Development of a Reduced-Order Model for Reacting Gas-Solids Flow Using Proper Orthogonal Decomposition

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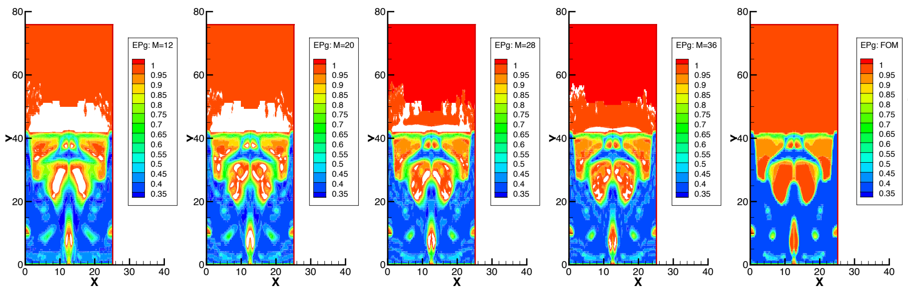
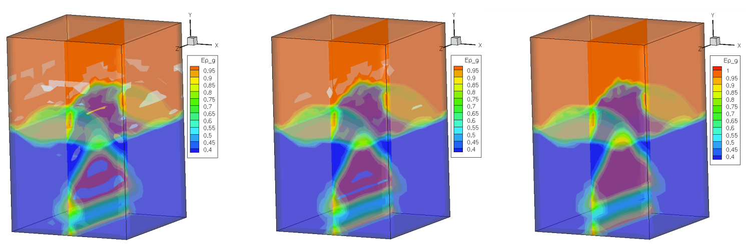
Nonphysical predictions of void fractions leads to solution divergence



(a) (b) (c) (d) (e)

Void fraction contours: ROM with (a) 12, (b) 20, (c) 28, (d) 36 POD modes, and (e) FOM



(a) (b) (c)

Void fraction contours: (a) ROM with 20 POD modes, (b) ROM with 40 POD modes, (c) FOM

Constrained POD

Linear Problem

First-order wave equation

$$u_t + cu_x = 0, \quad x \in [0,1], \quad c > 0$$

with initial condition $u(x,0) = f(x) \geq 0$.
Approximate $u(x,t)$ using POD method

$$u(x,t) \approx \sum_{i=1}^{m} a_i(t)\phi_i(x)$$

such that

$$\dot{a}_i\phi_i + ca_i\phi_i' = 0$$

Apply Galerkin projection

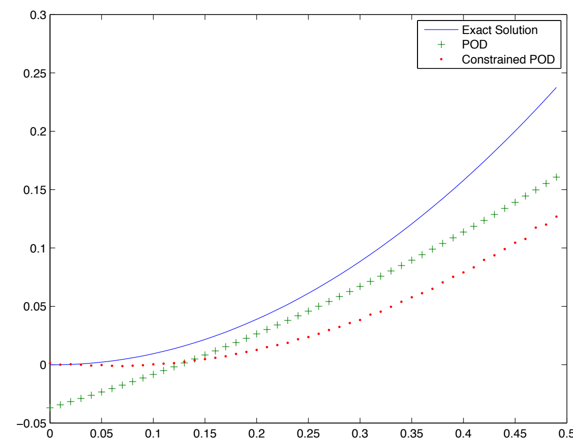
$$\int_0^1 \dot{a}_i\phi_i\phi_j dx + \int_0^1 ca_i\phi_i'\phi_j dx = 0$$

reduces due to orthogonality of POD basis functions to

$$\dot{a}_j + c\left(\int_0^1 \phi_i'\phi_j dx\right) a_i = 0$$

or in vectorial form

$$\underline{\dot{a}} + \boldsymbol{B}\underline{a} = \underline{0}$$



First-order wave equation: FOM, unconstrained and constrained ROM; m=4, N=100

where $\underline{a} \in \mathbb{R}^m, \boldsymbol{B} \in \mathbb{R}^{m\times m}$ and $\boldsymbol{B}_{ij} = c\left(\int_0^1 \phi_i'\phi_j dx\right)$.
Using an implicit time integration scheme

$$(\boldsymbol{I} + \Delta t\ \boldsymbol{B})\underline{a}^{n+1} - \underline{a}^n = \underline{0}, \quad \underline{a}^n := \underline{a}(t^n)$$

or

$$\boldsymbol{C}\underline{a}^{n+1} - \underline{a}^n = \underline{0}$$

Karush-Kuhn-Tucker Condition

Because of the initial condition, $u \geq 0$ always.
Using Karush-Kuhn-Tucker condition, the non-negativity requirement is

$$\underline{\lambda}^T\boldsymbol{\Phi}\underline{a}^{n+1} \geq 0$$

$\boldsymbol{\Phi} = [\underline{\phi}_1 \ldots \underline{\phi}_m]$, $\boldsymbol{\Phi} \in \mathbb{R}^{N\times m}$ - matrix of POD modes
N - number of spatial points
$\underline{\lambda}$ - vector of Lagrange multipliers, $\underline{\lambda} \in \mathbb{R}^N$.
Minimize the functional

