

Spectrally-consistent regularization modeling of turbulent natural convection flows

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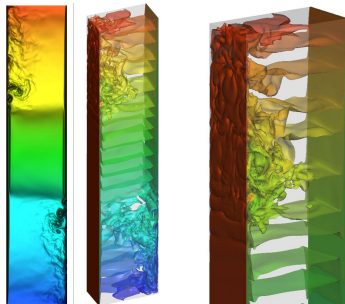
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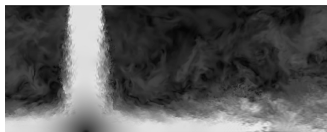
DNS of turbulent incompressible flows

Main features of the DNS code:

- Structured staggered grids
- High-order symmetry-preserving schemes
- Fully-explicit second-order time-integration method
- Poisson solver for 2.5D problems: FFT + PCG
- Hybrid MPI+OpenMP parallelization
- OpenCL-based extension for its use on GPGPU

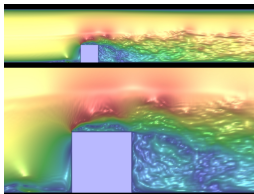


Air-filled DHC of aspect ratio 5 at $Ra = 4.5 \times 10^{10}$ (36M grid points)

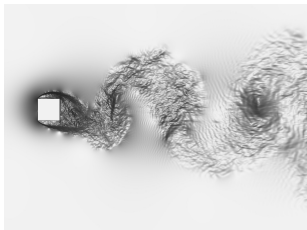


Plane impingement jet at $Re = 20000$ (102M grid points)

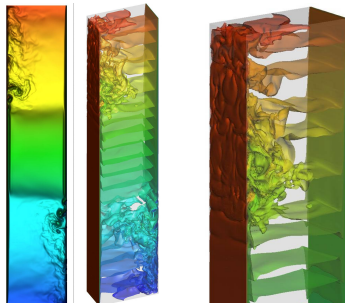
DNS of turbulent incompressible flows



Wall-mounted cube at $Re = 7240$ (17M grid points)



Square cylinder at $Re = 22000$ (75M grid points)

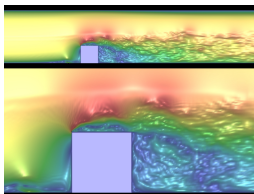


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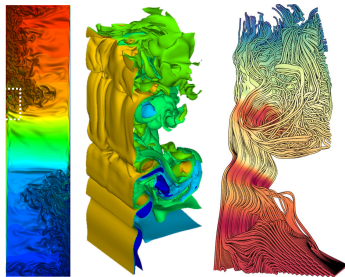


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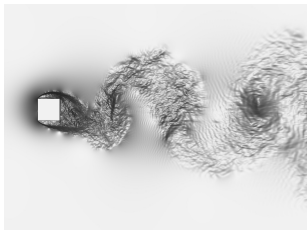
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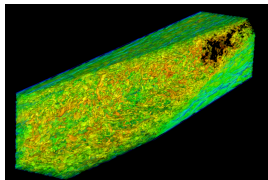
Wall-mounted cube at $Re = 7240$ (17M grid points)



Air-filled DHC of aspect ratio 4 at $Ra = 10^{11}$ (111M grid points)

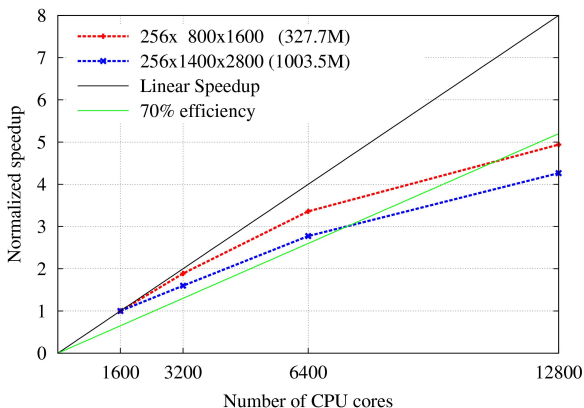


Square cylinder at $Re = 22000$ (75M grid points)



