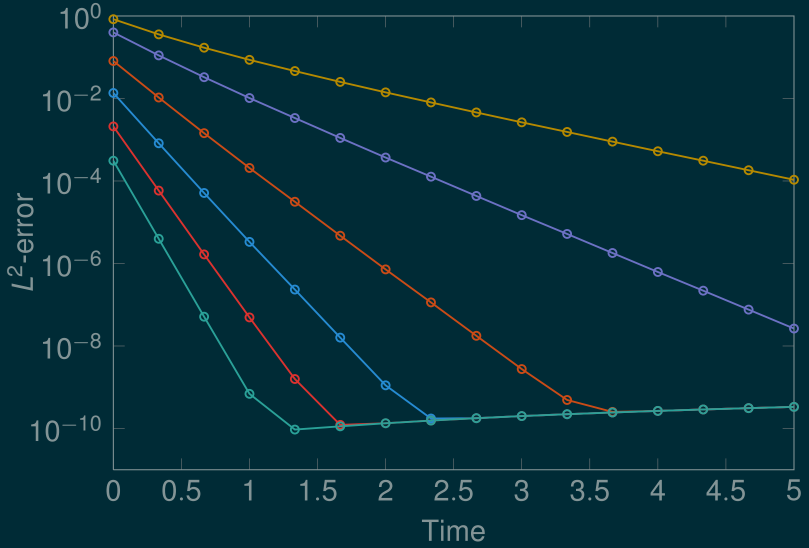

$\mathbf{v}'$
$\arg(\mathbf{v} + \mathbf{v}')$
$\mathbf{w}'$

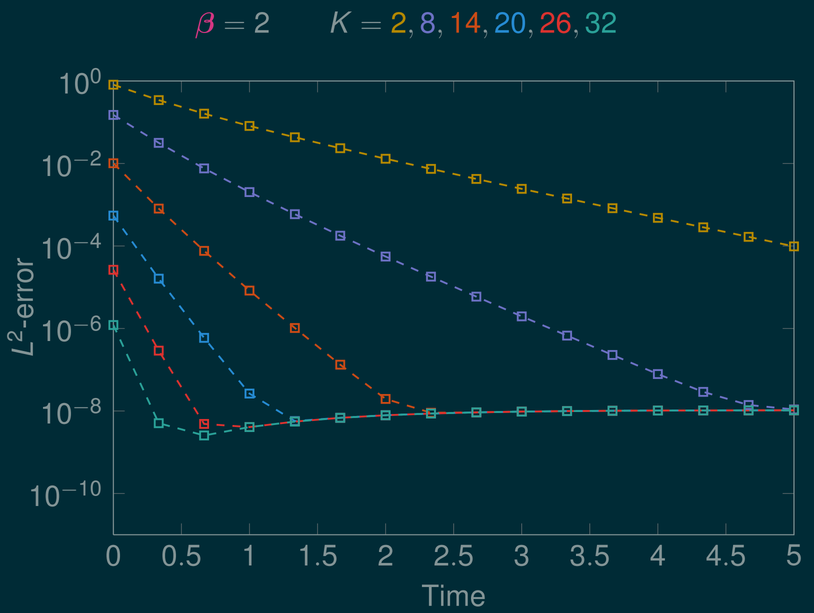
Verification (BKW)

$$f(t, \mathbf{v}) = \frac{1}{2\pi s} \left(1 - \frac{1-s}{2s} \left(2 - \frac{|\mathbf{v}|^2}{s} \right) \right) e^{-|\mathbf{v}|^2/2s}$$

