



Supplement of

High-performance geodynamics on GPUs using the PETSc CUDA backend (GAUZZ v1.0.0)

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Supplement

Contents of this file

- Figures S1 to S5
- Tables S1 to S5

Introduction

This document provides supplementary information to accompany the main manuscript. The figures present the velocity and pressure fields of the velocity subproblem and the SolCx benchmark, the root-mean-square velocity evolution of the 3D thermo-mechanical convection benchmark, the temporal evolution of the 3D Rayleigh–Taylor instability, and the wall times of the 3D Rayleigh–Taylor, sticky-air, and subduction benchmarks under four processor configurations. The tables list the memory bandwidth measured on the CPU and GPU hardware, the pre-assembly memory across 3D mesh resolutions, the dimensional parameters of the sticky-air and subduction models, and the wall times of the 3D thermo-mechanical convection benchmark.

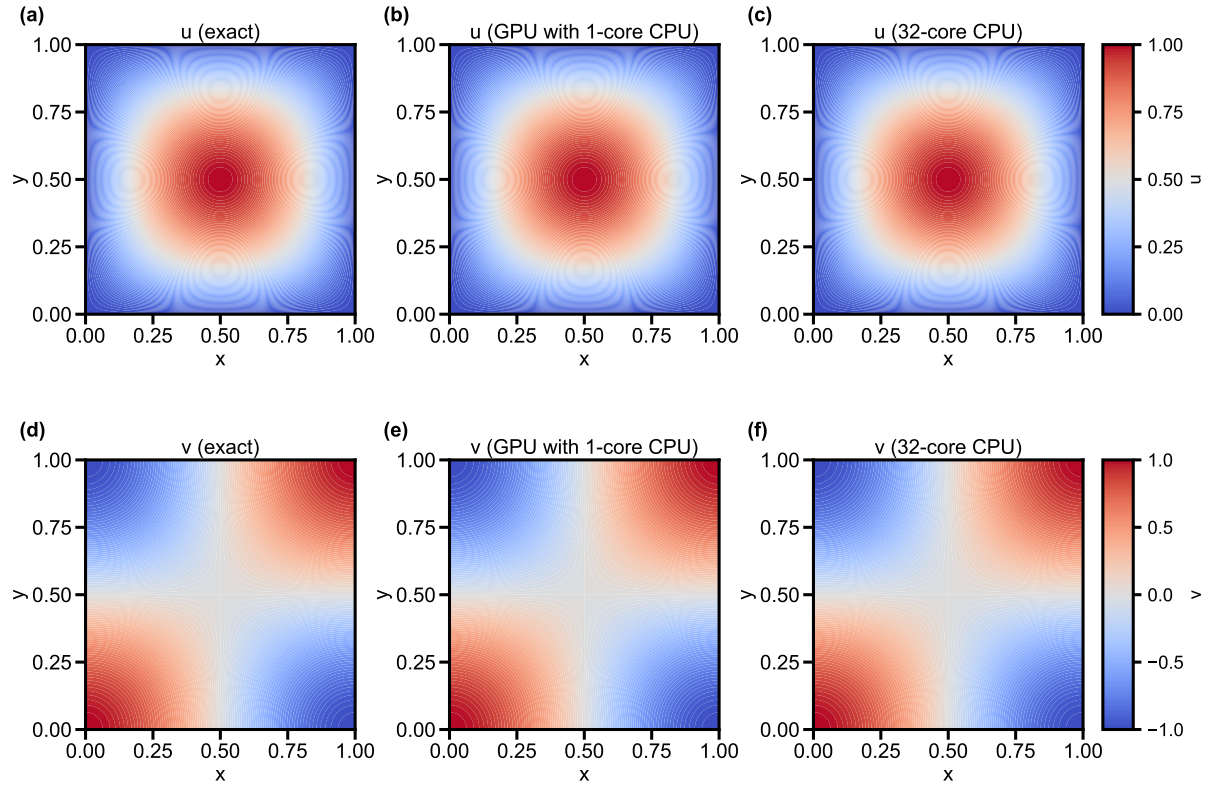


Figure S1: Velocity fields in the x - and y -directions from the velocity subproblem: exact solution (a and d), GPU (b and e), and CPU (c and f).

