An HPC Framework for Bayesian Uncertainty Quantification of Flows Across Scales

Ursula Rasthofer

with: Petros Koumoutsakos, Diego Rossinelli, Lina Kulakova, Dmitry Alexeev, Sergey Litvinov, Panagiotis Angelikopoulos, Panagiotis Hadjidoukas, Costas Papadimitriou, Jonas Sukys
HPC in Science and Engineering

- computationally expensive models (e.g., fluid flow, molecular dynamics, ...)

- uncertainties in numerical model and predictions
  - models based on parameters: how to choose? do we trust them?
  - sources of randomness in problem statement: how reliable are predictions?

- large number of model evaluations for Uncertainty Quantification (UQ)
Outline

• Bayesian UQ for Blood Flow
• MLMC-UQ for Compressible Multicomponent Flow
• Conclusions
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CANCER

8M deaths/year

90% due to metastasis
Separation of Circulating Tumor Cells
Dissipative Particle Dynamics

- stochastic, mesoscale approach to simulate soft matter
- consistent coarse-graining of molecular dynamics
- forces: N-body interactions + stochastic

\[
\mathbf{F}_i = \sum_{n=1,n \neq i}^{N} \mathbf{F}_{i,n}^{C,DPD} + \mathbf{F}_{i,n}^{D,DPD} + \mathbf{F}_{i,n}^{R,DPD} \\
+ \sum_{k=1,k \neq i}^{K} \mathbf{F}_{i,k}^{C,FSI} + \mathbf{F}_{i,k}^{D,FSI} + \mathbf{F}_{i,k}^{R,FSI} \\
+ \sum_{m=1,m \neq i}^{M} \mathbf{F}_{i,m}^{C,wall} + \mathbf{F}_{i,m}^{D,wall} + \mathbf{F}_{i,m}^{R,wall}
\]

Red Blood Cell Model

\[ F_{\text{cell}} = \sum_{n=1}^{N} F_{\text{dihedral,1}}^{0,n-1,n,n+1} + F_{\text{dihedral,2}}^{0,n,N+n,n+1} + F_{\text{triangle}}^{0,n,n+1} + F_{\text{bond}}^{0,n} \]

\[ F_{\text{bond}}^{0,n} = -\frac{k_B T}{p} \left( \frac{1}{4(1-x_n)^2} - \frac{1}{4} + x_n \right) + \frac{k_p}{x_0 l_0} + 2\sqrt{k_B T \gamma} \frac{T}{dW_{ij}^S} \]

\[ x_n = \frac{b_n}{l_0/x_0} \]

[spring-like force]

[disssipative force]

\[ dW_{ij}^S = dW_{ij}^S - tr[dW_{ij}^S]1/3 \]

[J. Li et al. 2005]

calibrate for:

maximum spring extension \( x_0 \)
persistence length \( p \)
Bayesian Uncertainty Quantification

Which parameters are “good” for the model?

Result: a distribution over all possible parameters of the model.

Model with parameters:

Input → Output

Data:
Compare with data and decide

Prediction error equation:
\[ D = M(\theta) + \varepsilon \]
\[ \varepsilon \sim \mathcal{N}(0, \Sigma) \]

Likelihood:
\[ p(D|\theta) \]

Bayes’ Theorem:
\[ p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} \]
Red Blood Cell Model

data: stretching experiment (Suresh et al., 2005)

![Image of RBCs]

extracted from: Suresh et al. 2005

![Data graph]

data extracted from: Suresh et al. 2005

simulation: uDeviceX

https://github.com/uDeviceX/uDeviceX

stochastic forward model:

\[
D = M(\theta) + \varepsilon, \varepsilon \sim \mathcal{N}(0, \Sigma),
\]

\[
\Sigma = \text{diag}(\sigma_1^2 + \tau_1^2 + \omega_1^2, \ldots, \sigma_2^2 + \tau_1^2 + \omega_1^2, \sigma_2^2 + \tau_2^2 + \omega_2^2, \ldots, \sigma_2^2 + \tau_2^2 + \omega_2^2)
\]
Transmit Markov Chain Monte Carlo (TMCMC)

Bayesian Inference Algorithm

[Ching & Chen 2007]

Sample from the prior PDF $f(\theta|MD_i)$

Set annealing parameter: $p = 0$

Initialise

$p \geq 1$?