Square duct at $Re_\tau = 1200$ (172M grid points)

Scaling? Yes¹, we can... but never enough



¹A. Gorobets et al. "Hybrid MPI+OpenMP parallelization of an FFT-based 3D Poisson solver with one periodic direction" **Computers&Fluids**, 49:101-109, 2011

Governing equations

Incompressible Navier-Stokes equations:

$$\begin{aligned}\nabla \cdot \mathbf{u} &= 0 \\ \partial_t \mathbf{u} + \mathcal{C}(\mathbf{u}, \mathbf{u}) &= \mathcal{D}\mathbf{u} - \nabla p\end{aligned}$$

where the **nonlinear convective** term is given by

$$\mathcal{C}(\mathbf{u}, \phi) = (\mathbf{u} \cdot \nabla)\phi$$

and the **linear dissipative** term is given by

$$\mathcal{D}\phi = \nu \Delta \phi$$

Stopping the vortex-stretching²

Taking the curl of momentum equation the **vorticity transport equation** follows

$$\partial_t \omega + \mathcal{C}(u, \omega) = \mathcal{C}(\omega, u) + \mathcal{D}(\omega)$$

²F.X. Trias *et al.* **Computers&Fluids**, 39:1815-1831, 2010

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Let us now consider an arbitrary part of the flow domain, Ω , with **periodic boundary conditions**. Then, taking the L^2 innerproduct with $\omega = \nabla \times u$ leads to the **enstrophy equation**

$$\frac{1}{2} \frac{d}{dt} (\omega, \omega) = (\omega, \mathcal{C}(\omega, u)) - \nu (\nabla \omega, \nabla \omega)$$

where $(a, b) = \int_{\Omega} a \cdot b d\Omega$.

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where $(a, b) = \int_{\Omega} a \cdot b d\Omega$. Unless, the grid is fine enough convection dominates diffusion

$$(\omega, \mathcal{C}(\omega, u)) > \nu (\nabla \omega, \nabla \omega)$$

²F.X. Trias *et al.* **Computers&Fluids**, 39:1815-1831, 2010

Stopping the vortex-stretching

The **vortex-stretching** term can be expressed in terms of the invariant $R = -1/3\text{tr}(S^3) = -\det(S)$

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Then, recalling that $\nabla \times \omega = \nabla(\nabla \cdot u) - \Delta u$ and the **boundary contribution vanishes***, the **diffusive term** is given by the $L^2(\Omega)$ -norm of Δu

$$\begin{aligned} (\nabla \omega, \nabla \omega) &\stackrel{*}{=} -(\omega, \Delta \omega) = (\omega, \nabla \times \nabla \times \omega) \\ &\stackrel{*}{=} (\nabla \times \omega, \nabla \times \omega) = (\Delta u, \Delta u) = \|\Delta u\|^2 \end{aligned}$$

Stopping the vortex-stretching

The **overall damping** introduced by a model should be given by

$$H^\Omega = \min \left\{ \frac{\nu \|\Delta u\|^2}{4|\tilde{R}|}, 1 \right\}$$

where $\tilde{R} = \int_{\Omega} R d\Omega$.

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- Laminar flows ($R \rightarrow 0$)
- 2D flows ($\lambda_2 = 0 \rightarrow R = 0$)
- In the wall (near-wall behavior is given by $R \propto y^1$ and $\|\Delta u\|^2 \propto y^0$)

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³Roel Verstappen, **Journal of Scientific Computing**, 49:94-110, 2011

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One possible solution would consist on an **eddy-viscosity** type LES model:

$$\nu_e \approx \frac{4|\tilde{R}|}{\|\Delta u\|^2}$$

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Taking $\|\Delta u\|^2 \leq -\lambda_\Delta(\omega, \omega) = 4\lambda_\Delta \tilde{Q}$, it becomes the eddy-viscosity model³ based on the invariants $R = -1/3\text{tr}(S^3) = -\det(S)$ and $Q = -1/2\text{tr}(S^2)$.

$\lambda_\Delta < 0$ is the largest (smallest in absolute value) non-zero eigenvalue of Laplacian operator Δ on Ω . In a periodic box of size h , $\lambda_\Delta = -(\pi/h)^2$.