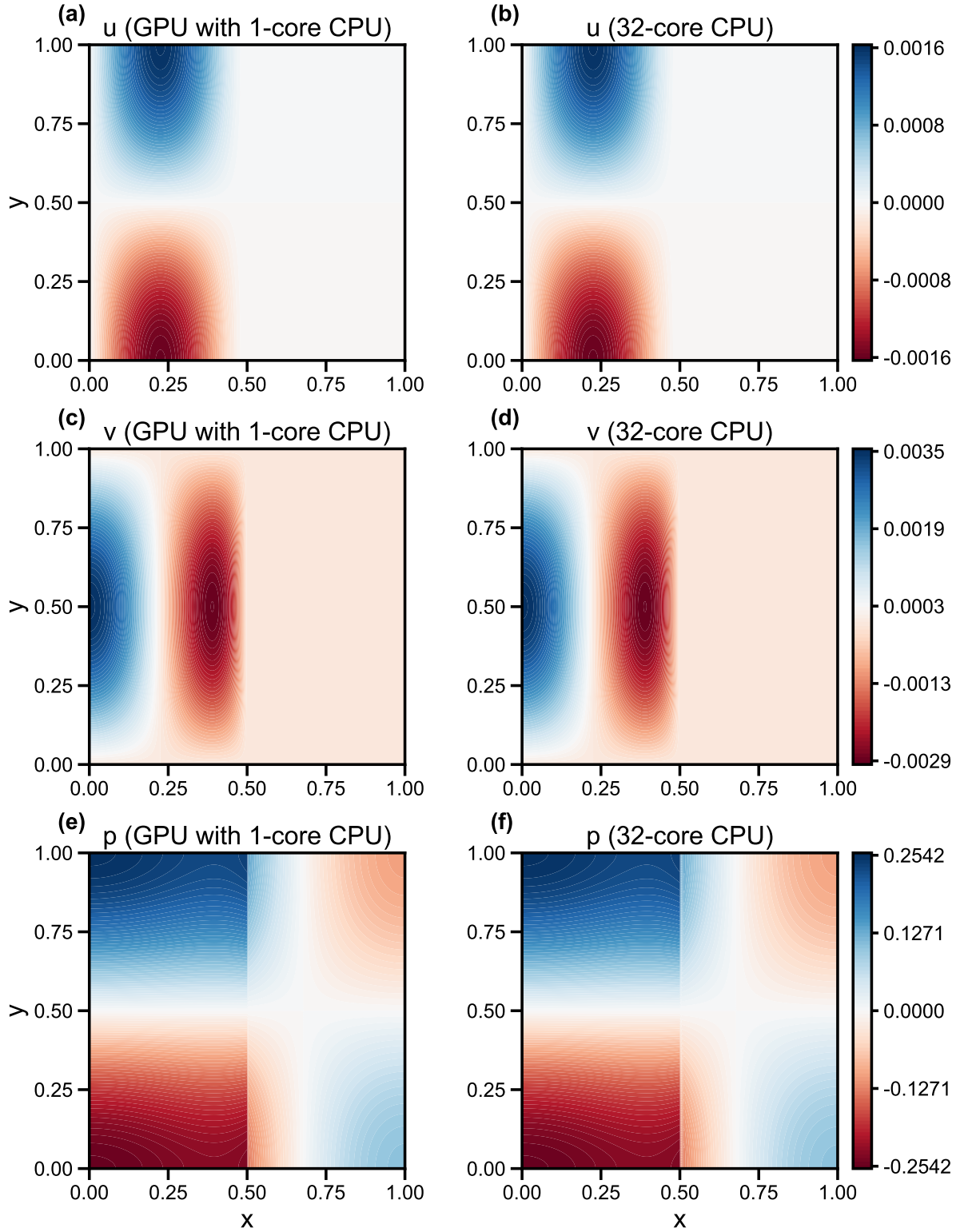


Figure S2: SolCx benchmark x - and y -velocity and pressure computed on the GPU (a, c, and e) and CPU (b, d, and f).

