A Reduced Ordel Model for Aerosol Coagulation

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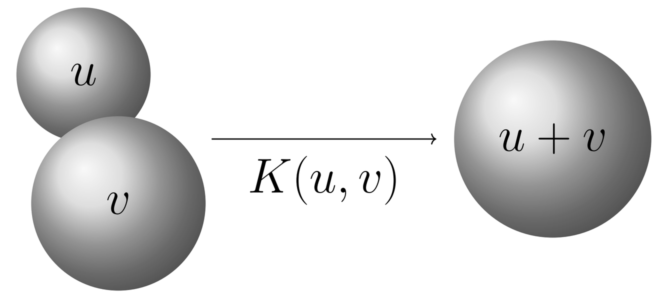
Coagulation

Coagulation is a process affecting the size distribution of particles, describing the rate of collisions of particles and the formation of larger particles over time.
It behaves **non-linearly** and **non-locally** [Smo16], leading to prohibitive computational demands for high-resolution simulations.



$$\frac{\partial n}{\partial t}(v,t) = \frac{1}{2}\int_0^v K(u, v-u)\, n(u,t)\, n(v-u,t)\,\mathrm{d}u - n(v,t)\int_0^\infty K(v,u)\, n(u,t)\,\mathrm{d}u \quad (1)$$

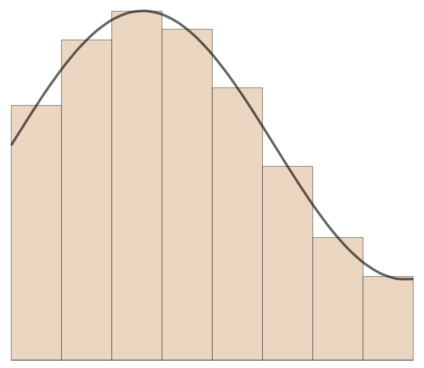
Relevance to many domains of physics

Coagulation is involved in many types of interacting particle systems, such as

- Atmospheric aerosol and air quality [SP16]
- Cloud droplets [CS98]
- Polymerization in colloidal systems [Ada95]
- Protoplanet accretion [Cha43]

Full order model

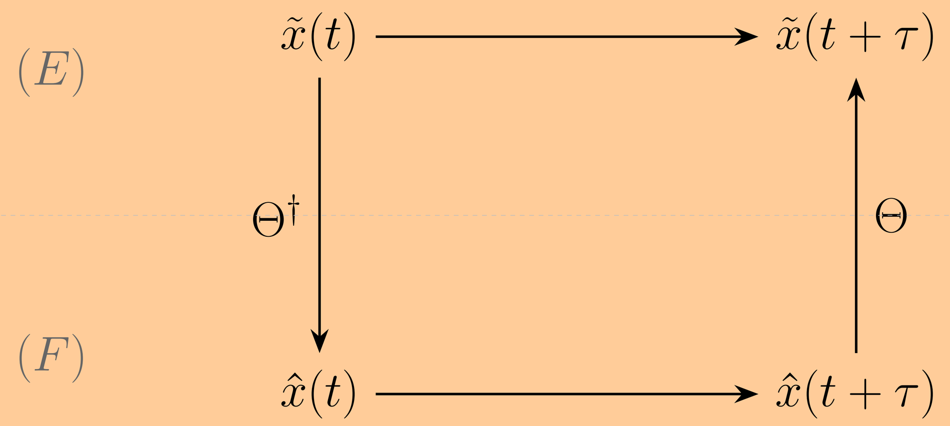
Let $E = Span\{\phi_1, \dots, \phi_N\}$ a reference approximation subspace, for instance a finite element approximation supported on a fine mesh.
Let $\tilde{n}(v,t) = \sum_{i=1}^{N} \phi_i(v)\tilde{x}_i(t)$ the approximation of (1) in E.
We are interested in the solution set $\mathcal{S}$ corresponding to a given a set of initial conditions $\mathcal{X}_0$



$$\mathcal{S} = \{\tilde{n}(v,t) \,|\, \tilde{n}(v,0) \in \mathcal{X}_0\} \quad (2)$$