Update $p$

Yes

No

Set annealing parameter: $p = 0$

$\text{Sample with weights proportional to the scaled likelihood } p(D|\theta(n)^{dp})$

$\text{Run MH from every selected sample: } \text{MH}(\mathcal{N}(\theta_i, \Sigma_g))$

Stop

Rejuvenate

$\text{Sample from the prior PDF } f(\theta|MD_i)$

$\text{Set annealing parameter: } p = 0$

$\text{Run MH from every selected sample: } \text{MH}(\mathcal{N}(\theta_i, \Sigma_g))$

$\text{Sample with weights proportional to the scaled likelihood } p(D|\theta(n)^{dp})$

Stop

Rejuvenate
HPC Approach: TORC

- runs on various architectures ranging from laptops to clusters
- automatic load-balancing
- integrable with external software used for model evaluation (e.g., uDeviceX)
- task-based parallelism
- easy to write parallel code

Task graph of a population-based sampling algorithm

[P. Hadjidoukas et al. 2012]
Pi4U: UQ Library on Top of TORC

- open-source library distributed under LGPL licence
- available at [http://www.cse-lab.ethz.ch/software/Pi4U](http://www.cse-lab.ethz.ch/software/Pi4U)
- algorithms:
  - **TMCMC** (for exact Bayesian inference)
  - **ABC-SubSim** (for approximate Bayesian inference)
  - **CMA-ES** (for optimization)
  - **Subset Simulation** (for rare events sampling)
  - **A-PNDL** (for adaptive parallel numerical differentiation)
Red Blood Cell Model

1024 samples per stage, 128 GPU nodes on Piz Daint (CSCS), 5 hours of wall-clock time per stage. CUDA + TORC workers.

(0.49, 4.86) (our calibration) vs (0.45, 1.99) (Fedosov, PhD thesis, 2010)

posterior distribution of the parameters

robust prediction

prediction is within error bars
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Power of Cavitation

extracted from: Brennen, Hydrodynamics of pumps, Oxford University Press, 1994

https://de.wikipedia.org/wiki/Kavitation
https://www.forddoctorsdts.com

extracted from: Bazan-Peregrino et al., Cavitation-enhanced delivery of a replicating oncolytic adenovirus to tumors using focused ultrasound, Journal of Controlled Release Volume 169, Issues 1–2, 2013, 40-47

https://en.wikipedia.org/wiki/Extracorporeal_shock_wave_lithotripsy
https://de.wikipedia.org/wiki/Knallkrebse

engineering

biomedical applications

nature
50K Bubbles, 64 Billion Cells

25K time steps, 72h x 32K cores
Governing Equations

\[
\begin{align*}
\frac{\partial \alpha_1 \rho_1}{\partial t} + \nabla \cdot (\alpha_1 \rho_1 \mathbf{u}) &= 0 \\
\frac{\partial \alpha_2 \rho_2}{\partial t} + \nabla \cdot (\alpha_2 \rho_2 \mathbf{u}) &= 0 \\
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I}) &= 0 \\
\frac{\partial E}{\partial t} + \nabla \cdot ((E + p) \mathbf{u}) &= 0 \\
\frac{\partial \alpha_2}{\partial t} + \mathbf{u} \cdot \nabla \alpha_2 &= K \nabla \cdot \mathbf{u}
\end{align*}
\]

where

\[
K = \frac{\alpha_1 \alpha_2 (\rho_1 c_1^2 - \rho_2 c_2^2)}{\alpha_1 \rho_2 c_2^2 + \alpha_2 \rho_1 c_1^2}
\]

and

\[
\alpha_1 + \alpha_2 = 1
\]

Thermodynamic Closure

- stiffened equation-of-state (EoS) for pure fluids

\[ p_k = (\gamma_k - 1) \rho_k e_k - \gamma_k p_{c,k} \]

[Menikoff & Plohr 1989, ...]