$$s(t) = 1 - \frac{1}{2} e^{-t/8}$$

$\beta = 1 \qquad K = 2, 8, 14, 20, 26, 32$



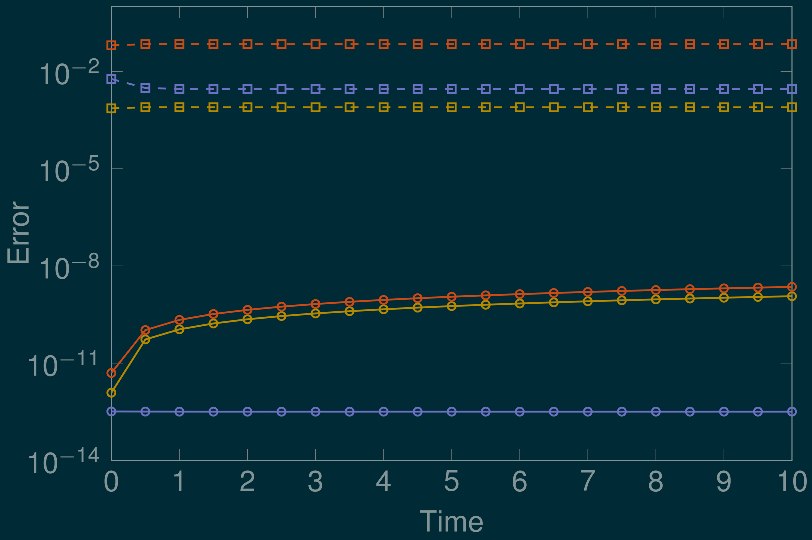

$\beta = 2$ $K = 2, 8, 14, 20, 26, 32$
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
L^2-error
0 0.5 1 1.5 2 2.5 3 3.5 4 4.5 5
Time

Crossed streams

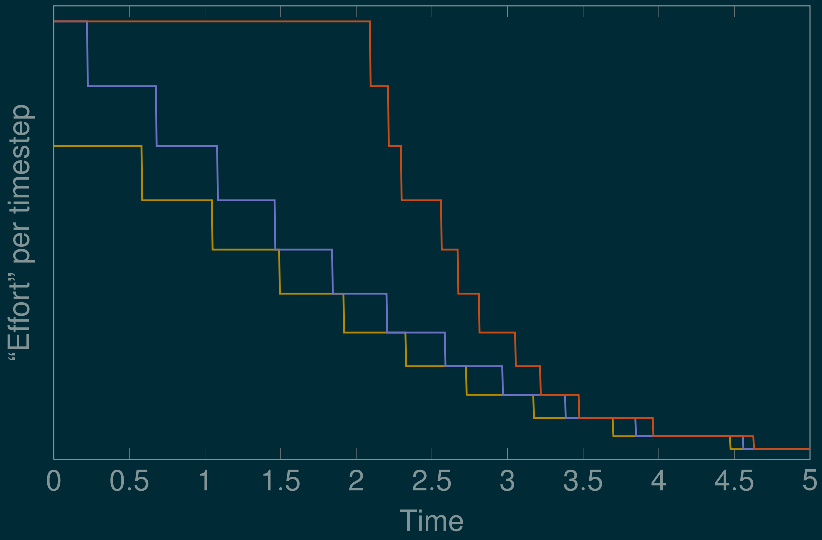
$$f_0(\boldsymbol{v}) = \exp\left[-S(v_1 - R)^2 - (v_2 - R)^2\right] + \exp\left[-(v_1 + R)^2 - S(v_2 + R)^2\right]$$

$\rightarrow$ video.

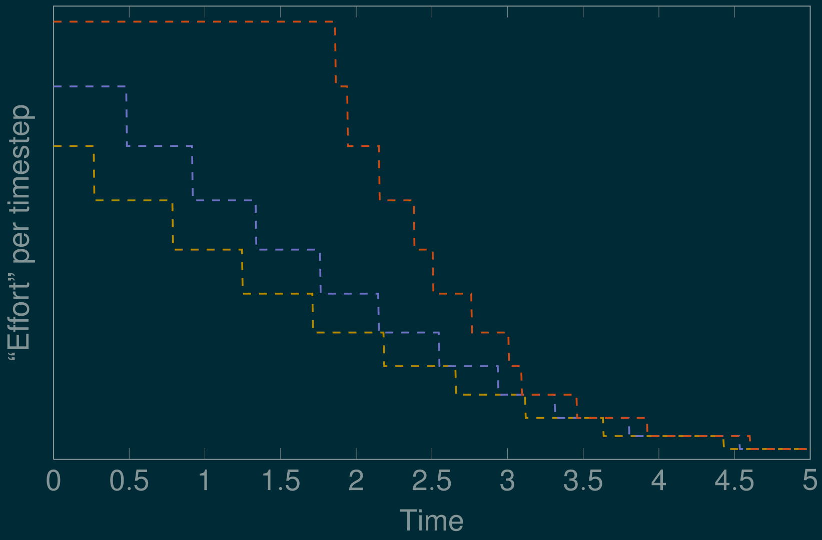
Mass, momentum and energy.



Adaptivity



Adaptivity



Summary

Fourier based methods are

- usually faster for comparable problems
- currently available for $d > 2$

Laguerre based methods are

- free of aliasing and truncation
- naturally adaptive for long times
- fully conservative ($\beta = 1$)