Model order reduction

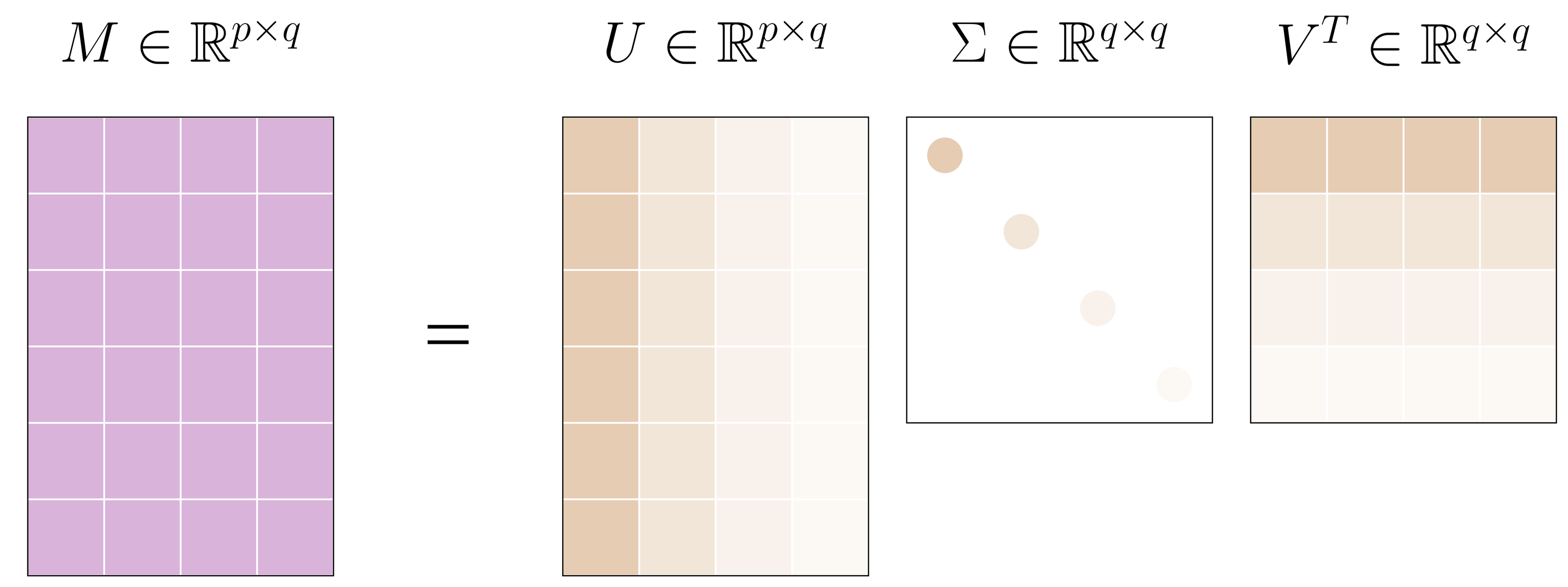
Our goal is to find a subspace F with reduced dimension such that $\mathcal{S}$ is well approximated, but time-evolution in F can be performed at a lower cost.



Let $F = Span\{\varphi_1, \dots, \varphi_R\} \subset E$ with $\varphi = \phi\Theta$, with $\Theta \in \mathbb{R}^N$. We are looking for the optimal Θ such that $\|\tilde{n} - \hat{n}\|_2$ is minimized.

Identification of a suitable subspace

Singular Value Decomposition (SVD) :



The truncated SVD up to rank R provides the optimal R dimensional approximation in a least square sense.

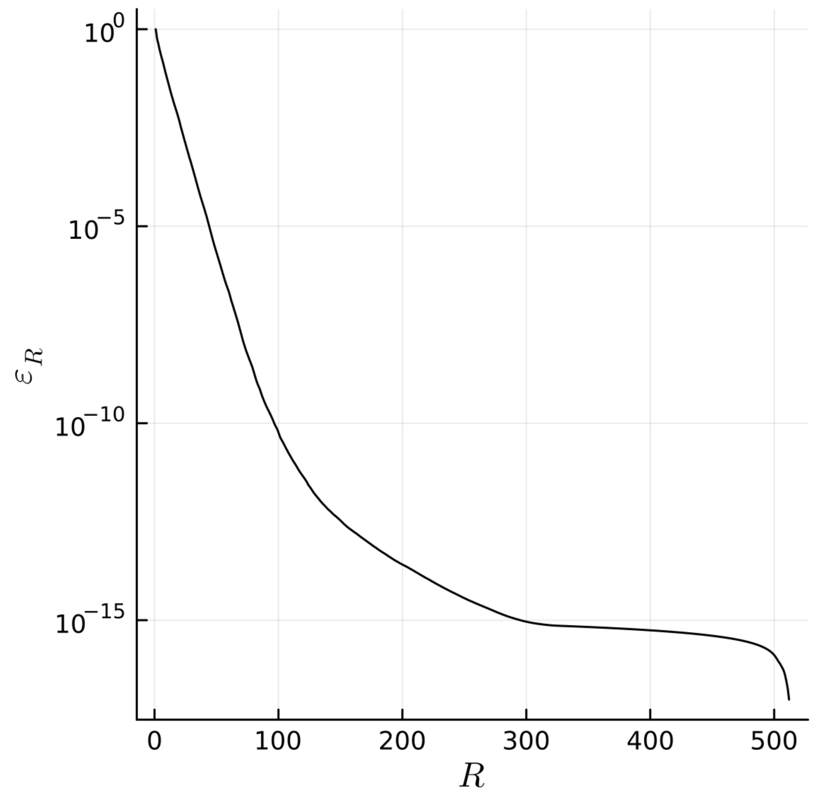


Figure 1. L^2 error associated with rank-R approximation of $\mathcal{S}$.