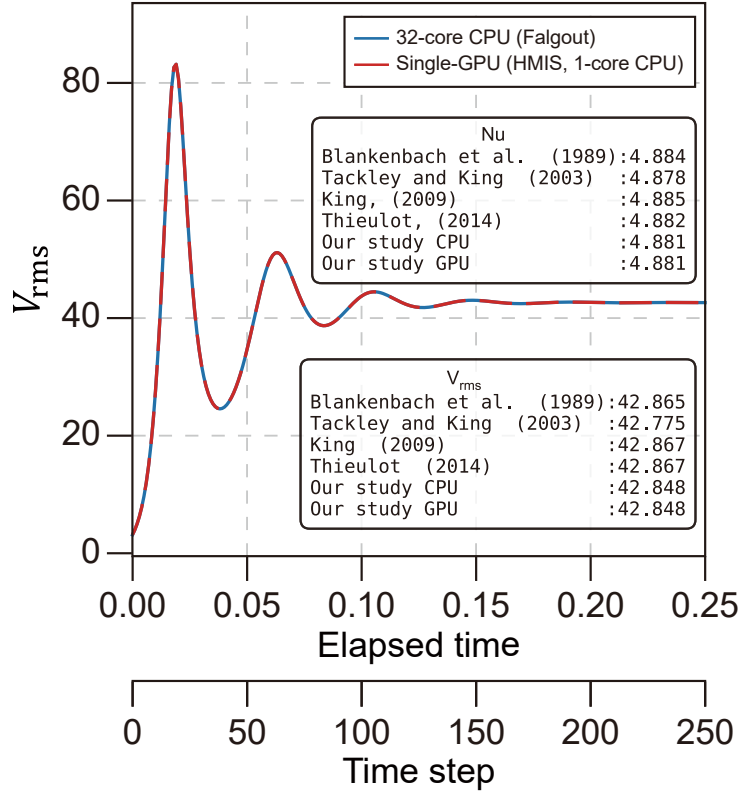


Figure S3: Time evolution of the global root-mean-square velocity (V_{rms}) for the 3D thermo-mechanical convection benchmark of Blankenbach et al. (1989) on the single-GPU (HMIS) with 1-core CPU and on the 32-core CPU (Falgout) environments. Reference values of V_{rms} and the Nusselt number (Nu) reported by Blankenbach et al. (1989), Tackley and King (2003), King (2009), and Thieulot (2014) are included for comparison.