³Roel Verstappen, **Journal of Scientific Computing**, 49:94-110, 2011

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Alternatively, **regularizations** of the non-linear convective term results into a damping of vortex-stretching term, *i.e.* $f^{reg} |\tilde{R}|$ (where $0 < f \leq 1$)

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Or a combination of both?

Symmetry-preserving regularization modeling

We consider smooth approximations (regularizations) of the nonlinearity,

$$\partial_t u_\epsilon + \tilde{\mathcal{C}}(u_\epsilon, u_\epsilon) = \mathcal{D}(u_\epsilon) - \nabla p_\epsilon$$

that conserve the following inviscid invariants

- Kinetic energy : (u, u)
- Enstrophy (in 2D) : (ω, ω)
- Helicity (in 3D) : (ω, u)

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The **approximate convective operator** must **preserve** the basic **symmetry** properties:

$$\begin{aligned}(\mathcal{C}(u, v), w) &= -(\mathcal{C}(u, w), v) \\(\mathcal{C}(u, v), \Delta v) &= (\mathcal{C}(u, \Delta v), v) \quad \text{in 2D}\end{aligned}$$

Symmetry-preserving regularization models

Following these principles a family of \mathcal{C}_4^γ regularizations can be derived³. Here we consider the \mathcal{C}_4 approximation⁴,

$$\partial_t u_\epsilon + \mathcal{C}_4(u_\epsilon, u_\epsilon) = \mathcal{D}(u_\epsilon) - \nabla p_\epsilon$$

where the convective term is smoothed according to:

$$\mathcal{C}_4(u, v) = \mathcal{C}(\bar{u}, \bar{v}) + \overline{\mathcal{C}(\bar{u}, v')} + \overline{\mathcal{C}(u', \bar{v})}$$

where $u' = u - \bar{u}$ and $\mathcal{C}_4(u, v) = \mathcal{C}(u, v) + \mathcal{O}(\epsilon^4)$ for **any symmetric filter**.

High-frequencies need to be effectively damped.

But how much?

³F.X. Trias *et al.* **Journal of Physics: Conference Series**, 318: art.042060, 2011

⁴Roel Verstappen, **Computers & Fluids**, 37 (7): 887-897, 2008

Symmetry-preserving regularization models

Answer: Again the balance between **vortex-stretching** contribution and **physical dissipation** provides a proper value for the damping

$$f_4(\hat{g}_k(\epsilon)) \approx \min \left\{ \frac{\nu \|\Delta u\|^2}{4|\tilde{R}|}, 1 \right\}$$

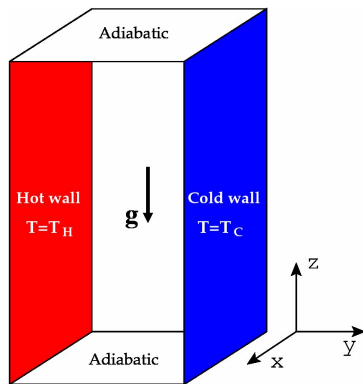
where

$$(\omega, \mathcal{C}_4(\omega, u)) \approx f_4(\hat{g}_k(\epsilon))(\omega, \mathcal{C}(\omega, u))$$

Test-case: Differentially Heated Cavity

Boundary conditions:

- **Isothermal vertical walls**
- **Adiabatic horizontal walls**
- **Periodic** boundary conditions in the spanwise direction



Dimensionless governing numbers:

- $Ra = \beta \Delta T L_z^3 g / (\alpha \nu)$
- $Pr = \nu / \alpha$
- Height aspect ratio $A_z = L_z / L_y$
- Depth aspect ratio $A_x = L_x / L_y$

DNS^{5,6} results for $Ra = 10^{11}$, $Pr = 0.71$

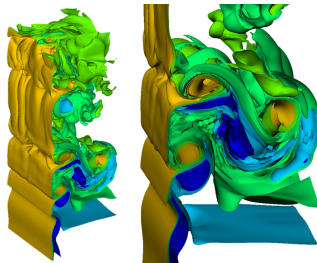


Some details about **DNS**:

- Mesh size: $128 \times 682 \times 1278$
- ≈ 3 months - 256 CPUs
- 4th-order symmetry-preserving scheme
- $A_z = 4$

Complexity of the flow:

- Boundary layers
- Stratified cavity core
- Internal waves
- Recirculation areas



⁵F. X. Trias *et al.* Int. Journal of Heat and Mass Transfer, 53:665-673, 2010

⁶F. X. Trias *et al.* Int. Journal of Heat and Mass Transfer, 53:674-683, 2010

Results for differentially heated cavity at $Ra = 10^{11}$

- Regularization model \mathcal{C}_4 is tested.
- Two coarse meshes are considered

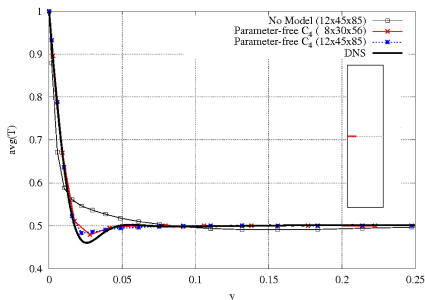
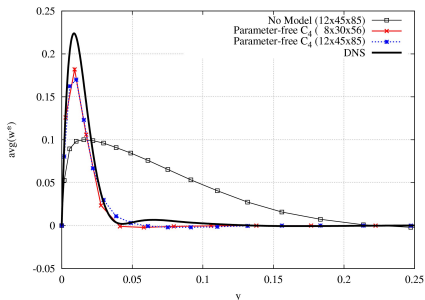
	DNS	RM1	RM2
N_x	128	12	8
N_y	682	45	30
N_z	1278	85	56

- The **discrete linear filter**⁷ is based on polynomial functions of the discrete diffusive operator, \mathbf{D}

⁷F.X. Trias and R.W.C.P. Verstappen, **Computers & Fluids**, 40:139-148, 2011

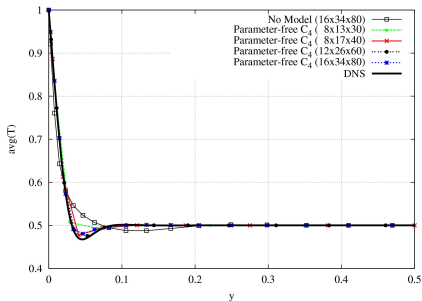
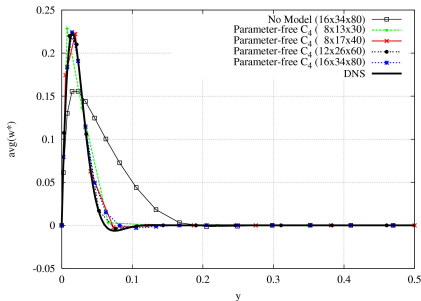
Results for differentially heated cavity at $Ra = 10^{11}$

Profiles



Averaged vertical velocity and temperature profiles at the horizontal mid-height plane.

How does the parameter-free \tilde{C}_4 regularization modeling behave for other grids and Ra -numbers?

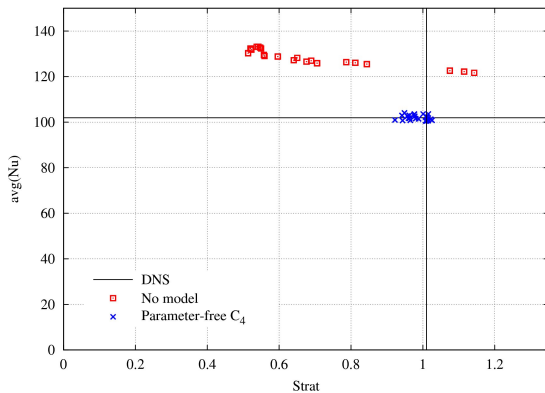


Averaged vertical velocity and temperature profiles at the horizontal mid-height plane at $Ra = 10^{10}$.

Even for a **very coarse** $8 \times 13 \times 30$ grid **reasonable results** are obtained!

⇒ Results for different grids show the **robustness** of the method.