- mixture relations

\[ \rho = \alpha_1 \rho_1 + \alpha_2 \rho_2 \]
\[ \rho e = \alpha_1 \rho_1 e_1 + \alpha_2 \rho_2 e_2 \]

- pressure equilibrium \( p = p_k \)

- mixture speed of sound

\[ \frac{1}{\rho c^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2} \]

[Wood 1930]
Cubism-MPCF

- compressible multicomponent flow solver tailored to HPC systems [Rossinelli et al. 2013]
- 3D structured-grid finite volume solver
- wavelet-based compression of simulation data

TIME TO SOLUTION (no I/O)

Tw = 1.8
Tw = 29.7 (TUM)
Tw = 16.3 - 39.0 (Stanford)

PFLOPS (% Peak)

14 (172%) (TUM)
21 - 41% (Stanford)

I/O COMPRESSION

10-100X

SIZE

1.3 E13 - 15K bubbles
1.2 E08 - 0.15K bubbles
0.4 E13 - Turbulence

ACM Gordon Bell Prize 2013
Godunov-Type Finite Volume Method

- reformulation of gas-volume-fraction equation
  [Johnsen & Colonius 2006]
- high-order reconstruction of face values of primitive variables using WENO3/5
  [Liu et al. 1994, Jiang & Shu 1998]
- approximate HLLC Riemann solver for flux reconstruction
  [Toro et al. 1994]
- low-storage 3rd-order Runge-Kutta scheme for time discretization
  [Gottlieb et al. 2001]
Cubism-MPCF: Software Layout

- cluster (MPI)
- node (OpenMP)
- core (SIMD): WENO, HLLC
Collapsing Bubble Clouds

- average radius
  \[ R_{\text{avg}} = \frac{1}{N} \sum_{i=1}^{N} R_i \]

- equivalent radius
  \[ R_{\text{eq}} = \sqrt[3]{\frac{3}{\pi} \sum_{i=1}^{N} R_i^3} \]

- gas volume fraction
  \[ \alpha = \frac{1}{V_c} \sum_{i=1}^{N} \frac{4}{3} \pi R_i^3 \]

- cloud interaction parameter
  \[ \beta = \alpha \left( \frac{R_{\text{eq}}}{R_{\text{avg}}} \right)^2 \]

- cloud generation
  - locations: uniform distribution
  - radii: log-Gaussian
2500 Bubbles - Collapse Process

- cloud interaction parameter of 15
- low pressure ratio
- bubble radius resolved by 10 to 15 cells
Collapse of 2 Random Clouds

spherical clouds of 100 equally sized (R=75µm) cavities uniformly distributed (random) cavity positions
Collapse of 2 Random Clouds

maximum pressure

significant variations

spherical clouds of 100 equally sized (R=75µm) cavities

uniformly distributed (random) cavity positions
MultiLevel Monte Carlo (MLMC)

- variance reduction technique using sampling on hierarchy of mesh resolutions
- further improvement by optimal control variate coefficients due to minimization of variance reduction costs for weakly correlated resolution levels

[Heinrich 1999, Giles 2008]

**Step of MLMC:**

1. generate i.i.d. samples of random input quantities for each resolution level 0…L
2. for each level and sample, solve for approximate solutions using Cubism-MPCF
3. assemble MLMC estimator for statistics of quantities of interest
Inner Working of MLMC

- majority of samples computed on lowest levels of resolution (reduced budget)
- optimization problem for given tolerance or computational budget  
  [Giles 2008]

adaptive number of warmup samples

230x speedup for OCV-MLMC even for less correlated levels
Results MLMC: Bubble Clouds

uncertainty quantification (i.e., mean, confidence intervals) of various quantities of interest

vapor volume

no significant uncertainty

pressure sensor

wide 90% confidence interval
100 MPa - 600 MPa
Results MLMC: Bubble Clouds

Secondary cavitation observed at epicenter immediately after final collapse

Vapor volume fraction sensor

Average pressure over spherical shells

“Secondary cavitation” region after the final cloud collapse

Pressure peak reflects at cloud center sharp drop - “Secondary cavitation”
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Summary and Outlook

- **uDeviceX**: dissipative particle dynamics solver to simulate blood flow capable of ~1.4 billion deformable red blood cells
- **Cubism-MPCF**: finite volume solver for compressible, multicomponent flow simulations capable of ~13 trillion cells
- **Pi4U and TORC**: efficient exploitation of HPC architectures for Bayesian inference in large-scale models
  - **TMCMC** to calibrate parameters of red blood cell model
  - **MLMC** to quantify uncertainties in peak pressures of clouds under random initial conditions (currently implemented into Pi4U with TORC framework)
Thank you for your attention!