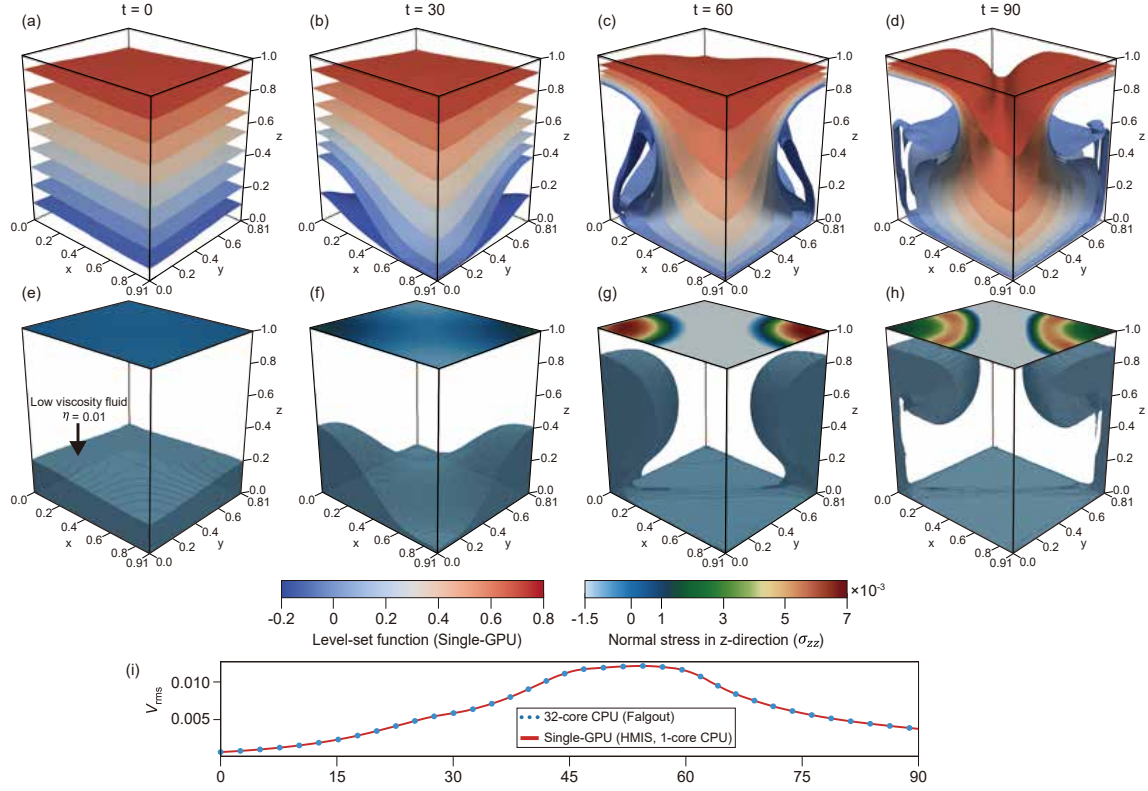


Figure S4: Temporal evolution of the 3D Rayleigh–Taylor instability derived from the GPU (HMIS) with 1-core CPU. (a–d) Snapshots of level-set function isosurfaces at nondimensional times $t = 0, 30, 60,$ and 90 . (e–h) Evolution of the interface between two compositions and the distribution of normal stress in the z -direction on the top surface. (i) Root-mean-square velocity (V_{rms}) measured in the GPU and 32-core CPU environments.

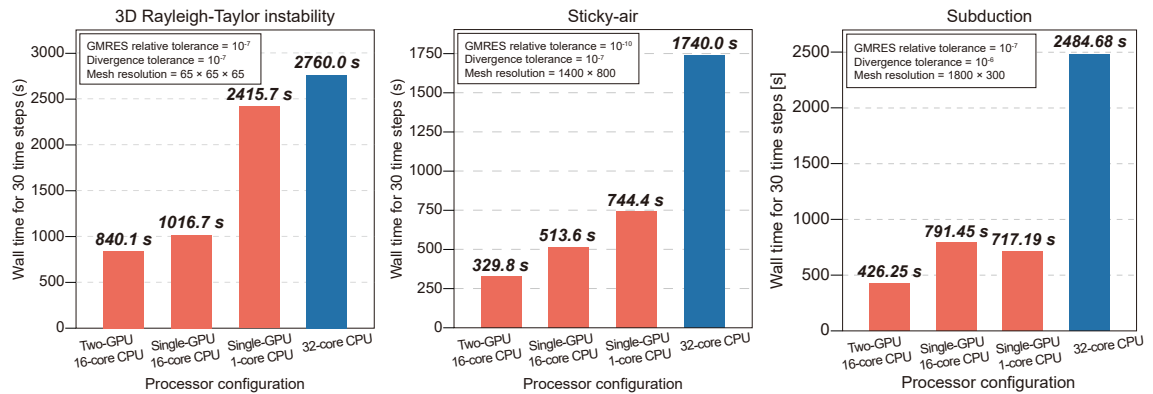


Figure S5: Wall time for 30 time steps under four processor configurations: two-GPU with 16-core CPU, single-GPU with 16-core CPU, single-GPU with 1-core CPU, and 32-core CPU (CPU-only).