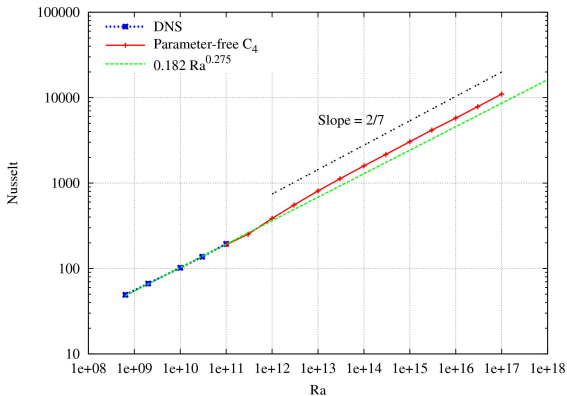
Challenging C_4 : mesh independence analysis



The overall Nusselt number and the centerline stratification for 50 randomly generated coarse grids with fixed stretching at $Ra = 10^{10}$.

$$8 \leq N_x \leq 16, 17 \leq N_y \leq 34, \text{ and } 40 \leq N_z \leq 80.$$

Performance at very high Rayleigh numbers



Meshes have been generated with the criteria of keeping the same number of points in the BL than for $Ra = 10^{10}$.

Towards a simple LES model

On the other hand, a **new eddy-viscosity** type model

$$\partial_t \bar{u} + \mathcal{C}(\bar{u}, \bar{u}) = \mathcal{D}\bar{u} - \nabla \bar{p} - \nabla \cdot \tau(\bar{u}) ; \quad \nabla \cdot \bar{u} = 0$$

$$\tau(\bar{u}) = -2\nu_t S(\bar{u})$$

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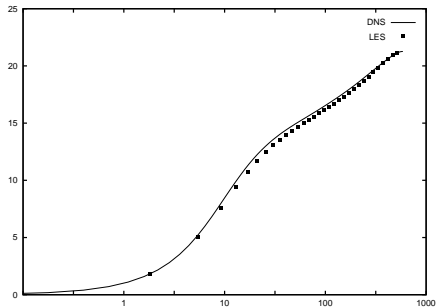
has also been derived following the same principles

$$\nu_t = \max \left\{ \frac{4|\tilde{R}| - \nu \|\Delta \bar{u}\|^2}{\|\Delta \bar{u}\|^2}, 0 \right\}$$

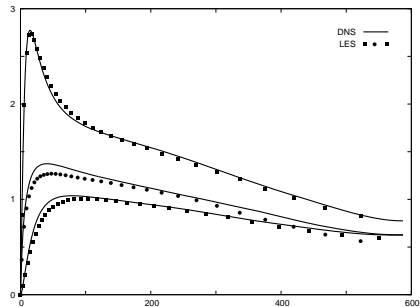
Turbulent channel flow

 $Re_\tau = 590$

DNS Moser et al.

LES 64^3 

mean velocity



rms fluctuations

Conclusions

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Conclusions and Future Research

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- Test the performance of new eddy-viscosity type LES for other configurations.

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- Based on this, **a new eddy-viscosity type** LES models has been derived.

- Test the performance of new eddy-viscosity type LES for other configurations.
- Try to properly combine **regularization modeling** and **LES**.

Thank you for you attention

Further reading about C_4 regularization

- Roel Verstappen, “*On restraining the production of small scales of motion in a turbulent channel flow*”, *Computers & Fluids*, 37 (7): 887-897, 2008
- F. X. Trias *et al.*, “*Parameter-free symmetry-preserving regularization modeling of a turbulent differentially heated cavity*”, *Computers & Fluids*, 39:1815-1831, 2010.
- F. X. Trias and R.W.C.P. Verstappen, “*On the construction of discrete filters for symmetry-preserving regularization models*”, *Computers & Fluids*, 40:139-148, 2011.
- F. X. Trias *et al.*, “*Numerical simulation of turbulence at lower cost: Regularization modeling*”, *Computers & Fluids*, (published online).