Reduction of the time-evolution operator

The time-evolution operator for the ROM can be precomputed *offline* such that the *online* cost scales only with R, independently of N.

Full order model $$\left[\frac{\partial \tilde{x}}{\partial t}\right]_i = \sum_{j,k=1}^{N} \tilde{\chi}_{ijk}\,\tilde{x}_j\tilde{x}_k \quad (3)$$

Reduced order model $$\left[\frac{\partial \hat{x}}{\partial t}\right]_i = \sum_{j,k=1}^{R} \hat{\chi}_{ijk}\,\hat{x}_j\hat{x}_k \quad (4)$$

with precomputed tensors

$$\tilde{\chi}_{ijk} = \sum_{i'=1}^{N}\left[g_\phi^{-1}\right]_{i,i'}\langle \phi_{i'}, \mathcal{B}[\phi_j, \phi_k]\rangle \qquad \tilde{\chi} \in \mathbb{R}^{N\times N\times N} \quad (5)$$

$$\hat{\chi}_{ijk} = \sum_{i'=1}^{R}\left[g_\varphi^{-1}\right]_{i,i'}\langle \varphi_{i'}, \mathcal{B}[\varphi_j, \varphi_k]\rangle \qquad \hat{\chi} \in \mathbb{R}^{R\times R\times R} \quad (6)$$

Mass-conservation

Mass conservation can be casted as an orthogonality condition :

$$M(t) = \int_0^\infty v\, n(v,t)\,\mathrm{d}v \quad (7)$$

$$\frac{dM}{dt} = \int_0^\infty v\,\frac{\partial n}{\partial t}(v,t)\,\mathrm{d}v = \left\langle v, \frac{\partial n}{\partial t}\right\rangle = 0 \quad (8)$$

A sufficient condition for mass conservation is that $v \mapsto v \in F$. Classical reduction does not lead to a mass conservative ROM. However, it can always be enforced from a non conservative one, at the cost of one extra degree of freedom.

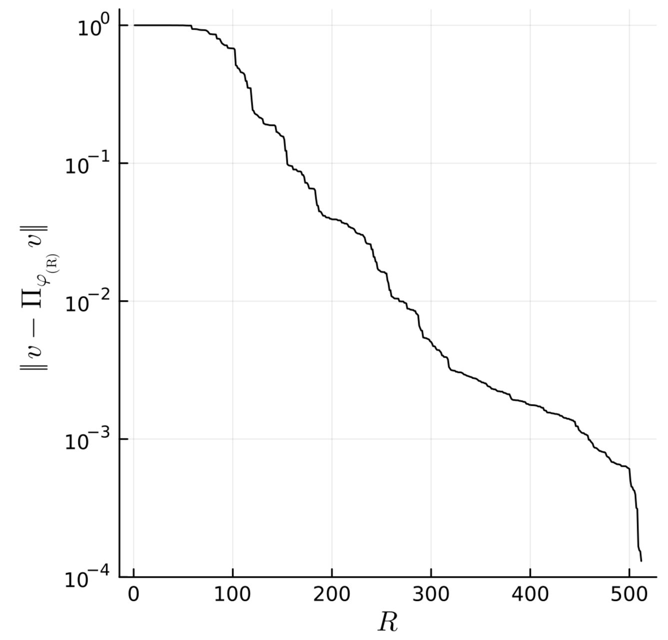


Figure 2. Projection error associated to mass imbalance

Certification through *a posteriori* error estimates

Quality of the ROM outputs can be certified by using *a posteriori* error estimates [HRS16]. The norm of the residual between the dynamics projected on E and F can be computed from the knowledge of $\hat{x}$ only, at a cost independent of N.

$$\hat{r}[\hat{n}](v) = \Pi_E\mathcal{B}[\hat{n},\hat{n}](v) - \Pi_F\mathcal{B}[\hat{n},\hat{n}](v) \quad (9)$$

$$R = \|\hat{r}\| = \left(\sum_{i,j,k,l=1}^{R} \Delta_{ijkl}\,\hat{x}_i\hat{x}_j\hat{x}_k\hat{x}_l\right)^{1/2} \quad (10)$$

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