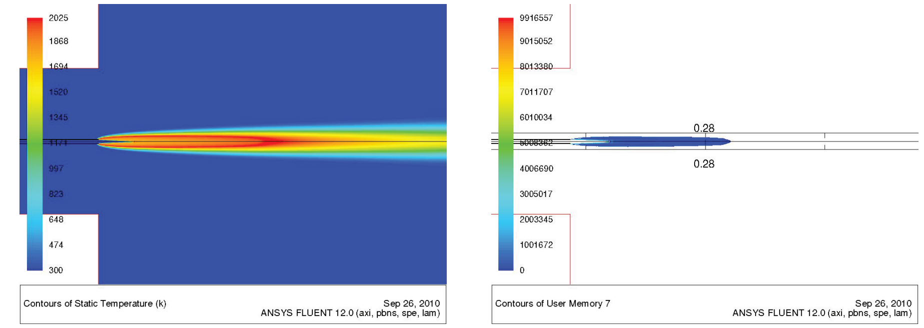
$$J = ||\boldsymbol{C}\underline{a}^{n+1} - \underline{a}^n||^2 + \underline{\lambda}^T\boldsymbol{\Phi}\underline{a}^{n+1}$$

which requires that

$$J_{\underline{a}^{n+1}} = 2\boldsymbol{C}\underline{a}^{n+1} - 2\underline{a}^n + \boldsymbol{\Phi}^T\underline{\lambda} = 0$$
$$J_{\underline{\lambda}} = \boldsymbol{\Phi}\underline{a}^{n+1} = 0$$

Obtain time coefficients and Lagrange multipliers from

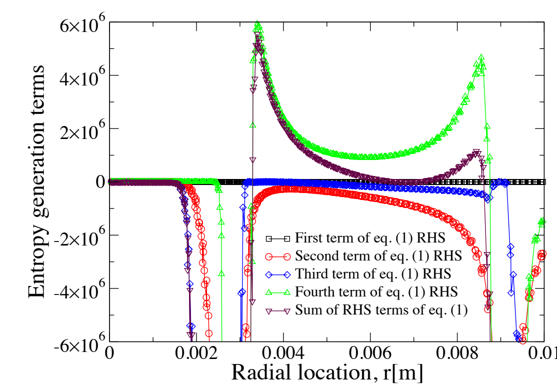
$$\begin{bmatrix} 2\boldsymbol{C} & \boldsymbol{\Phi}^T \\ \boldsymbol{\Phi} & \underline{0} \end{bmatrix} \left\{ \begin{matrix} \underline{a}^{n+1} \\ \underline{\lambda} \end{matrix} \right\} = \left\{ \begin{matrix} 2\underline{a}^n \\ \underline{0} \end{matrix} \right\}$$



(a) (b)

Sandia Flame A: (a) static temperature, (b) magnitude of entropy violation

$$-\mathrm{tr}[(\mathbf{T}+P\mathbf{I})\cdot\mathbf{D}]+\frac{1}{T}\boldsymbol{\epsilon}\cdot\nabla T + cRT\sum_{B=1}^{N}\mathbf{j}_{(B)}\cdot\frac{\mathbf{d}_{(B)}}{\rho_{(B)}}+\sum_{j=1}^{K}\sum_{B=1}^{N}\mu_{(B)}r_{(B,j)}\le 0$$



Terms of Differential Entropy Inequality

Assume $f(x) = x^2$ and introduce 0wo errors in the model:

1. $f(x) = x^2$ replaced by $x^2 - 10^{-4}$;
2. POD basis functions perturbed by 10^{-4}.

Nonlinear Problem

Burgers equation

$$u_t + uu_x = 0, \quad x \in [0,1]$$

Using the POD approximation and Galerkin projection yields

$$\dot{a}_k + a_ia_jG_{ijk} = 0, \quad i,j,k = 1,m \tag{1}$$

where $G_{ijk} = \int_0^1 \phi_j\phi_i'\phi_k dx$. For two POD modes, that is, m=2, the discretized form of (1) becomes:

$$\begin{bmatrix} 1 + a_i^nG_{i11}\Delta t & a_i^nG_{i21}\Delta t \\ a_i^nG_{i12}\Delta t & 1 + a_i^nG_{i22}\Delta t \end{bmatrix} \left\{ \begin{matrix} a_1^{n+1} \\ a_2^{n+1} \end{matrix} \right\} = \left\{ \begin{matrix} a_1^n \\ a_2^n \end{matrix} \right\}$$

$$\mathcal{C}_{n\ell}\,\underline{a}^{n+1} - \underline{a}^n = \underline{0}$$

$$\mathcal{C}_{n\ell} = \begin{bmatrix} 1 + a_i^nG_{i11}\Delta t & a_i^nG_{i21}\Delta t \\ a_i^nG_{i12}\Delta t & 1 + a_i^nG_{i22}\Delta t \end{bmatrix}$$

Constrain time coefficients of gas void fraction such that the POD reconstructed gas void fraction, $\epsilon \in [0.38, 1]$.