Symmetry-preserving regularization models

Regularizations of the non-linear convective term can be constructed

$$\tilde{C}(u, v) = \sum_{i,j,k=0}^1 a_{ijk} \tilde{C}_{ijk}(u, v)$$

where $\tilde{C}_{ijk}(u, v) = \varphi_k(C(\varphi_i(u), \varphi_j(v)))$ and $\varphi_i(u) = \begin{cases} u, & \text{if } i = 0 \\ \bar{u}, & \text{if } i = 1 \end{cases}$

$\bar{(\cdot)}$ is a **self-adjoint** filter that **commutes** with differential operators.

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$\bar{(\cdot)}$ is a **self-adjoint** filter that **commutes** with differential operators.

Among all possible combinations we find the regularization proposed by Leray, $\mathcal{C}(\bar{u}, u) : a_{100} = 1$ (with the rest of $a_{ijk} = 0$)

\implies Eight coefficients a_{ijk} need to be determined.

Symmetry-preserving regularization models

$$\tilde{\mathcal{C}}(u, v) = \sum_{i,j,k=0}^1 a_{ijk} \tilde{\mathcal{C}}_{ijk}(u, v)$$

$$\sum_{i,j,k=0}^1 a_{ijk} = 1 \quad \longrightarrow \quad \tilde{\mathcal{C}}(u, v) = \mathcal{C}(u, v) + \mathcal{O}(\epsilon^n) \quad \text{with } n \geq 2$$

$$\left(\tilde{\mathcal{C}}(u, v), w \right) = - \left(\tilde{\mathcal{C}}(u, w), v \right) \quad \longrightarrow \quad a_{ijk} = a_{ikj}$$

$$\left(\tilde{\mathcal{C}}(u, v), \Delta v \right) = \left(\tilde{\mathcal{C}}(u, \Delta v), v \right) \quad \text{in 2D} \quad \longrightarrow \quad a_{ijk} = a_{kji}$$

⁸Roel Verstappen, **Computers & Fluids**, 37 (7): 887-897, 2008

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$$\sum_{i,j,k=0}^1 a_{ijk} = 1 \quad \longrightarrow \quad \tilde{\mathcal{C}}(u, v) = \mathcal{C}(u, v) + \mathcal{O}(\epsilon^n) \quad \text{with } n \geq 2$$

$$\left(\tilde{\mathcal{C}}(u, v), w \right) = - \left(\tilde{\mathcal{C}}(u, w), v \right) \quad \longrightarrow \quad a_{ijk} = a_{ikj}$$

$$\left(\tilde{\mathcal{C}}(u, v), \Delta v \right) = \left(\tilde{\mathcal{C}}(u, \Delta v), v \right) \quad \text{in 2D} \quad \longrightarrow \quad a_{ijk} = a_{kji}$$

This leads to a family of $\mathcal{O}(\epsilon^2)$ -accurate regularizations. Among them⁸,

$$\mathcal{C}_2(u, v) = \tilde{\mathcal{C}}_{111}(u, v) = \overline{\mathcal{C}(\bar{u}, \bar{v})}$$

⁸Roel Verstappen, **Computers & Fluids**, 37 (7): 887-897, 2008

Symmetry-preserving regularization models

To cancel second-order terms, three additional conditions need to be imposed:

$$\sum_{j,k=0}^1 a_{1jk} = 0 \quad \sum_{i,k=0}^1 a_{i1k} = 0 \quad \sum_{i,j=0}^1 a_{ij1} = 0$$

$$\mathcal{C}_4^\gamma(u, v) = \frac{1}{2} ((\mathcal{C}_4 + \mathcal{C}_6) + \gamma(\mathcal{C}_4 - \mathcal{C}_6))(u, v)$$

where \mathcal{C}_4 and \mathcal{C}_6 read

$$\mathcal{C}_4(u, v) = \mathcal{C}(\bar{u}, \bar{v}) + \overline{\mathcal{C}(\bar{u}, v')} + \overline{\mathcal{C}(u', \bar{v})}$$

$$\mathcal{C}_6(u, v) = \mathcal{C}(\bar{u}, \bar{v}) + \mathcal{C}(\bar{u}, v') + \mathcal{C}(u', \bar{v}) + \overline{\mathcal{C}(u', v')}$$