Table S1: Memory bandwidth measured using vector operations on the CPU and GPU. Percentages in parentheses indicate the fraction of the theoretical peak memory bandwidth.

Operation		32-core CPU [GB s ⁻¹]	GPU [GB s ⁻¹]	GPU/CPU ratio
Copy	$c = a$	115.4 (75%)	800.9 (83%)	6.9
Scale	$b = s \cdot c$	104.1 (68%)	800.3 (83%)	7.7
Add	$c = a + b$	109.1 (71%)	822.2 (86%)	7.5
Update	$a = a + s \cdot b$	113.2 (74%)	824.0 (86%)	7.3

Table S2: Comparison of DOFs and pre-assembly memory requirements for different mesh resolutions.

Mesh resolution	DOFs	Memory for pre-assembly (MB)
$100 \times 15 \times 100$	3,352,864	510.0
$100 \times 20 \times 100$	4,456,884	680.0
$100 \times 25 \times 100$	5,560,904	850.0
$100 \times 30 \times 100$	6,664,924	1014.0
$100 \times 35 \times 100$	7,768,944	1176.0
$100 \times 40 \times 100$	8,872,964	1336.0

Table S3: Parameters used to nondimensionalize the sticky-air benchmark.

Descriptions	Symbols	Values
Reference viscosity	η_0	$10^{18} \text{ Pa} \cdot \text{s}$
Reference density	ρ_0	$0 \text{ kg} \cdot \text{m}^{-3}$
Characteristic length	D	800 km
Thermal diffusivity	κ	$10^{-6} \text{ m}^2 \cdot \text{s}^{-1}$
Gravitational acceleration	g	$10 \text{ m} \cdot \text{s}^{-2}$

Table S4: Parameters used to nondimensionalize the subduction model.

Descriptions	Symbols	Values
Reference viscosity	η_0	$3.5 \times 10^{23} \text{ Pa} \cdot \text{s}$
Reference density	ρ_0	$3230 \text{ kg} \cdot \text{m}^{-3}$
Characteristic length	D	600 km
Thermal diffusivity	κ	$10^{-6} \text{ m}^2 \cdot \text{s}^{-1}$
Gravitational acceleration	g	$10 \text{ m} \cdot \text{s}^{-2}$

Table S5: Comparison of computational wall times for 3D thermo-mechanical convection simulations across different hardware configurations (GPU, CPU) and ASPECT.

3D thermo-mechanical convection	GPU (two-GPU, 16-core)	GPU (single-GPU, 16-core)	CPU (32-core)	ASPECT (32-core)
Total wall time	195.360 s	319.069 s	1013.739 s	1123.000 s
Initialization / mesh	0.573 s	0.607 s	0.770 s	1.440 s
Setup DoF systems	0.212 s	0.214 s	0.200 s	0.138 s
Setup initial conditions	0.373 s	0.401 s	0.080 s	0.116 s
Setup matrices/KSP	0.019 s	0.013 s	0.041 s	1.060 s
Assemble/update Stokes system	3.356 s	3.401 s	5.083 s	269.000 s
Build Stokes preconditioner	1.439 s	2.618 s	0.082 s	1.850 s
Solve Stokes system	126.620 s	247.352 s	961.005 s	471.000 s
Assemble temperature system	49.941 s	48.552 s	42.726 s	312.000 s
Build temperature preconditioner	0.553 s	0.596 s	0.277 s	6.990 s
Solve temperature system	6.138 s	7.639 s	1.046 s	3.260 s

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